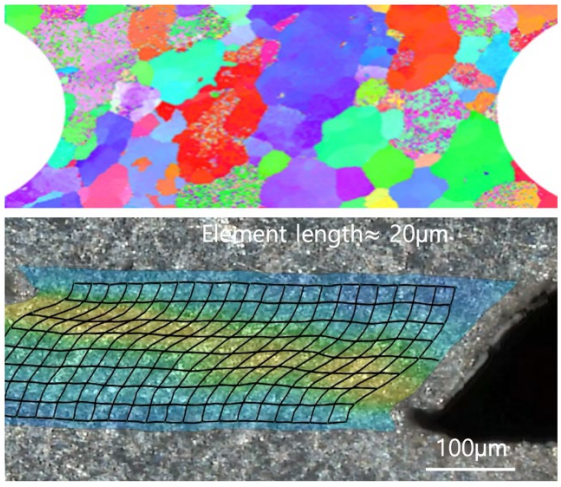
# Physics & Mechanics of Plasticity, Damage & Fracture

Proceedings of ICPDF '26:
The 29th International Conferences on
Plasticity, Damage, and Fracture

*Editors*
Jeong Whan Yoon & Akhtar S. Khan

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# PREFACE

This proceeding book contains over two hundred abstracts of papers that are expected to be presented at ICPDF '26 by scientists from around the world. After 41 years of constant efforts, the conference has a balanced representation from mechanics and material science communities of plasticity, damage and fracture. Presentations include recent developments in mechanisms and mechanics of plastic deformation, damage and fracture; results in a new and growing other topics in plasticity, damage and fracture; and in bordering domains of the mechanical behavior of materials. These new directions for this conference, can be seen in papers on dislocation theory based modeling of microstructure evolution, plasticity of textured poly-crystals, microstructure-based models of plastic deformation, continuum and discrete dislocation dynamics and in-situ characterization in nano-mechanics and radiation damage multi-scale modeling. These papers also contain progress made in traditional plasticity areas such as advances in mechanics for materials forming, multi-axial deformation and formability, and multi-scale materials modeling and experimental characterization of mechanical behavior of poly-crystals, etc.

The symposium series was conceived and initiated, to provide an international informal forum for research results dissemination with ample time duration for presentation and discussion. This symposium includes twelve distinguished key-note lectures of Forty-five minutes duration. Also, each session of this symposium series is designed to include invited key-note lectures of thirty minutes and invited papers of fifteen minutes durations. The invited key-note lectures provide a review of the sub-topic area including lecturer's own new research results. Previous conferences in the series of International Symposium on Plasticity and Its Current Applications, now renamed since 2017 to International Conference on Plasticity, Damage & Fracture (ICPDF), were held in Norman, Oklahoma (1984), Mie University at Tsu Japan (1989), Grenoble France (1991), Baltimore Maryland (1993), Osaka Japan (1995), Juneau Alaska (1997), Cancun Mexico (1999), Whistler Resort Canada (2000), Aruba (2002), Quebec City Canada (2003), Kauai Hawaii (2005), Halifax in Nova Scotia Canada (2006), Girdwood Alaska (2007), Kona Hawaii (2008), St. Thomas USA (2009), St. Kitts West indies (2010), Puerto Vallarata Mexico (2011), San Juan USA (2012), Nassau Bahamas (2013), Freeport Bahamas (2014), Montego Bay in Jamaica (2015), Kona in Hawaii (2016), Puerto Vallarta Mexico (2017), San Juan Puerto-Rico (2018), Panama City Panama (2019), Cancun Mexico (2020), Punta Cana in Dominican Republic (2023), and Panama City Panama (2024).

From 1984 to 2020, Akhtar Khan served as the Conference Chair. Late Professors Jean- Paul Boehler and Masataka Tokuda, and Professor Shinji Tanimura co-chaired and co- organized some of these conferences. Professors Satya Atluri, late Daniel Drucker, Rodney Clifton, Albert Kobayashi, Jean-Louis Chaboche, Lallit Anand, Dave McDowell, Nobutada Ohno, Hussein Zbib, Rob Wagoner, Fred Barlat, Paul van Houtte, George Voyiadjis, Georges Cailletaud, Tome Carlos, Valery Levitas, Surya Kalidindi, and Huseyin Sehitoglu have served as past Honorary Chairmen. From ICPDF2023, Jeong Whan Yoon has been serving as Chair and Akhtar Khan has been continuously supporting the ICPDF as Co-Chair or Honorary Chair. The Army Research Office, the National Science Foundation, the Office of Naval Research, GM, Deakin University, and numerous other professional organizations, host institutions and industries have sponsored some of these events. These symposia and now ICPDF, except the first one, had two hundred fifty to four hundred presentations, most of them have over three hundred presenters. Thus, this Conference has become the largest gathering of distinguished and young plasticity, damage and fracture researchers. The series has maintained a high level of quality presentations by including speakers by invitation only. Locations have been chosen to give almost pollution free and relaxed atmosphere, but at economical prices, to discuss exciting new results in various plasticity areas.

A number of special symposiums are organized as listed below, with the names of the organizers given for each. We are personally thankful to these members of the International Organizing Committee. These include some symposiums in honor of distinguished colleagues as also noted below, i.e.,

**Ming Wang Fu (Hong Kong), Yinan Cui (China):** "Physics-Based Modelling and AI-enabled simulation"; **Qi Hu, Yanshan Lou (China):** "Characterization of Plasticity and Failure under Linear and Non-linear Loading Path"; **Lin Hua, Fei Yin (China):** "AI Modeling for Plastic Forming with Multi-Energy Fields"; **Abigail Hunter (USA), Gi-Dong Sim (Korea), Nate Mate (USA):** "Khan Medal Symposium in Honor of Irene Beyerlein: Understanding Deformation Mechanisms at the Mesoscale via Modelling and Experiments"; **Kaan Inal (Canada), Dirk Mohr (Switzerland):** "Advances in ML-based Applications for Plasticity, Damage and Fracture"; **Guozhen Kang, Xu Zhang (China):** "Cyclic Plasticity and Fatigue: Mechanisms, Modeling, and Design"; **Myoung-Gyu Lee (Korea), Hojun Lim (USA), Junying Min (China):** "Integrating Length Scales: Constitutive Modeling and Plasticity Strategies"; **Valery Levitas (USA):** "Material Transformations and Plasticity"; **Guisen Liu (China), Jian Wang (USA):** "Multiscale Plasticity of Materials Under Extreme Conditions"; **Valentina Salomoni, Massimiliano Ferronato (Italy):** "Numerical Strategies for Nonlinear Coupled Hydro-Poromechanics and Thermo-Mechanics Problems"; **T. A. Venkatesh, Wei Cai, Ming Dao (USA):** "Hydrogen Effects on Deformation, Fatigue and Fracture"; **Qing Zhou, Kaikai Song, Jichao Qiao (China):** "Multi-Scale Insights into Strengthening, Plasticity, and Damage in Multi-Principal Element Alloys".

The plenary lecture, introduced for the first time in the conference in Halifax (2006), is given by the winner of Khan International Award for outstanding contribution to the field of plasticity over last twenty-four years period (endowed by Mrs. (Dr.) Tanveer A. Khan and Professor Akhtar S. Khan), will be given this year by Professor Ming Wang Fu. Previous winners of this award are Dr. Jean-Louis Chaboche, ONERA, France (2006); Professor Lallit Anand (2007); Professor David McDowell (2008), Professor Nobutada Ohno (2009), Professor Hussein Zbib (2010), Professor Rob Wagoner (2011), Professor George Voyiadjis (2012), Professor Fred Barlat (2013), Professors Paul van Houtte (2014) & Georges Cailletaud (2015), Dr. Carlos Tome (2016), Professor Valery Levitas (2018), Professor Surya Kalidindi (2019), Professor Huseyin Sehitoglu (2020), Professor Jeong Whan Yoon (2023), and Irene Beyerlein (2024). Last, but not the least, Yinan Cui (Tsinghua University) for 2026 will receive the 20$^{th}$ International Journal of Plasticity Young Researcher Awards respectively for excellent contributions to the field of plasticity, damage and fracture over a five year period. The first nineteenth winners of this award were Professors Frederic Barlat (2006), Young Huang (2007), Jeong Whan Yoon (2008), Peidong Wu (2009), Mark Horstemeyer, (2010), Sean Agnew (2011), Jeff Kysar (2012), Irene Beyerlein (2013), Myoung-Gyu Lee (2014), Jian Wang (2015), Dirk Mohr (2016), Nathan Mara (2017), Laurent Capolungo (2018), Stephen R. Niezgoda (2019), Marko Knezevic (2020), Yanshan Lou (2021), Waqas Muhammad (2022), Giacomo Po (2023), and Xu Zhang (2024).

It is our pleasure to gratefully acknowledge the support of the International Journal of Plasticity, School of Engineering at Deakin University, the Department of Mechanical Engineering at Korea Advanced Institute of Science and Technology (KAIST), the Department of Mechanical Engineering at the University of Maryland Baltimore County (UMBC), Numerical Engineering Analysis and Testing (NEAT) Inc. We are grateful for various helps provided by Georgina Fatouros and Jess Holmes at Deakin University, Wonjin Park and Daecheon Cho at KAIST. It is truly our pleasure to finally thank the most important contributors to this conference and the proceeding volume, over two hundred scientists from around the world. They have been backbone of the success of this conference series and for advancing the plasticity, damage and fracture related research globally.

Jeong Whan Yoon (Chair, Associate Editor for Int. J. Plasticity)

Akhtar S. Khan (Honorary Chair, Editor-in-Chief for Int. J. Plasticity)

## International Organizing Committee at ICPDF '26 (Jan. 3-8, 2026)

### Chair: Jeong Whan Yoon (S. Korea / Australia)

### Honorary Chair: Akhtar S. Khan (USA)

### Members and organized Symposiums:

**Ming Wang Fu (Hong Kong), Yinan Cui (China):** "Physics-Based Modelling and AI-enabled simulation"

**Qi Hu, Yanshan Lou (China):** "Characterization of Plasticity and Failure under Linear and Non-linear Loading Path"

**Lin Hua, Fei Yin (China):** "AI Modeling for Plastic Forming with Multi-Energy Fields"

**Abigail Hunter (USA), Gi-Dong Sim (Korea), Nate Mate (USA):** "Khan Medal Symposium in Honor of Irene Beyerlein: Understanding Deformation Mechanisms at the Mesoscale via Modelling and Experiments"

**Kaan Inal (Canada), Dirk Mohr (Switzerland):** "Advances in ML-based Applications for Plasticity, Damage and Fracture"

**Guozhen Kang, Xu Zhang (China):** "Cyclic Plasticity and Fatigue: Mechanisms, Modeling, and Design"

**Myoung-Gyu Lee (Korea), Hojun Lim (USA), Junying Min (China):** "Integrating Length Scales: Constitutive Modeling and Plasticity Strategies"

**Valery Levitas (USA):** "Material Transformations and Plasticity"; **Guisen Liu (China), Jian Wang (USA):** "Multiscale Plasticity of Materials Under Extreme Conditions"

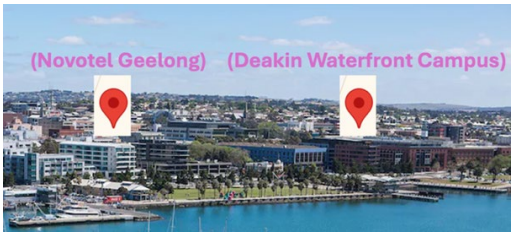
**Valentina Salomoni, Massimiliano Ferronato (Italy):** "Numerical Strategies for Nonlinear Coupled Hydro-Poromechanics and Thermo-Mechanics Problems"

**T. A. Venkatesh, Wei Cai, Ming Dao (USA):** "Hydrogen Effects on Deformation, Fatigue and Fracture"

**Qing Zhou, Kaikai Song, Jichao Qiao (China):** "Multi-Scale Insights into Strengthening, Plasticity, and Damage in Multi-Principal Element Alloys".

**TENTATIVE PROGRAM: ICPDF 2026, Geelong Australia, Jan. 3-8**
Ver.2, December 29, 2025

We are delighted to be welcoming you to the International Conference on Plasticity, Damage, and Fracture 2026 Geelong on January 3 to 8, 2026.




**Conference Venue - 3 to 4 January**
Address: Novotel Geelong, 10/14 Eastern Beach Rd, Geelong, Victoria 3220

**Conference Venue - 5 to 7 January**
Address: Deakin University Waterfront Campus, 1 Gheringhap Street, Geelong, Victoria 3220

**Registration desk**
The registration desk will be open daily from 8:30am to 5pm on Saturday 3 January, and from 8am to 5pm on the remaining conference days for registration and questions. **If you have not provided the conference secretary with a copy of your passport, please have this ready for presentation upon registration.**

**Accommodation**
If you have not yet arranged your accommodation, we urge you to do so as soon as possible. Please kindly refer the discount codes sent by the conference secretary.

**Presentation**
If you are presenting at the conference, please upload a copy of your presentation slides here **following the release of the final program which will be announced on December 26**. To assist us, please save your file with your presentation time and full name eg: Saturday_1100_JohnSmith. If you are unable to upload via Dropbox, please email your slides or bring them to the registration desk on a USB device. **All presentations will be deleted after presentations on a daily basis.**

Please note that the general secretary office is closed from December 23 until January 3 for the Christmas & holiday period. **During the period, the chairs can respond you only for the conference program.**

**Transfer from Melbourne Airport to Geelong**
Gull bus operates regular shuttle bus services between Melbourne Airport and Geelong with a one-way adult fare of $35 (AUD). You can reserve Gull Bus at https://gull.com.au/ Please consult a driver for the closest stop from your hotel location. Geelong Railway Station is the closest to Novotel Geelong (10 mins. walk).

**Cultural Excursion on 8 January**
The conference offers Cultural Excursion to Great Ocean Road on 8 January. It is complimentary and limited to max. 50 people. Application is available on 3 and 4 January at the registration desk.

# Saturday, Jan. 3, 2026

**08:30 - 10:30 Registration and Coffee**

**10:30 - 10:50 <u>Orientation on Novotel Venue by Chair</u> …….. Room (Peninsula)**

| *Room* | **Peninsula** | **Bellarine** | **Ceres** |
|---|---|---|---|
| | ***(Sym) Characterization of Plasticity and Failure under Linear and Non-linear Loading Path (I)*** | ***(Sym) Material Transformations and Plasticity (I)*** | ***(Sym) Integrating Length Scales: Constitutive Modeling and Plasticity Strategies (I)*** |
| *Chairs* | ***Yanshan Lou ++ & Zhidong Chang*** | ***Qingping Sun & Jian-Feng Nie*** | ***Giang Nguyen & Ibrahim Jawahir*** |
| 11:00 ~ 11:30 | * Songchen Wang, Jeong Whan Yoon, **<u>Yanshan Lou</u>**<br><br>LODE-DEPENDENT FUNCTION FOR CHARACTERIZATION OF ANISOTROPY, STRENGTH DIFFERENTIAL EFFECT AND YIELD SURFACE EVOLUTION | **<u>* Qingping SUN</u>**<br><br>CYCLIC TRANSFORMATION-INDUCED PLASTICITY, ELASTOCALORIC COOLING AND SYSTEM PERFORMANCE DEGRADATION | **<u>* Giang D. Nguyen</u>**, Ha H. Bui<br><br>BRIDGING THE SCALES IN CONSTITUTIVE MODELLING OF GEOMATERIALS - |
| 11:30 ~ 11:45 | + **<u>Zhidong Chang</u>**, JunGongwei Shi, Ziying Ding, Dayong An, Yongbing Li, Jun Chen<br><br>ROOM-TEMPERATURE PRECIPITATION STRENGTHENING IN AL-2.5MG-0.4FE SHEET INDUCED BY CYCLIC SEVERE PLASTICITY DEFORMATION | **<u>* Levente Balogh</u>**, Lucas Ravkov, Thalles Lucas, Shengze Yin, Arash Nikniazi, Vahid Fallah<br><br>USING HIGH-RESOLUTION SYNCHROTRON X-RAY DIFFRACTION TO CHARACTERIZE DISLOCATION CELLS IN ADDITIVELY MANUFACTURES HASTELLOY-X | + **<u>Wonjin Park</u>**, Youngung Jeong, Jeong Whan Yoon<br><br>ANISOTROPY PREDICTION OF SHEET METALS WITH A TEXTURE-BASED POTENTIAL MODEL |
| 11:45 ~ 12:00 | + **<u>Jiajun Chen</u>**, Xiongqi Peng<br><br>AN ANISOTROPIC CONSTITUTIVE MODEL FOR CARBON FABRIC-REINFORCED SHAPE MEMORY POLYMER COMPOSITES BASED ON PHASE TRANSITION CONCEPT | | + **<u>Dat G. Phan</u>**, Giang D. Nguyen, Ha H. Bui, Terry Bennett<br><br>CONSTITUTIVE MODEL FOR CAPTURING PRE AND POST-LOCALISATION RESPONSES OF PARTIALLY SATURATED SOILS |
| 12:00 ~ 12:15 | + **<u>Xinxi Liu</u>**, Dayong An, Xifeng Li, Jun Chen<br><br>MICROSTRUCTURE AND PROPERTY CONTROL OF METALLIC MATERIALS VIA THERMOMECHANICAL-COUPLED INCREMENTAL FORMING | **<u>* Jian-Feng Nie</u>**<br><br>FORMATION AND STRENGTEHNING MECHANISMS OF PLATE-SHAPED PRECIPITATES IN LIGHT ALLOYS | + **<u>Yin Du</u>**, Hanming Wang, Tao Yang, Qing Zhou, Haifeng Wang<br><br>INVESTIGATION INTO THE EFFECT OF CRYOGENIC TEMPERATURES ON WEAR BEHAVIORS OF EUTECTIC ALCOCRFENI2.1 HIGH ENTROPY ALLOY |
| 12:15 ~ 12:30 | + Xiaoguang Fan, Li Wang, **<u>Yunteng Xiao</u>**, Mei Zhan<br><br>MACRO-MICRO ANISOTROPY INDUCED BY LOADING PATH VARIATION IN HOT WORKING OF TITANIUM ALLOYS: INTERPRETABLE AND PHYSICS-INFORMED MODELING | | * Alper Uysal, **<u>Ibrahim Jawahir</u>**<br><br>A VARIABLE FLOW STRESS SLIP-LINE MODEL AND EXPERIMENTAL VALIDATION FOR MACHINING PROCESSES |
| 12:30 ~ 12:45 | - | **<u>* Donald W. Brown</u>**, D.T. Carver, B. Clausen, D.J. Savage, N. Peterson, C.R. Lear, S. Checchia, M. Di Michiel<br><br>HEATING RATE DEPENDENT RECOVERY AND RECRYSTALLIZATION OF ROLLED TITANIUM AND AM'ed Ti-6Al-4V | |
| 12:45 ~ 13:00 | | | - |

**13:00 – 14:00 <u>Lunch</u>**

| *Room* | **Peninsula** | **Bellarine** | **Ceres** |
|---|---|---|---|
| | ***(Sym) Characterization of Plasticity and Failure under Linear and Non-linear Loading Path (II)*** | ***(Sym) Material Transformations and Plasticity (II)*** | ***(Sym) Hydrogen Effects on Deformation, Fatigue and Fracture (I)*** |
| *Chairs* | ***Qi Hu ++ & Baodong Shi*** | ***Valery Levitas ++ & Wayne Chen*** | ***Wen Meng & Donald Brown*** |
| 14:00 ~ 14:30 | *** Qi Hu**, Jeong Whan Yoon, Takeshi Nishiwaki, Jun Chen<br><br>AN EXTENDED ANISOTROPIC DISTORTIONAL HARDENING MODEL FOR THE FLEXIBLE BAUSCHINGER EFFECT UNDER NONLINEAR STRAIN PATHS | ***** Valery I. Levitas**<br><br>RECENT ADVANCES IN SEVERE PLASTIC DEFORMATIONS, STRAIN-INDUCED PHASE TRANSFORMATIONS, AND MICROSTRUCTURE EVOLUTION AT HIGH PRESSURE | *** W.J. Meng**, B. Zhang, C.F.O. Dahlberg, J.W. Hutchinson, W. Xu, A. Kaveh<br><br>PROBING MICRON SCALE PLASTIC RESPONSE UNDER NON-PROPORTIONAL LOADING AND HYDROGEN CHARGING EFFECTS USING SMALL SCALE MECHANICAL TESTING |
| 14:30 ~ 14:45 | + **Zexiong Zhang**, Chun-mei Liu, Xun-zhong Guo, Tao Tao, Wang Yun<br><br>RESEARCH ON DOUBLE-SIDED INCREMENTAL AND ELECTRO-AGING FLEXIBLE FORMING TECHNOLOGY FOR Al-Li ALLOY | | + **Liangyun Lan**, Xiangwei Kong, Andrej Atrens<br><br>HYDROGEN AFFECTED FRACTURE TOUGHNESS OF X52 PIPELINE STEEL WITH ITS MECHANISM OF PLASTICITY DEGRADATION |
| 14:45 ~ 15:15 | *** Yong Hou**, Zhenkai Mu, Wei Wang, Shuangjie Zhang, Baoyu Wang, Shibo Ma<br><br>A NOVEL HILL48 YIELD CRITERION FRAMEWORK USING STRESS ADJUSTMENT TO CAPTURE STRESS-STATE-DEPENDENT PLASTIC ANISOTROPY | *** Wayne Chen**, Andrew Roginski, Cody Kirk<br><br>MONITORING PHASE TRANSITION DURING HIGH-RATE PLASTIC DEFORMATION | * Lawrence Cho, Yuran Kong, Pawan Kathayat, John G. Speer, Kip O. Findley, **Donald W. Brown**, Samantha K. Lawrence, Bjørn Clausen, Sven C. Vogel, Joseph A. Ronevich, Chris W. San Marchi, Levente Balogh, Lucas Ravkov<br><br>UNDERSTANDING THE ROLE OF HYDROGEN ON THE DEFORMATION MECHANISMS AND DISLOCATION STRUCTURE EVOLUTION IN HIGH MN AUSTENITIC STEELS THROUGH NEUTRON DIFFRACTION LINE PROFILE ANALYSIS |
| 15:15 ~ 15:30 | *** Baodong Shi**<br><br>ANISOTROPIC YIELD LOCI AND INVERSE SWIFT EFFECT IN EXTRUDED AZ31 MG ALLOY | *** Klaus Hackl**, Philipp Junker<br><br>A RELAXATION-BASED APPROACH TO DAMAGE MODELING | + Hyoungryul Park, Yifan Wang, Inseo Woo, Wei Cai, J.C Stinville, **Keonwook Kang**<br><br>THE EFFECT OF AN ATOMIC HYDROGEN ON THE KINK MIGRATION IN A <111>{110} SCREW DISLOCATION IN BCC TUNGSTEN: ATOMISTIC STUDY |
| 15:30 ~ 15:45 | | | |
| 15:45 ~ 16:15 | * Yue Wu, Chenxin Gao, Renhao Wu, **Haiming Zhang**<br><br>MICROSTRUCTURE-RESOLVED PLASTICITY HETEROGENEITIES AND DAMAGE INITIATION IN NEAR-A Ti60 UNDER NON-LINEAR LOADING PATHS | - | - |

## 19:00 – 21:00 Welcome Dinner (Novotel Peninsula)

*** 45 minutes Distinguished keynote lecture, * 30 minutes keynote lecture,
+ 15 minutes invited presentation, ++ Symposium Organizer

# Sunday, Jan. 4, 2026

| *Room* | **Peninsula** | **Bellarine** | **Ceres** |
|---|---|---|---|
| | ***(Sym) AI Modeling for Plastic Forming with Multi-Energy Fields (I)*** | ***(Sym) Material Transformations and Plasticity (II)*** | ***(Sym) Integrating Length Scales: Constitutive Modeling and Plasticity Strategies (II)*** |
| *Chairs* | ***Lin Hua ++ & Fei Chen*** | ***Yann Le Godec & Alexander Soldatov*** | ***Hyuk Jong Bong & Dongchan Jang*** |
| 8:30 ~ 9:00 | *** Fei Yin, **Lin Hua**<br><br>PHYSICS-INFORMED MACHINE LEARNING OF THERMAL STABILITY IN GRADIENT NANOCRYSTALLINE 316L STAINLESS STEEL | *** Yann Le Godec**<br><br>EXPLORING EXTREME CHEMISTRY AND EARTH PROCESSES WITH NEXT-GENERATION PORTABLE LARGE VOLUME HIGH P-T-STRESS SYNCHROTRON CELLS | *** Hyuk Jong Bong**, Kyung Mun Min, Seonghwan Choi<br><br>ON THE DIRECTION-DEPENDENT FORMABILITY OF AN ULTRA-THIN COMMERCIALLY PURE TITANIUM SHEET |
| 9:00 ~ 9:15 | | *** Alexander V. Soldatov**<br><br>GRAPHITE UNDER SEVERE SHEAR DEFORMATION-ENROUTE SYNTHESIS OF HEXAGONAL DIAMOND | *** Yuqiang Chen**<br><br>CONTRIBUTION OF LATTICE ROTATION AND RECRYSTALLIZATION MECHANISM TO THE TRANSFORMATION OF ORIENTATION PREFERENCE IN ALUMINUM SINGLE CRYSTAL DURING ECAP |
| 9:15 ~ 9:30 | + **Qifa Chen**, Tao Wang, Jinyu Zhao<br><br>INVAR 36 ALLOY ULTRA-THIN STRIP ROLLING PROCESS AND THE INFLUENCE MECHANISM OF SURFACE DEFECTS ON THE HOLE FORMATION RATE | | |
| 9:30 ~ 10:00 | *** Fei Chen**<br><br>MACHINE LEARNING FRAMEWORK TO PREDICT THE COARSE GRAIN FORMATION DURING HOT WORKING | * Haoxiang Liu, Xudong Liu, Yaoqing Zhang, **Yixuan He**<br><br>EVADING STRENGTH-DUCTILITY TRADE-OFF IN EUTECTIC HIGH ENTROPY ALLOYS THROUGH HETERIGENEOUS STRUCTURE INDUCED MARTENSITIC TRANSFOAMATION | *** Dongchan Jang**, Hadi Ghaffarian, Daehyeok Ahn<br><br>DEFECT-DRIVEN PLASTICITY IN IRRADIATED NANOTWINNED Cu |
| 10:00 ~ 10:15 | + **Wei Feng**, Ruikun Wang, Yuhao Zhang, Xinghui Han, Lin Hua<br><br>EFFECT OF HIGH TEMPERATURE QUENCHING TEMPERATURE ON THE WEAR PERFORMANCE OF AVIATION GEAR STEEL 15Cr14Co12Mo5Ni2 | - | - |
| 10:15 ~ 10:30 | + **Zhihui Gao**, Tao Wang, Hui Niu, Qingshan Ding<br><br>COUPLED STRENGTHENING MECHANISMS IN Ti/Al CLADDING TUBES WITH DUAL HETEROGENEOUS STRUCTURES FABRICATED BY THREE-ROLL SKEW ROLLING | | |

## 10:30 – 11:00 Coffee Break

| *Room* | **Peninsula** | **Bellarine** | **Ceres** |
|---|---|---|---|
| | ***(Sym) AI Modeling for Plastic Forming with Multi-Energy Fields (II)*** | ***(Sym) Physics-Based Modelling and AI-enabled simulation (I)*** | ***(Sym) Multiscale Plasticity of Materials Under Extreme Conditions (I)*** |
| *Chairs* | ***Junying Min & Tao Wang*** | ***Yinan Cui ++ & Heng Li*** | ***Yao Shen & Jia Li*** |
| 11:00 ~ 11:30 | *** Junying Min**, Xianglu Zhang, Xiaolong Ma, Bo Chen<br>HARNESSING ELECTRICAL ASSISTANCE IN FORMING OF ULTRA-THIN TITANIUM SHEETS | ***** Yinan Cui**, Xin Liu, Fushang Tan, Zhun Liang, Enrique Martinez Saez, Yang Li, Nikhil Chandra Admal, Giacomo Po<br>DATA-DRIVEN MULTISCALE MODELING OF HETEROGENEITY EFFECTS ON ALLOY STRENGTH AND FATIGUE | * Shuqing Yang, Guisen Liu, **Yao Shen**, Jianbo Hu, Wenjun Zhu<br>A POLYCRYSTALLINE THERMO-ELASTO-PLASTIC CONSTITUTIVE MODEL BASED ON EULERIAN STRAIN FRAMEWORK: THEORY, NUMERICAL IMPLEMENTATION, AND APPLICATION FOR SHOCK AND QUASI-ISENTROPIC LOADING |
| 11:30 ~ 11:45 | + **Xiaomiao Niu**, Chenchen Zhao, Tao Wang, Qingxue Huang<br>EFFECT OF PULSED CURRENT ON THE DEFORMATION AND INTERFACIAL BONDING OF COPPER/STAINLESS STEEL STRIPS IN ROLLING | | + Tianyou Wang, Qiankun Li, **Li Jin**, Chuanlai Liu, Jian Zeng, Fulin Wang, Shuai Dong, Fenghua Wang, Jie Dong<br>INTERPRETABLE MACHINE LEARNING FOR PREDICTING TENSILE TWINNING AND REVEALING MICROSTRUCTURAL INFLUENCES IN PURE Mg |
| 11:45 ~ 12:15 | *** Tao Wang**<br>ROLLING TECHNOLOGIES AND EXTREME MANUFACTURING | *** Heng Li**, Ronghai Wu, Zhao Zhang<br>MECHANICAL RESPONSE-MICROSTRUCTURE-CRACKING RELATION OF POWDER METALLURGY NI-BASED SUPERALLOYS UNDER LOW CYCLE FATIGUE | *** Jia Li**, Weizheng Lu, Xiaoai Yi, Yuan Chen, and Qihong Fang<br>MULTISCALE DEFORMATION MECHANISMS IN HIGH-ENTROPY ALLOYS FOR ENHANCED STRENGTH AND DUCTILITY |
| 12:15 ~ 12:30 | + **Yan Wen,** Chang Liu, Fei Yin, Lechun Xie, Lin Hua<br>IN-SITU MANIPULATING MECHANISM OF ELECTROMAGNETIC FIELD ON THE MICROSTRUCTURE AND HARDNESS OF TITANIUM ALLOY DURING LASER MELTING DEPOSITION | *** Chaoyang Sun**, Huijun Liang, Lingyun Qian, Chunhui Wang, Peipei Li<br>A PHYSICAL-BASED CRYSTAL PLASTICITY MODEL FOR HIGH-MANGANESE STEEL CONSIDERING γ-ε-α' MARTENSITIC TRANSFORMATION | + **Guisen Liu**, Yao Shen<br>MESOSCALE MODELING ON IRRADITION HARDENING OF METALLIC MATERIALS |
| 12:30 ~ 12:45 | + **Luoqi Wu**, Xiaobin Feng, Guodong Li<br>SYNERGISTICAL IMPROVEMENT OF STRENGTH AND PLASTICITY OF CADMIUM TELLURIDE SEMICONDUCTOR MATREILAS THROUGH INTERFACE MODIFICATION ENGINEERING SUCH AS GRADIENT STRUCTURE AND ALLOYING | | - |
| 12:45 ~ 13:00 | + **Daohan Lin**, Yixi Zhao, Xuan Cheng, Dan Shao, Jianzhi Sun<br>PATH-PLANNING FOR INDUCTION STRAIGHTENING PROCESS BASED ON REINFORCEMENT LEARNING APPROACH | + **Xiaoqing Shang**, Shengyi Zhong, Xiaoqin Zeng<br>UNVEILING DEFORMATION MECHANISM OF METAL COMPOSITE USING COMBINED IN-SITU DIFFRACTION EXPEREIMENTS AND FULL-FIELD CRYSTAL PLASTICITY MODELING | |
| 13:00 ~ 13:15 | + **Huiling Wang**, Dongsheng Qian, Feng Wang, Lin Hua<br>DAMAGE EVOLUTION OF MULTI-TYPE VOIDS DURING PLASTIC DEFORMATION OF HIGH-CARBON STEEL USING CRYSTAL PLASTICITY FINITE ELEMENT MODELING | + **Xinxin Sun**, Wentao Yan, Ming Wang Fu<br>A FULLY COUPLED MULTI-PHYSICS MULTI-PHASE FIELD CRYSTAL PLASTICITY FINITE ELEMENT MODEL (MPF-CPFEM) FOR PREDICTING MICROSTRUCTURE EVOLUTION AND THERMOMECHANICAL BEHAVIOR IN ADDITIVE MANUFACTURING | |

## 13:15 – 14:15 Lunch

| *Room* | **Peninsula** | **Bellarine** | **Ceres** |
|---|---|---|---|
| | ***(Sym) Characterization of Plasticity and Failure under Linear and Non-linear Loading Path (III)*** | ***(Sym) Multi-Scale Insights into Strengthening, Plasticity, and Damage in Multi-Principal Element Alloys (I)*** | ***Fatigue & Fracture*** |
| *Chairs* | ***Jeong Whan Yoon & Zhutian Xu*** | ***Jichao Qiao ++ & Yajuan Duan*** | ***Satyam Suwas & Wei Lu*** |
| 14:15 ~ 14:45 | ***** Jeong Whan Yoon**<br><br>ADVANCES IN MATERIALS CHRACTERIZATION | *** Jichao Qiao**<br><br>INTEGRATED MULTISCALE MODEL FOR THE VISCOELASTIC BEHAVIOR AND MICROSTRUCTURAL EVOLUTION OF METALLIC GLASSES: INSIGHTS FROM CYCLIC LOADING, CREEP AND THERMO-MECHANICAL COUPLING | *** Satyam Suwas**, S. Tejanath Reddy, K.U. Yazar, A. Bhattacharjee<br><br>MICROSTRUCTURAL ORIGIN OF DWELL-FATIGUE DEBIT IN NEAR- α TITANIUM ALLOYS |
| 14:45 ~ 15:00 | | + **Yajuan Duan**, Jichao Qiao, Eloi Pineda<br><br>ON THE CONNECTION BETWEEN MECHANICAL RELAXATION AND EQUILIBRATION KINETICS IN A HIGH-ENTROPY METALLIC GLASS | + **Di Song**, Heinz Thomas Beier, Michael Vormwald<br><br>UNIFIED LOW-CYCLE FATIGUE BEHAVIOR AND LIFE PREDICTION OF HIGH-MANGANESE TWIP STEELS UNDER COMPLEX LOADING CONDITIONS |
| 15:00 ~ 15:15 | *** Zhutian Xu**, Chuanzheng Li, Linfa Peng<br><br>FRACTURE OF NANO-COATINGS ON POLYCRYSTALLINE METALLIC SUBSTRATES IN PLASTIC DEFORMATION AND ITS MODELING | + Yixuan He, **Haoxiang Liu**, Xudong Liu<br><br>TAILORING MARTENSITIC TRANSFORMATION KINETICS IN Co36.8Ni39.2Al24 HYPEREUTECTIC MEDIUM ENTROPY ALLOY THROUGH HEAT TREATMENT | + **Jiangshuai Meng**, Xu Li, Sheng Jiang, Daniel Dias-da-Costa, Luming Shen<br><br>IMAGE-BASED QUANTIFICATION OF FRAGMENT KINETIC ENERGY IN DYNAMIC FAILURE OF BRITTLE MATERIALS |
| 15:15 ~ 15:30 | | + **Guo-Jian Lyu**, Guanghui Xing, Jichao Qiao<br><br>STUDY ON THE COUPLING MECHANISM OF DYNAMIC RELAXATION AND INELASTIC DEFORMATION IN METALLIC GLASSES | + **Thomas Virazels**, Navab Hosseini, Nicolas Jacques, José A. Rodríguez Martínez<br><br>THE EFFECT OF MICROSTRUCTURAL INERTIA ON PLASTIC LOCALIZATION AND VOID GROWTH IN POROUS SOLIDS |
| 15:30 ~ 15:45 | + **Guofeng Han**, Jeong Whan Yoon<br><br>EVALUATING SHEAR STRAIN UNDER NONIDEAL SIMPLE SHEAR DEFORMATION | + **Bing Wang**, Jinyi Zhang, Jichao Qiao<br><br>REJUVENATION MECHANISM INDUCED BY CYCLIC LOADING IN SIMULATION | *** Wei Lu**<br><br>ELECTRODE FRACTURE AND ITS EFFECT ON BATTERY PERFORMANCE |
| 15:45 ~ 16:00 | + **Enzhen Ren**, Ji He<br><br>MACHINE LEARNING-ASSISTED NON-PARAMETRIC FULL-FIELD STRESS-STRAIN IDENTIFICATION FOR HIGH-THROUGHPUT DATA ACQUISITION OF SHEET METALS | - | |
| 16:00 ~ 16:15 | + **Jianyu Wang**, Feifan Li, Shifeng Wen<br><br>MULTI-SCALE INVESTIGATIONS ON DAMAGE AND ANISOTROPIC TENSILE BEHAVIOR OF TITANIUM MATRIX COMPOSITES WITH A NOVEL TIB-NETWORK ARCHITECTURE AT HIGH TEMPERATURE | | + **Thomas Virazels**, Javier García-Molleja, Juan Carlos Nieto-Fuentes, Manny Gonzales, Federico Sket, José A. Rodríguez-Martínez<br><br>HIGH-VELOCITY FRAGMENTATION AND SPALL FRACTURE OF STEEL AF9628 |
| 16:15 ~ 16:30 | + **Kehuan Wang**, Wentao Chen, Gang Liu<br><br>BREAKING THE STRENGTH-DUCTILITY TRADE-OFF IN 600 ℃ HIGH-TEMPERATURE TITANIUM ALLOYS VIA RAPID HEATING | | - |

*** 45 minutes Distinguished keynote lecture, * 30 minutes keynote lecture,
+ 15 minutes invited presentation, ++ Symposium Organizer

# Monday, Jan. 5, 2026

## 08:00 - 08:20 Orientation on Deakin Venue by Chair …… Room (D2.304 Costa Hall Lecture Theatre)

| *Room* | **D2.304 Costa Hall Lecture Theatre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***(Sym) Characterization of Plasticity and Failure under Linear and Non-linear Loading Path (IV)*** | ***(Sym) Numerical Strategies for Nonlinear Coupled Hydro-Poromechanics and Thermo-Mechanics Problems*** | ***(Sym) Integrating Length Scales: Constitutive Modeling and Plasticity Strategies (III)*** | ***(Sym) Cyclic Plasticity and Fatigue: Mechanisms, Modeling, and Design (I)*** |
| *Chairs* | ***Cunsheng Zhang & Thomas Stoughton*** | ***Valentina Salomoni ++ & Massimiliano Ferronato ++*** | ***Eun-Ho Lee & Dayong Li*** | ***Guozheng Kang ++ & Yanyao Jiang*** |
| 08:30 ~ 09:00 | * **Cunsheng Zhang**, Zinan Cheng<br>EXTENSIVE MODIFICATION AND APPLICATION OF VISCOPLASTIC SELF-CONSISTENT MODEL IN VARIOUS FIELDS | * **Valentina A. Salomoni**, Gianluca Mazzucco, Giovanna Xotta, Riccardo Fincato, Beatrice Pomaro, Nico De Marchi, Jiangkun Zhang, Alberto Antonini<br>MODELING POROUS/NON-POROUS MEDIA AT DIFFERENT SCALES FOR SUSTAINABLE APPLICATIONS | * **Eun-Ho Lee**, Sung-Hyun Oh, Jae-Uk Lee, Hyun-Dong Lee, Hoo-Jeong Lee<br>CONSTITUTIVE MODELING FOR MULTI-SCALE SIMULATION OF BUMPLESS HYBRID BONDING PROCESSES IN SEMICONDUCTOR DIE STACKING FOR HIGH-PERFORMANCE COMPUTING SYSTEM | *** **Guozheng Kang**, Yu Lei, Ziyi Wang, Binghui Hu, Chao Yu<br>EXPERIMENTAL AND THEORETICAL STUDY ON TEMPERATURE-DEPENDENT RATCHETTING-FATIGUE INTERACTION OF EXTRUDED AZ31 MAGNESIUM ALLOYM ALLOY |
| 09:00 ~ 09:15 | + **Wen Zhang**, Huan Wu, Xincun Zhuang, Zhen Zhao<br>A DAMAGE EVOLUTION FRAMEWORK BASED ON SHAPE AND VOLUME CHANGES OF SPHERICAL VOIDS UNDER NON-PROPORTIONAL LOADING CONDITIONS | * **Massimiliano Ferronato**, Eduardo Da Silva Castro, Andrea Franceschini, Daniele Moretto<br>MULTI-PHYSICS AND MULTI-DOMAIN SIMULATIONS OF COUPLED PROCESSES IN POROUS MEDIA | * Guowei Zhou, Qi Wang, **Dayong Li**, Peidong Wu<br>NEURAL NETWORK BASED MESOSCALE PLASTICITY MODEL FOR HCP MATERIAL WITH SLIP AND TWINNING MECHANISMS | |
| 09:15 ~ 09:30 | **+ Yue Liu**, Kang Zhanga, Kaichao Zhangb, Na Xiaoc, Hongshou Huangd, Hao Wange<br>SHEAR-TAILORED MACROSCOPIC HETEROGENEOUS STRUCTURE DELIVERS EXCEPTIONAL SUPERPLASTICITY IN DUAL-PHASE TITANIUM ALLOYS | | | + **Hyemin Ryu**, Jiaqi Dong, Kelvin Y. Xie, Gi-Dong Sim<br>PHASE TRANSFORMATION-MEDIATED TRANSITION FROM LOW- TO HIGH-CYCLE FATIGUE IN Ni-RICH NiTi THIN FILMS |
| 09:30 ~ 09:45 | * **Thomas B. Stoughton**, Jeong-Whan Yoon<br>APPLICATION OF DIGITAL IMAGE CORRELATION TECHNOLOGY FOR CHARACTERIZATION OF ELASTO-PLASTICITY, NECKING, AND FRACTURE PROPERTIES OF SHEET METAL | + **Yukai Xiong**, Xu Zhang<br>COUPLED CRYSTAL PLASTICITY-PHASE FIELD MODELING OF MULTI-MECHANISM DEFORMATION IN FCC METALS: INSIGHTS INTO TWINNING-MEDIATED PLASTICITY | * **Guowei Zhou**, Dayong Li, Peidong Wu<br>MODELLING OF CONTINUOUS DYNAMIC RECRYSTALLIZATION OF ALUMINUM ALLOY WITH CRYSTAL PLASTICITY FINITE ELEMENT CONSIDERING EXPLICIT SUBGRAIN STRUCTURE EVOLUTIONS | * **Yanyao Jiang**, Yuxuan Song, Zengliang Gao<br>MATAL FATIGUE AND CYCLIC PLASTICITY: FROM A MACROSCOPIC PERSPECTIVE |
| 09:45 ~ 10:00 | | + **Mei-Cen Chen**, Eun-Ho Lee<br>MODELING OF INTERFACIAL FRACTURE IN STACKED THIN FILMS WITH STRAIN-RATE AND HYGROTHERMAL EFFECTS | | |
| 10:00 ~ 10:15 | + Jing-Hua Zheng, **Yueyulong Fang**, Ruodie Yu, Qian Bai, Kailun Zheng<br>A NOVEL CONSTITUTIVE MODEL FOR ALUMINUM ALLOYS UNDER COMPRESSION & SHEAR COUPLED DEFORMATION | - | * **Xincun Zhuang**, Ruizhi Deng, Huachao Yang, Wen Zhang, Zhen Zhao<br>EFFECTS OF TENSION-COMPRESSION ASYMMETRY IN R-VALUE ON PLASTIC FLOW BEHAVIOR: EXPERIMENTS AND MODELING | + **Sita Choudhary**, Prasanth Soundappan, Aarya Kedar Sathe, I. Balasundar, Satyam Suwas<br>MICROMECHANICAL RESPONSE OF AN ADDITIVELY MANUFACTURED NEAR-α Ti-6242 ALLOY UNDER CYCLIC LOADING: INSIGHTS FROM EXPERIMENTS AND CRYSTAL PLASTICITY SIMULATIONS |
| 10:15 ~ 10:30 | + **Daecheon Cho**, Heonyong Lim, Kanghyeok Choi, Jeong-Whan Yoon<br>INVESTIGATION OF THE MECHANISM FOR EDGE CRACK REDUCTION AND ANALYSIS OF THE EFFECT OF MAJOR PROCESS VARIABLES IN EQUAL-SPEED ASYMMETRIC ROLLING | | | - |

## 10:30 – 11:00 Coffee Break

| *Room* | **D2.304 Costa Hall Lecture Theatre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***Deformation Mechanisms in Hexagonal Metals*** | ***(Sym) Multi-Scale Insights into Strengthening , Plasticity, and Damage in Multi -Principal Element Alloys (II)*** | ***(Sym) Integrating Length Scales: Constitutive Modeling and Plasticity Strategies (IV)*** | ***(Sym) Multiscale Plasticity of Materials Under Extreme Conditions (II)*** |
| *Chairs* | **Matthew R. Barnett & Orcun K. Celebi** | **Zhangwei Wang & Laichang Zhang** | **Heung Nam Han & R.E. Jones** | **Fulin Wang & Jiao Luo** |
| 11:00 ~ 11:30 | *** **Matthew R. Barnett**, Jun Wang, Peter Lynch, Andrew Stevenson<br><br>OBSERVING CO-ORDINATED BURSTS OF PLASTICITY IN BULK MAGNESIUM ALLOYS | * **Zhangwei Wang**<br><br>COMPOSITIONALLY COMPLEX ALLOYS—TOWARD THE DESIGN OF EXCEPTIONAL MATERIALS | * **Heung Nam Han**, Kyung Mun Min, Seonghwan Choi, Jee Hyuk Ahn, Hyuk Jong Bong, Myoung-Gyu Lee<br><br>TOWARD AN INTEGRATED MODELING FRAMEWORK FOR RECRYSTALLIZATION-DRIVEN MICROSTRUCTURE CONTROL | * **Fulin Wang**, Fenghua Wang, Jian Zeng, Chuanlai Liu, Shuai Dong, Li Jin, Jie Dong<br><br>LOCAL STRAIN MODULATION BY THE LPSO PHASE OF LAMELLAR AND BLOCKY MORPHOLOGY IN MG ALLOYS |
| 11:30 ~ 11:45 | | | | |
| 11:45 ~ 12:00 | + **Orcun K. Celebi**, Tolga B. Celebi, Daegun You, Ashley Bucsek, Huseyin Sehitoglu<br><br>CROSS-SLIP AND EASY-GLIDE CRSS DETERMINATION IN TITANIUM: THEORETICAL PREDICTIONS AND IN-SITU EXPERIMENTAL MEASUREMENTS | * **Laichang Zhang**<br><br>ADDITIVE MANUFACTURING AND MECHANICAL BEHAVIOR OF TINBTAZRMO REFRACTORY HIGH-ENTROPY ALLOY | * **R.E. Jones**, J.N. Fuhg, D.T. Seidl<br><br>A NEURAL NETWORK FRAMEWORK FOR THERMOVISCOPLASTICITY | * **Anirban Patra**, Namit Pai, Youngung Jeong, Carlos N. Tomé<br><br>ELASTO-VISCOPLASTIC MODELING OF DEFORMATION IN DUAL PHASE STEELS: FROM MICROSTRUCTURES TO COMPONENTS |
| 12:00 ~ 12:15 | + **Daegun You**, Ahmed Sameer Khan Mohammed, Minoru Nishida, Huseyin Sehitoglu<br><br>ORIGIN OF TWINNING MODE HIERARCHY IN NITI – A CRITICAL UNDERSTANDING | + **Yang Chen**, Shuo Wang, Jing Peng, Qihong Fang<br><br>ON THE INVESTIGATION OF STRENGTHENING AND IRRADIATION DAMAGE IN MULTI-PRINCIPAL ELEMENT ALLOYS: MULTISCALE DISLOCATIONS DYNAMICS SIMULATIONS | + **Zeran Hou**, Jinheung Park, Yong Hou, Yushi Yang, Myoung-Gyu Lee, Junying Min<br><br>A TEMPERATURE-EXPLICIT CRYSTAL PLASTICITY FRAMEWORK FOR PREDICTING MECHANICAL BEHAVIOR OF QP1500 | + **Jingya Wang**, Hongwei Xiong, Javier LLorca, Xiaoqin Zeng<br><br>OVERCOMING THE SPECIFIC STIFFNESS/DUCTILITY TRADE-OFF IN ZX50/SIC MAGNESIUM COMPOSITES THROUGH SOLUTE-SEGREGATION INTERFACE STRENGTHENING |
| 12:15 ~ 12:30 | + **Hao Wang**, Jinhu Zhang, Xuexiong Li, Jianke Qiu, Shujun Li, Jianrong Liu, Dongsheng Xu, Rui Yang<br><br>DESIGN OF TITANIUM ALLOYS INTEGRATING MECHANISM AND INTELLIGENCE | + **LingYun Qian**, JiaXiang Zhang, Jie Xu, XinYu Liu, ChaoYang Sun<br><br>ESTABLISHMENT OF A UNIFIED ELASTOPLASTIC CONSTITUTIVE MODEL FOR SiC/AL COMPOSITES AND THREE-DIMENSIONAL FINITE ELEMENT MODELING BASED ON MICROSTRUCTURE | + **Mohamed Magdy**, Xianglu Zhang, Junying Min<br><br>INTEGRATED CRYSTAL PLASTICITY-PHASE FIELD FRAMEWORK FOR PREDICTING ELECTRICALLY INDUCED RECRYSTALLIZATION AND GRAIN GROWTH IN POLYCRYSTALLINE TITANIUM | + **Jingyu Zhang**, Mingxin Huang<br><br>STRAIN-RATE EFFECTS ON THE STRENGTH AND FRACTURE OF ADVANCED HIGH-STRENGTH STEELS |
| 12:30 ~ 12:45 | - | * **Qing Zhou**<br><br>REVEALING THE MECHANISMS OF DISLOCATION-GRAIN BOUNDARY INTERACTIONS IN A COCRNI MEDIUM-ENTROPY ALLOY: A COMBINED SIMULATION AND EXPERIMENTAL STUDY | + **Jong-Hyeok Kwon**, Dae-Seo Kwon, Dong-Kyu Kim<br><br>AI-ASSISTED UNVEILING MICROMECHANICAL FAILURE MECHANISMS IN METAL MATRIX COMPOSITE: IN SITU ACOUSIC EMISSION AND NEUTRON DIFFRACTION | + **Chengyi Dan**<br><br>IN SITU HIGH THROUGHPUT CHARACTERIZATION AND ANALYSIS OF ALUMINUM ALLOYS |
| 12:45 ~ 13:00 | | | + Zhiyu Xiang, Hongwei Li, **Xin Zhang**<br><br>MULTISCALE MODELING OF ELECTRICALLY ASSISTED DEFORMATION IN Ni-BASED SUPERALLOY ALLOY THROUGH ELECTRON-ATOM COLLISION MECHANISM | * Ke Chen, **Jiao Luo**, Junjie Li, Jin Yang<br><br>MULTISCALE MODELING AND SIMULATION OF γ PHASE DURING GRADIENT STRAIN AND TEMPERATURE OF GH4586 SUPERALLOY USING INTEGRATED FINITE ELEMENT AND PHASE-FIELD METHOD |
| 13:00 ~ 13:15 | | - | - | |

## 13:15 – 14:30 Lunch

| *Room* | **D2.304 Costa Hall Lecture Theatre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***(Sym) Khan Medal Symposium in Honor of Irene Beyerlein: Understanding Deformation Mechanisms at the Mesoscale via Modelling and Experiments (I)*** | ***(Sym) AI Modeling for Plastic Forming with Multi-Energy Fields (III)*** | ***(Sym) Hydrogen Effects on Deformation, Fatigue and Fracture (II)*** | ***High Entropy Alloys*** |
| *Chairs* | **Irene J. Beyerlein & Gi-Dong Sim ++** | **Khanh Chau Le & Lechun Xie** | **Wei Cai ++ & Shigenobu Ogata** | **Alan Xu & Li Li** |
| 14:15 ~ 14:45 | ***** Irene J. Beyerlein**<br>FUNDAMENTAL PROPERTY EFFECTS ON CRITICAL RESOLVED SHEAR STRESSES IN REFRACTORY MULTI-PRINCIPAL ELEMENT ALLOYS | *** Khanh Chau Le**<br>DATA-DRIVEN APPROACH TO DISLOCATION MEDIATED PLASTICITY | *** Muhammad Arafin**<br>RECENT DEVELOPMENT ON LINEPIPE FOR HYDROGEN TRANSPORTATION | *** Alan Xu**, Michael Moschetti, David Miskovic, Tao Wei, Mihail Ionescu, Zhiyang Wang, Tim Palmer, Dhriti Bhattacharyya, Peidong He, Xiaopeng Li, Bernd Gludovatz, Michael Ferry<br>IMPROVED IRRADIATION RESISTANCE OF A LOW ACTIVATION REFRACTORY MEDIUM ENTROPY ALLOY, VCrFeW0.2, FOR FUSION APPLICATIONS DEMONSTRATED BY MICRO-TENSILE TESTING |
| 14:45 ~ 15:00 | | + **Lechun Xie**, Jian Zhou, Fei Yin, Lin Hua<br>THE STUDY OF MICROPILLAR CYCLIC COMPRESSION DEFORMATION BEHAVIOR OF Ti-6.5Al-3.5Mo-1.5Zr-0.3Si ALLOY AFTER ELECTROMAGNETIC SHOCK TREATMENT | * Wurong Jian, **Wei Cai**<br>HYDROGEN EFFECT ON DISLOCATION MOBILITY IN SINGLE CRYSTAL NICKEL | *** Wei Jian**<br>PLASTIC BEHAVIOR OF REFRACTORY HIGH ENTROPY ALLOYS FROM NANOSCALE PERSPECTIVE |
| 15:00 ~ 15:15 | *** Dongwoo Lee**, Taeyeop Kim, Daegun You<br>COMBINATORIAL EXPERIMENTAL STUDY ON THE MECHANICAL BEHAVIOR OF Mo–Nb–Ti AND Ta–Nb–Ti COMPLEX-CONCENTRATED ALLOY THIN FILMS | + **Zhang Han**, Liu Yanxiong<br>DEFORMATION BEHAVIOR AND MICROSTRUCTURAL EVOLUTION OF HIGH-STRENGTH AND LOW-PLASTICITY MATERIALS UNDER COMPRESSION PROCESS WITH CONFINING PRESSURE | | |
| 15:15 ~ 15:30 | | + **Xiong Zhou**, Fengrui Chen, Guodong Li, Zhixiang Qi, Guang Chen<br>QUANTITATIVE EXPLANATION OF TWIN BOUNDARY INDUCED DUCTILITY IN γ-TiAl BASED ON THE COMPETITIVE MECHANISM OF DISLOCATION NUCLEATION | *** Jörg Neugebauer**, Ali Tehranchi, Tilmann Hickel<br>HYDROGEN ENHANCED CROSS SLIP (HECS): A NOVEL ATOMISTIC MECHANISM FOR HYDROGEN ASSISTED EMBRITTLEMENT IN NICKEL GRAIN BOUNDARIES | *** Li Li**, Yang Chen, Qihong Fang, Jia Li<br>AN ATOMICALLY INFORMED FINITE ELEMENT FRAMEWORK FOR LATTICE-DISTORTION-INDUCED STRAIN HARDENING IN HIGH-ENTROPY ALLOYS |
| 15:30 ~ 15:45 | *** Amit Misra**<br>EXPERIMENTAL CHARACTERIZATION OF GRAIN BOUNDARY STRENGTHENING IN POLYCRYSTALLINE MAGNESIUM ALLOYS | + **Yanqiu Yang**, Yanchao Zhao, Zhenwei Li, Li Yang, Zhixun Wen<br>HOT CORROSION-CREEP DEFORMATION BEHAVIOR OF NI-BASED SINGLE CRYSTAL SUPERALLOY CONSIDERING THE STRESS DEPENDENCE AND FILM COOLING HOLE | | |
| 15:45 ~ 16:00 | | + **Min Yi**<br>AN ELECTRO-THERMO-MECHANICALLY COUPLED CRYSTAL PLASTICITY MODEL FOR ELECTROPLASTICITY | *** Shigenobu Ogata**<br>ATOMISTIC MODELING OF HYDROGEN IMPACT ON DEFECT KINETICS IN MATALS | + **Qishan Huang**, Yixuan Zeng, Haofei Zhou<br>GRAIN BOUNDARY SEGREGATION-INDUCED TRANSITION OF DEFORMATION MECHANISMS IN FENICRCOCU HIGH-ENTROPY ALLOY |
| 16:00 ~ 16:15 | *** Gi-Dong Sim**, Injong Oh, Zion Lee, Hojang Kim<br>ALUMINUM-CARBON THIN FILMS WITH HIGH STRENGTH AND DUCTILITY | - | | - |
| 16:15 ~ 16:30 | | | + **Frank W. DelRio**, Manuel Schmitz-Elbers, Uwe Strohmeier, Thomas Straub<br>LOCAL FAILURE STRAIN AND REDUCTION OF AREA PROVIDE EARLY METRICS FOR HYDROGEN EMBRITTLEMENT IN MICROSCALE TENSILE SPECIMENS | |

*** 45 minutes Distinguished keynote lecture, * 30 minutes keynote lecture,
+ 15 minutes invited presentation, ++ Symposium Organizer

# Tuesday, Jan. 6, 2026

| *Room* | **D2.304 Costa Hall Lecture Theatre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***(Sym) Khan Medal Symposium in Honor of Irene Beyerlein: Understanding Deformation Mechanisms at the Mesoscale via Modelling and Experiments (II)*** | ***Multiscale Modeling (I)*** | ***(Sym) Hydrogen Effects on Deformation, Fatigue and Fracture (III)*** | ***Crystal Plasticity*** |
| *Chairs* | ***Abigail Hunter ++ & Keonwook Kang*** | ***Yoshiteru Aoyagi & Frank William DelRio*** | ***Neeraj S. Thirumalai & T. A. Venkatesh ++*** | ***Chuanlai Liu & Bjørn Holmedal*** |
| 08:30 ~ 09:00 | ***** Abigail Hunter**<br><br>MESOSCALE INVESTIGATION OF DISLOCATION-GRAIN BOUNDARY INTERACTIONS IN METALS AND ALLOYS | *** Yoshiteru Aoyagi**<br><br>MULTISCALE MODELING OF NONLINEAR VISCOELASTIC-VISCOPLASTIC BEHAVIOR IN GLASSY POLYMERS BASED ON INTRAMOLECULAR CHAIN ROTATION | *** Neeraj S. Thirumalai**<br><br>HYDROGEN EMBRITTLEMENT IN ENERGY INDUSTRY: PERSPECTIVE ON MECHANISMS AND EMERGING CHALLENGES IN H2 and CO2 TRANSPORTATION | *** Chuanlai Liu**<br><br>MICROSTRUCTURE-SENSITIVE CRYSTAL PLASTICITY AND PHASE-FIELD MODELING OF PLASTIC DEFORMATION, FRACUTRE, RECRYSTALLIZATION IN Mg ALLOYS |
| 09:00 ~ 09:15 | | *** Frank W. DelRio**, William M. Mook, Paul G. Kotula, Jeffery A. Greathouse, Eric D. Hintsala, Douglas D. Stauffer, Henry Q. Afful, Corinne E. Packard, Anastasia G. Ilgen<br><br>VISUALIZING THERMOMECHANICAL WEAKENING OF MUSCOVITE MICA VIA MICROSCALE SHEAR TESTING | *** T. A. Venkatesh**, Xiaoli Wang, Guang Cheng, Wei Cai, Ming Dao<br><br>THE EFFECTS OF HYDROGEN TRAPPING AT GRAIN-BOUNDARIES AND PRECIPITATE INTERFACES ON MECHANICAL PROPERTIES: A MOLECULAR DYNAMICS STUDY | *** Bjørn Holmedal**, Hassan M. Asadkandi, Tomáš Mánik, Arash Imani Aria, Odd Sture Hopperstad<br><br>HIGH-RESOLUTION CRYSTAL-PLASTICITY SIMULATIONS OF INNER YIELD SURFACES AFTER PRE-DEFORMATION |
| 09:15 ~ 09:30 | **+ Deunbom Chung**, Minwoo Park, Wanchuck Woo, Seungcheol Oh, Kyeongjae Jeong, Heung Nam Han<br><br>FE-CNN FRAMEWORK FOR NON-DESTRUCTIVE CHARACTERIZATION OF RESIDUAL STRESS VIA SPHERICAL INDENTATION | | | |
| 09:30 ~ 09:45 | * Hyunggyu Lee , Jie Nan, Younggak Shin, Byeongchan Lee, **Keonwook Kang**<br><br>ATOMISTIC STUDIES OF CUMULATIVE IRRADIATION DAMAGES IN SINGLE-CRYSTILLINE TUNGSTEN AND EVOLUTION OF SECONDARY DEFECTS | **+ S. Caleb Foster**, Justin W. Wilkerson, José A. Rodríguez-Martínez<br><br>A MULTISCALE FINITE ELEMENT ANALYSIS OF THE DYNAMIC FRAGMENTATION OF ADDITIVELY MANUFACTURED POROUS METAL RINGS | *** Mira Todorova**, Sudarsan Surendralal, Florian Deißenbeck, Stefan Wippermann, Jing Yang and Jörg Neugebauer<br><br>AB-INITIO INSIGHTS INTO THE INTERACTIONS OF HYDROGEN WITH METALS IN ELECTROCHEMICAL ENVIRONMENT | **+ Haruki Ohashi**, Hojun Lim, Yoshiteru Aoyagi, Aashique A. Rezwan<br>CRYSTAL PLASTICITY – PHASE FIELD DAMAGE SIMULATION: INVESTIGATING DUCTILE FRACTURE BEHAVIOR INDUCED BY CRYSTALLOGRAPHIC ORIENTATION AND PRECIPITATED PARTICLE |
| gpa09 :45 ~ 10:00 | | + **Nomun Gerel-Erdene**, Yoshiteru Aoyagi<br><br>MULTISCALE PLASTICITY SIMULATION OF POLYLACTIC ACID SPHERULITES USING THREE-DIMENSIONAL LAMINATE THEORY INCORPORATING CRYSTALLINITY AND MICROSTRUCTURE | | + **Rui Zhao**, Changke Li, Qiji Guo, Yimeng Xu, Min Wan<br><br>MACRO-MICRO ANISOTROPIC ANALYSIS OF BASED ON CRYSTAL PLASTICITY FINITE ELEMENT METHOD |
| 10:00 ~ 10:15 | *** Leyun Wang**, Dongfang Shi, Xiaoqin Zeng, Huamiao Wang+, Zhefeng Zhang<br><br>ENHANCED PYRAMIDAL SLIP IN MAGNESIUM ALLOYS VIA GADOLINIUM ALLOYING AND ITS EFFECT ON PLASTIC DEFORMATION | **+ Yuntong Huang**, Shuyang Dai, Chuqi Chen, Yang Xiang<br><br>A MULTI-SCALE PHASE FIELD MODEL FOR AMORPHIZATION AS A DEFORMATION MECHANISM IN NANOCRYSTALLINE MATERIALS | *** Rama Srinivas Varanasi**<br><br>HYDROGEN-INDUCED FAST FRACTURE IN A 1.5 GPa DUAL-PHASE STEEL | - |
| 10:15 ~ 10:30 | | + **Cheng Luo**, Huang Yuan, Xingxing Zhang<br><br>ANISOTROPIC MULTISCALE PLASTICITY BEHAVIORS OF ADDITIVELY MANUFACTURED SUPERALLOYS: SYNCHROTRON X-RAY DIFFRACTION AND DISLOCATION-BASED CRYSTAL PLASTICITY MODELING | | |

## 10:30 – 11:00 Coffee Break

| *Room* | **D2.304 Costa Hall Lecture Theatre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***(Sym) Khan Medal Symposium in Honor of Irene Beyerlein: Understanding Deformation Mechanisms at the Mesoscale via Modelling and Experiments (II)*** | ***Plasticity at High Strain Rate*** | ***(Sym) Integrating Length Scales: Constitutive Modeling and Plasticity Strategies (V)*** | ***Polymer & Composite*** |
| *Chairs* | ***Curt A. Bronkhorst & Lei Cao*** | ***Henryk Paul & Justin S. Wark*** | ***Myoung-Gyu Lee & Shihoon Choi ++*** | ***Guoqiang Li & Theo Tervoort*** |
| 11:00 ~ 11:30 | *** **Curt A. Bronkhorst**, Noah J. Schmelzer, Sam D. Dunham, Raymond Rasmussen, Stephen Yang, Janith Wanni, Charles Adkins, Dan J. Thoma<br><br>STATISTICAL THERMOMECHANICS OF DUCTILE DAMAGE FOR DYNAMIC LOADING CONDITIONS | * **Henryk Paul**, Sandra Puchlerska, Robert Chulist<br><br>ROLE OF LATTICE RE-ORIENTATION IN THE FORMATION OF SHEAR BANDS DURING HIGH STRAIN-RATE DEFORMATION | * **Myoung-Gyu Lee**, Seonghwan Choi, Seungwoo Kim, Jehyun You<br><br>UNDERSTANDING ANISOTROPIC PLASTICITY IN POLYCRYSTALLINE METALS THROUGH MICROSTRUCTURE-PROPERTY RELATIONSHIPS | * **Guoqiang Li**<br><br>CONSTITUTIVE MODELING OF SHAPE MEMORY POLYMERS |
| 11:30 ~ 11:45 | | * **Makoto Uchida**, Mei Toji, Keito Oya, Yoshihisa Kaneko<br><br>NUMERICAL MODELING OF THERMAL HISTORY– AND STRAIN RATE– DEPEDENT DOUBLE YIELDING BEHAVIOR OF SEMI-CRYSTALLINE POLYMER | * Hyeonbin Moon, Donghyuk Cho, Jeong Whan Yoon, **Seunghwa Ryu**<br><br>PHYSICS-INFORMED DISCOVERY OF YIELD FUNCTIONS IN PLASTICITY USING PHYSICS-INFORMED NEURAL NETWORKS | * **Theo Tervoort**, Arturo Winters, Jan Vermant<br><br>AN ELASTO-VISCOPLASTIC APPROACH TO POLYMER RHEOLOGY |
| 11:45 ~ 12:00 | + **Ronghai Wu,** Heng Li<br><br>PREDICTING DISLOCATION PATTERNS AND DISCOVERING THE LAW OF SIMILITUDE BY MACHINE LEARNING | | | |
| 12:00 ~ 12:15 | * **Lei Cao**<br><br>TRANSFORMATION-ASSISTED TWIN NUCLEATION IN METALS | * **Justin S. Wark**, Patrick G. Heighway<br><br>FEMTOSECOND X-RAY DIFFRACTION STUDIES OF PLASTICITY AT EXTREME PRESSURES AND STRAIN RATES | * Saurabh Pawar, K. U. Yazar., Khushahal Thool, Wi-Geol Seo, Chang-Gon Jeong, Yoon-Uk Heo, **Shi-Hoon Choi**<br><br>ANISOTROPIC COMPRESSION BEHAVIOR OF 316L STAINLESS STEEL AT CRYOGENIC TEMPERATURE | + **Ji Lin**, Rui Xiao<br><br>A THREE-DIMENSIONAL SHEAR TRANSFORMATION ZONE THEORY FOR GLASSY POLYMERS |
| 12:15 ~ 12:30 | | | | + **Zefeng Yu**, Shan Tang<br><br>MDVP: A MECHANISM-BASED DATA-DRIVEN VISCOPLASTIC CONSTITUTIVE MODEL FOR GLASSY POLYMERS |
| 12:30 ~ 12:45 | * **Nathan A. Mara**, Mauricio De Leo, Nicolas Fuchs-Lynch, Justin Y. Cheng, Shuozhi Xu, Irene J. Beyerlein<br><br>ENHANCING STRENGTH AND DUCTILITY OF HCP/BCC AND FCC/BCC NANOLAMINATES VIA THICK 3D INTERFACES | + **Hamed Sadeghi**, Jiayu Chen, Keith Davey, Yongxiang Hu<br><br>SIZE EFFECTS IN HIGH-STRAIN RATE BEHAVIOR OF SINGLE CRYSTAL ALUMINUM: A FINITE SIMILITUDE APPROACH | + Yong Hou, **Jinheung Park**, Junying Min, Zhenkai Mu, Yannis Korkolis<br><br>A SIMPLE YET FLEXIBLE POLY6 YIELD CRITERION FOR PLASTIC ANISOTROPY IN SHEET METALS | - |
| 12:45 ~ 13:00 | | - | + **Yao Xiao**, Yunhui Geng, Chao Yu<br><br>TAILORING THE THERMAL EXPANSION PERFORMANCE OF NiMnGa FERROMAGNETIC SHAPE MEMORY ALLOY THROUGH ROTARY MAGNETIC FIELD: EXPERIMENT AND THEORETICAL MODEL | |
| 13:00 ~ 13:15 | - | | + **Yixing Zhao**, Jeong-Hwan Moon, Min-Seong Kim, Meiling Geng, Lihong Cai, Namsu Park, Jinwoo Lee, Sung-Tae Hong<br><br>CRYOGENIC DEFORMATION BEHAVIOR AND MICROSTRUCTURAL MECHANISMS IN AA6061T6 | |

## 13:15 – 14:15 Lunch

| *Room* | **D2.304 Costa Hall Lecture Theatre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***(Sym) Advances in ML-based Applications for Plasticity, Damage and Fracture (I)*** | ***Constitutive Modeling (I)*** | ***Novel Experiment & Modeling / Additive Manufacturng*** | ***Damage in Plasticity*** |
| *Chairs* | ***Alfonso H.W. Ngan & Hansohl Cho*** | ***Lidiia Nazarenko & Arash Yavari*** | ***J.A. Rodriguez-Martinez & Chaoyue Jin*** | ***Rui Xiao & Katarzyna Kowalczyk-Gajewska*** |
| 14:15 ~ 14:45 | *** **Alfonso H.W. Ngan**, Wei Li, Shuang Lyu, Yuanhang Xia, Mengzhen Cao, Yue Chen, Yuqi Zhang<br><br>DISLOCATIONS IN COMPLEX CONCENTRATED ALLOYS – STATISTICAL MECHANICS AND MACHINE LEARNING OF RESISTANCES | * **Lidiia Nazarenko**, Aleksandr Yurievich Chirkov, Holm Altenbach<br><br>MIXED FINITE ELEMENT METHOD FOR A SIMPLIFIED GRADIENT ELASTIC-PLASTIC MODEL: FORMULATION, IMPLEMENTATION, AND APPLICATION TO REPRESENTATIVE PROBLEMS | * **J. A. Rodríguez-Martínez**, T. Virazels, J. García-Molleja, B. Lukić, A. Rack, S. Puerta*, D. Pedroche, F. Sket<br><br>REAL-TIME IN-SITU X-RAY IMAGING OF PORE COMPACTION AND SPALL FRACTURE IN PLATE IMPACT TESTS ON ADDITIVELY MANUFACTURED METALS" | * **Rui Xiao**<br><br>DAMAGE OF TOUGH ELASTOMERS AND GELS: INSIGHTS FROM MECHANOCHEMISTRY |
| 14:45 ~ 15:00 | | * **Arash Yavari**<br><br>NONLINEAR CAUCHY ELASTICITY | + **Chaoyue Jin**, Shurong Ding, Xiaobin Jian<br><br>ON THE MECHANICAL PROPERTY DEGRADATION OF POST-IRRADIATED U-MO ALLOYS | * **Katarzyna Kowalczyk-Gajewska**, Saketh Virupakshi, Xinzhu Zheng, Michał Kursa, Sandra Musiał, Michał Maj, Ibrahim Karaman, Ankit Srivastava<br><br>FULL-FIELD ANALYSES OF PLASTICITY AND VOID GROWTH IN MATERIALS DEFORMING BY SLIP AND TWINNING |
| 15:00 ~ 15:15 | * **Abhijit Brahme,** Johann B. Scheepers, Kaan Inal<br><br>DEEP LEARNING BASED SURROGATE MODELING FOR CRYSTAL-PLASTICITY DRIVEN PREDICTION OF ALUMINUM ALLOY FRACTURE SURFACES | | + **Zion Lee**, Hojang Kim, Sunkun Choi, Injong Oh, Jaehong Park, Gi-Dong Sim<br><br>ACHIEVING HIGH STRENGTH IN 6061 ALUMINUM ALLOY THIN FILMS THROUGH INTERSTITIAL CARBON INCORPORATION. | |
| 15:15 ~ 15:30 | | + **Jiawen Zhang**, Zhangtao Li, Yuwei Zhang, Yinan Cui, Xufei Fang, Wenjun Lu<br><br>SCALE-BRIDGING DISLOCATION PLASTICITY IN MGO AT ROOM TEMPERATURE | + **Wenbho Sha**, Jun Yua, Xin Lina, Lilin wanga, Liang Maa, Yang Zhoua, Yufeng Zhanga, Shuoqing Shia, Qiaodan Yana<br><br>MOLTEN POOL SHAPE AND IN-SITU NANO (Nb,Ti)C PRECIPITATION ON MECHANICAL PROPERTIES IN LASER DIRECTED ENERGY DEPOSITED IN718/TICP COMPOSITE | + **Bingxin Zhao**<br><br>THERMO-MECHANICAL DEFORMATION AND EARLY-STAGE DAMAGE IN ROTATING COMPOSITE SPACE STRUCTURES |
| F | * **Hansohl Cho**, Seunghyeon Lee, Thao Nguyen, Darby J. Luscher, Saryu J. Fensin, John S. Carpenter<br><br>STATISTICAL INFERENCE AND UNCERTAINTY QUANTIFICATION FOR MODELING OF BODY-CENTERED-CUBIC SINGLE CRYSTALS | + **Xiao-Lei Cui**, Qianxi Sun, Shijian Yuan<br><br>OVERCOMING LIMITATIONS IN PREDICTING BIAXIAL TENSION OF ANISOTROPIC ALUMINUM ALLOY TUBES USING BARLAT89 YIELD CRITERION | + **Yuguang Chen**, Wei Fan, Hua Tan, Xin Lin<br><br>COUPLING OPTIMIZED SOLIDIFICATION AND HEAT TREATMENT ENABLES SUPERIOR STRENGTH-DUCTILITY SYNERGY IN ADDITIVE MANUFACTURED NiTi ALLOYS | - |
| 15:45 ~ 16:00 | | - | + **Qian Wang**, Meng Wang, Yufan Shen, Xin Lin<br><br>MICROSTRUCTURE AND MECHANICAL PROPERTY OPTIMIZATION OF ADDITIVELY MANUFACTURED TI-MODIFIED HIGH-STRENGTH AL ALLOYS VIA MULTI-STAGE HEAT TREATMENT | |

## 16:15 – 17:15 Khan International Medal/Award Lecture by Ming Wang Fu :

*"Damage and Fracture in the Deformation of Materials"*

(Chair: Huseyin Sehitoglu, Room: D2.304 Costa Hall Lecture Theatre)

## 19:00 – 21:30 Conference Banquet (Geelong Stadium, Club Chin Chin)

*** 45 minutes Distinguished keynote lecture, * 30 minutes keynote lecture,
+ 15 minutes invited presentation, ++ Symposium Organizer

# Wednesday, Jan. 7, 2026

## 10:30 – 11:00 Morning Break

| *Room* | **D2.304 Costa Hall Lecture Thetre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***(Sym) Advances in ML-based Applications for Plasticity, Damage and Fracture (II)*** | ***(Sym) Hydrogen Effects on Deformation, Fatigue and Fracture (IV)*** | ***(Sym) Cyclic Plasticity and Fatigue: Mechanisms, Modeling, and Design (II)*** | ***Temperature Dependent Behaviors & Ni-based Alloy*** |
| *Chairs* | ***Yue Fan & Christian C. Roth*** | ***Ming Dao ++ & Guang Cheng*** | ***J.C. Stinville & Xu Zhang ++*** | ***Seid Koric & Zhuo Feng Lee*** |
| 11:00 ~ 11:30 | *** Yue Fan**<br><br>MACHINE LEARNING-AUGMENTED MODELING ON THE FORMATION OF NON-CONVENTIONAL NANO-PRECIPITATES IN FAST SOLIDIFIED Al ALLOYS | ***** Ming Dao**, Ting Yang, Cheng-Yuan Tsai, Wurong Jian, Yamini Mann, Wei Cai, T.A. Venkatesh<br><br>CRACK INITIATION OF HYDROGEN-CHARGED 304 STAINLESS STEELS UNDER MONOTONIC AND CYCLIC LOADING | * Dhruv Anjaria, Milan Heczko, Daegun You, Mathieu Calvat, Shuchi Sanandiya, Maik Rajkowski, Aditya Srinivasan Tirunilai, Huseyin Sehitoglu, Guillaume Laplanche, **J.C. Stinville**<br><br>FATIGUE-RESISTANT ALLOYS THROUGH DYNAMIC PLASTIC DEFORMATION DELOCALIZATION ACTIVATION | *** Seid Koric**, Qibang Liu, Jaewan Park, Amar A. Koric, Diab W. Abueidda<br><br>SEQUENTIAL DEEP OPERATOR NEURAL NETWORKS FOR PLASTIC AND THERMO-VISCOPLASTIC MATERIAL BEHAVIOR |
| 11:30 ~ 11:45 | *** Christian C. Roth**, Thomas Beerli, Xueyang Li, Vincent Grolleaua, Dirk Mohr<br><br>RATE-DEPENDENT DUCTILE FRACTURE OF DP-STEELS: STATIC AND DYNAMIC HIGH-THROUGHPUT EXPERIMENTS AND NEURAL NETWORK MODELING STATIC AND DYNAMIC HIGH-THROUGHPUT EXPERIMENTS AND NEURAL NETWORK MODELING | | *** Xu Zhang**, Yukai Xiong<br><br>PLASTIC DEFORMATION AND DAMAGE MECHANISMS IN PARTICLE-REINFORCED METAL MATRIX COMPOSITES: A CRYSTAL PLASTICITY-PHASE FIELD STUDY | + **Zhuo Feng Lee**, Hojang Kim, Yuhyun Park, Gi-Dong Sim<br><br>A HIGH-THROUGHPUT APPROACH TO ACQUIRE TENSILE AND COMPRESSIVE RESPONSES OF THIN FILMS AT ELEVATED TEMPERATURES |
| 11:45 ~ 12:00 | | *** Guang Cheng**, Kaiyuan Chen, Xuan Ding, Yajun Zhang, Jing Yang, Xiaolin Wang | | + **Xinyuan Yang**, Xiaoqing Shang, Shilong Liu, Haiming Zhang, Shengyi Zhong<br><br>CREEP MODELING FOR NICKEL-BASED SUPERALLOY ALIGNING GRAIN BOUNDARY EFFECT AND DISLOCATION MOVEMENT |
| 12:00 ~ 12:15 | + **Rui Barreira**, Dirk Mohr<br><br>MINIMAL STATE CELL RNN SURROGATE MODEL FOR ELASTOPLASTIC POROUS DUCTILE SOLIDS | HYDROGEN EMBRITTLEMENT UNDER EQUIVALENT HYDROGEN FUGACITY: A COMPARISON OF HYDROGEN CHARGING METHODS | + **Zinan Wang**, Xiangwei Kong, Chengying Zhao, Liu Cheng, Liyang Xie<br><br>AN ENHANCED MEAN STRESS EFFECT CORRECTION MODEL FOR FATIGUE LIFE PREDICTION OF NOTCHED COMPONENTS | + **Van Cong Phan**, Tu-Anh Bui-Thi, Thanh Thuong Do, Su Hyeon Choo, Jang Hyun Bae, Moon-Jo Kim, Changjoo Lee, Ki Seok Nam, Sung-Tae Hong<br><br>ELECTRICALLY ASSISTED SOLID-STATE SPOT JOINING OF A CAST A365 ALLOY: IMPROVEMENT OF JOINT PROPERTY BY LOCAL RAPID HEAT TREATMENT |
| 12:15 ~ 12:30 | + **Sandipkumar Dayani**, Waqas Muhammad, Abhijit Brahme, Kaan Inal<br><br>THERMODYNAMICALLY CONSISTENT CRYSTAL PLASTICITY MODEL COUPLING MARTENSITIC TRANSFORMATION AND DAMAGE EVOLUTION IN QP STEELS | - | + **Mengwei Zhang**, Weiping Hu, Zhixin Zhan, Qingchun Meng<br><br>A FREQUENCY-DOMAIN AND ENERGY-BASED DAMAGE MODEL FOR FATIGUE IN SPACECRAFT STRUCTURES INDUCED BY RANDOM VIBRATION | + **Qunzhi Zhai**, Dafan Du, Anping Dong, Jiaqi Ouyang, Baode Sun<br><br>MICROSTRUCTURAL EVOLUTION AND ENHANCED TENSILE PROPERTIES OF Ni-BASED SUPERALLOYS: A COMPARATIVE STUDY OF COUNTER-GRAVITY CASTING AND GRAVITY CASTING VIA IN-SITU SYNCHROTRON RADIATION |
| 12:30 ~ 12:45 | + **Xueyang Li**, Christian C. Roth, Vincent Grolleaua, Dirk Mohr<br><br>DETERMINING THE TAYLOR–QUINNEY COEFFICIENT AND ISOTHERMAL-TO-ADIABATIC TRANSITION FUNCTIONS FROM DYNAMIC IN-PLANE TORSION EXPERIMENTS ISOTHERMAL-TO-ADIABATIC TRANSITION FUNCTIONS FROM DYNAMIC IN-PLANE TORSION EXPERIMENTS | | - | - |

# 12:45 – 14:00 Lunch

| *Room* | **D2.304 Costa Hall Lecture Thetre** | **D2.194 Lecture Theatre** | **D2.330 Classroom** | **D3.211 Classroom** |
|---|---|---|---|---|
| | ***(Sym) Advances in ML-based Applications for Plasticity, Damage and Fracture (III)*** | ***Dislocation Plasticity*** | ***(Sym) Khan Medal Symposium in Honor of Irene Beyerlein: Understanding Deformation Mechanisms at the Mesoscale via Modelling and Experiments (IV)*** | ***(Sym) Physics-Based Modelling and AI-enabled simulation (II)*** |
| *Chairs* | ***Kaan Inal++ & Dirk Mohr ++*** | ***Huseyin Sehitoglu & Weizhong Han*** | ***Saryu Fensin & Michael Chandross*** | ***Giacomo Po & Xin Yan*** |
| 14:00 ~ 14:30 | *** Kaan Inal**<br><br>ADVANCES IN MACHINE LEARNING-BASED MICROMECHANICS: TOWARDS GENERALIZABLE MODELS FOR CRYSTAL PLASTICITY | *** **Huseyin Sehitoglu**, D. You, Gorkem Gengor a, O. Celebi, S. Pekol a, A.S.K. Mohammed<br><br>ATOMISTICS INFORMED CONTINUUM STRAIN FIELD OF DISLOCATIONS | *** Saryu Fensin**, Avanish Mishra<br><br>INFULENCE OF INTERFACE ROUGHNESS AND ORIENTATION ON THE DEFORMATION MECHANISMS OF Al-Ti BIMETALS | *** Giacomo Po**, Yang Li<br><br>MICROMECHANICS OF PLASTICITY IN HIGH-TEMPERATURE MATERIALS |
| 14:30 ~ 14:45 | *** Dirk Mohr**, Julian Heidenreich<br><br>TOWARDS IDENTIFYING DATA-DRIVEN CONSTITUTIVE MODELS FROM ROBOT-ASSISTED EXPERIMENTS: MINIMAL STATE CELL–BASED MODELING ENHANCED BY MULTI-TASK AND TRANSFER LEARNING | | *** Alejandro Strachan**, Jason Wilkening<br><br>STEADY-STATE ELASTIC PLASTIC SHOCK WAVES IN A LOW-SYMMETRY MOLECULAR CRYSTAL | **+ Xin Yan**, Yi Huang, Shiteng Zhao<br><br>ANISOTROPIC SHOCK RESPONSE AND TWIN-BOUNDARY-MEDIATED SPALLATION IN CrCoNi MEDIUM-ENTROPY ALLOY INSTRUCTIONS |
| 14:45 ~ 15:00 | | + **Mengzhen Cao**, Yuqi Zhang, David J Srolovitz, Alfonso H W Ngan<br><br>CORRELATING DISLOCATION WAVINESS AND STRENGTH WITH COMPOSITIONAL HETEROGENEITY VIA CONTINUOUS DISLOCATION DYNAMICS WITH SUB-CORE RESOLUTION | | + **Rui Barreira**, Marino Möckli, Dirk Mohr<br><br>EVOLUTION OF POLYCRYSTALLINE TEXTURES WITH MINIMAL STATE CELL RNN |
| 15:00 ~ 15:30 | *** Tomáš Mánik**, Bjørn Holmedal<br><br>FACET 2.0 – A NEURAL NETWORK-BASED YIELD SURFACE: A FLEXIBLE AND EFFICIENT CALIBRATIONS TO CRYSTAL PLASTICITY DATA | *** Weizhong Han**<br><br>RELATIVE MOBILITY OF SCREW VERSUS EEDGE DISLOCATIONS CONTROLS THE DUCTILE-TO-BRITTLE TRANSITION IN METALS | *** Michael Chandross**, Ian S. Winter, David Montes de Oca Zapain, John F. Curry<br><br>GRAIN BOUNDARY SEGREGATION IN NANOCRYSTALLINE ALLOYS | **+ Huanbo Weng**, Cheng Luo, Huang Yuan<br><br>MECHANISM-INFORMED NEURAL NETWORK MODELING OF RAFTED NICKEL-BASED SINGLE CRYSTAL ALLOYS |
| 15:30 ~ 16:00 | *** Yan Wang**<br><br>APPLICATION OF DEEP NEURAL NETWORK MOLECULAR DYNAMICS TO ELUCIDATE THE ATOMISTIC MECHANISMS OF LASER PROCESSING OF TWO-DIMENSIONAL MATERIALS | *** Jianquan Wan**, Xiaowei Zuo<br><br>EXCELLENT CRYOGENIC-TEMPERATURE STRENGTH AND DUCTILITY REALISED BY COUPLING DELTA PHASE AND TRIP EFFECT | *** Jianfeng Wang**<br><br>X-RAY MICROTOMORGRAPHY INVESTIGATIONS OF SAND PARTICLE BREAKAGE AIDED BY DISCRETE PARTICLE TRACKING | - |
| 16:00 ~ 16:15 | - | + **Ao Li**, Weiping Hu, Zhixin Zhan, Qingchun Meng<br><br>A DISLOCATION DENSITY-BASED CP-MPF UNIFIED FRACTURE MODEL OF NBSX ACROSS WIDE TEMPERATURE RANGES | - | |

# 16:30 – 18:00 Farewell Party (The Waterfront Café)

*** 45 minutes Distinguished keynote lecture, * 30 minutes keynote lecture,
+ 15 minutes invited presentation, ++ Symposium Organizer

## Thursday, Jan. 8, 2026

**08:30 – 18:30 Cultural Excursion to Great Ocean Road**
(Departing from Novotel Geelong)

- The conference offers Cultural Excursion to Great Ocean Road on 8 January. It is complimentary and limited to max. 50 people. Application is available on 3 and 4 January at the registration desk.

# TENTATIVE PARTICIPANTS, ICPDF 2026

Yoshiteru Aoyagi (Japan), Muhammad Arafin (USA), Levente Balogh (Canada), Matthew Barnett (Australia), Rui Barreira Morais Pinto (Switzerland), Irene Beyerlein (USA), Hyuk Jong Bong (Korea), Abhijit Brahme (Canada), Curt A. Bronkhorst (USA), Donald Brown (USA), Wei Cai (USA), Mengzhen Cao (China), Lei Cao (USA), Orcun Koray Celebi (Turkey), Michael Chandross (USA), Zhidong Chang (China), Wayne Chen (USA), Mei-Cen Chen (Korea), Yuguang Chen (China), Jiajun Chen (China), Fei Chen (China), Yang Chen (China), Qifa Chen (China), Yuqiang Chen (China), Guang Cheng (China), Hansohl Cho (Korea), Daecheon Cho (Korea), ShiHoon Choi (Korea), Sita Choudhary (India), Deunbom Chung (Korea), Yinan Cui (China), Xiao-Lei Cui (China), Chengyi Dan (Hong Kong), Ming Dao (USA), Sandipkumar Dayani (Canada), Frank William DelRio (USA), Yajuan Duan (China), Yue Fan (USA), Yueyulong Fang (China), Wei Feng (China), Saryu Fensin (USA), Massimiliano Ferronato (Italy), Caleb Foster (USA), Ming Fu (Hong Kong), Zhihui Gao (China), Nomun Gerel-Erdene (Japan), Yann Le Godec (France), Klaus Hackl (Germany), Heung Nam Han (Korea), Guofeng Han (Korea), Weizhong Han (China), Yixuan He (China), Bjørn Holmedal (Norway), Yong Hou (Germany), Zeran Hou (China), Qi Hu (China), Lin Hua (China), Yuntong Huang (China), Qishan Huang(China), Abigail Hunter (USA), Kaan Inal (Canada), Dongchan Jang (Korea), Ibrahim Jawahir (USA), Yandong Jia (China), Wei Jian (China), Yanyao Jiang (China), Li Jin (China), Chaoyue Jin (China), Reese Jones (USA), Guozheng Kang (China), Keonwook Kang (Korea), Xiangwei Kong (China), Seid Koric (USA), Katarzyna Kowalczyk-Gajewska (Poland), Jong-Hyeok Kwon (Korea), Liangyun Lan (China), Khanh Chau Le (Vietnam), Myoung-Gyu Lee (Korea), Dongwoo Lee (Korea), Zhuo Feng Lee (Korea), Zion Lee (Korea), Eun-Ho Lee (Korea), Valery Levitas (USA), Guoqiang Li (China), Jia Li (China), Ao Li (China), Dayong Li (China), Xueyang Li (Switzerland), Li Li (China), Heng Li (China), Daohan Lin (China), Ji Lin (China), David Littlefield (USA), Guisen Liu (China), Haoxiang Liu (China), Xinxi Liu (China), Yanxiong Liu (China), Chuanlai Liu (China), Yue Liu (China), Yanshan Lou (China), Wei Lu (USA), Cheng Lou (USA), Jiao Luo (China), Guojian Lyu (China), Mohamed Magdy Ibrahim Fadel (China), Tomas Manik (Norway), Nate Mara (USA), Jiangshuai Meng (Australia), Wen Meng (USA), Junying Min (China), Amit Misra (USA), Dirk Mohr (Switzerland), Lidiia Nazarenko (Germany), Jörg Neugebauer (Germany), Alfonso Ngan (UK), Giang Nguyen (Australia), Jian-Feng Nie (Australia), Xiaomiao Niu (China), Shigenobu Ogata (Japan), Haruki Ohashi (Japan), Namsu Park (Korea), Jinheung Park (Korea), Namsoo Park (Korea), Wonjin Park (Korea), Anirban Patra (India), Henryk Paul (Poland), Linfa Peng (China), Van Cong Phan (Korea), Dat G Phan (Australia), Giacomo Po (Canada), LingYun Qian (China), Jichao Qiao (China), Rama Srinivas Varanasi (India), Enzhen Ren (China), Jose Rodriguez-Martinez (Spain), Bernie Rolfe (Australia), Christian C. Roth (Switzerland), Dong Ruan (Australia), Seunghwa Ryu (Korea), Hyemin Ryu (Korea), Hamed Sadeghi (China), Valentina Salomoni (Italy), Huseyin Sehitoglu (USA), Wenbo Sha (China), Xiaoqing Shang (China), Yao Shen (China), Baodong Shi (China), Gi-Dong Sim (Korea), Alexander V. Soldatov (China), Di Song (China), Jean-Charles Stinville (USA), Thomas Stoughton (USA), Alejandro Strachan (USA), Qingping Sun (Hong Kong), Chaoyang Sun (China), Xinxin Sun (Hong Kong), Satyam Suwas (India), Theo Tervoort (Switzerland), Neeraj S. Thirumalai (USA), Mira Todorova (Germany), Makoto Uchida (Japan), Alper Uysal (Turkey), T Venkatesh (USA), Thomas Virazels (Spain), Jianquan Wan (China), Bing Wang (China), Fulin Wang (China), Hao Wang (China), Huiling Wang (China), Jianfeng Wang (Hong Kong), Jingya Wang (China), Jianyu Wang (China), Kehuan Wang (China), Leyun Wang (China), Qian Wang (China), Tao Wang (China), Yan Wang (USA), Yun Wang (China), Zhangwei Wang (China), Zinan Wang (China), Justin S. Wark (UK), Yan Wen (China), Ronghai Wu (China), Luoqi Wu (China), YueRui Xiao (China), Yao Xiao (China), Lechun Xie (China), Yukai Xiong (China), Alan Xu (Australia), Zhutian Xu (China), Xin Yan (China), Xinyuan Yang (China), Yanqiu Yang (China), Arash Yavari (USA), Min Yi (China), Fei Yin (China), Jeong Whan Yoon (Korea), Daegun You (USA), Zefeng Yu (China), Shuqing Yang (China), Qunzhi Zhai (China), Cunsheng Zhang (China), Haiming Zhang (China), Han Zhang (China), Jiawen Zhang (China), Jingyu Zhang (Hong Kong), Laichang Zhang (China), Mengwei Zhang (China), Wen Zhang (China), Xin Zhang (China), Xu Zhang (China), Ze-xiong Zhang (China), Rui Zhao (China), Bingxin Zhao (China), Guowei Zhou (China), Qing Zhou (China).

# MULTISCALE MODELING OF NONLINEAR VISCOELASTIC-VISCOPLASTIC BEHAVIOR IN GLASSY POLYMERS BASED ON INTRAMOLECULAR CHAIN ROTATION

**Yoshiteru Aoyagi**

**Department of Finemechanics, Tohoku University, 6-6-01 Aoba, Aramaki, Aoba-ku, Sendai, 980-8579, Janan. aoyagi@tohoku.ac.jp**

**ABSTRACT –** Recent advances in constitutive modeling of glassy polymers have improved the ability to reproduce their complex mechanical behavior, but many existing models suffer from increased complexity and a large number of material parameters. In this study, we propose a new constitutive model to describe the nonlinear viscoelastic-viscoplastic behavior of glassy polymers under loading, unloading, and cyclic loading conditions at temperatures below the glass transition temperature. The model introduces an anelastic strain component in addition to elastic and plastic strains, based on a three-state framework: a stable state, a metastable state in tension, and a metastable state in compression. This formulation enables a unified description of viscoelastic and viscoplastic phenomena through simple thermal activation processes. The model is capable of capturing nonlinear mechanical responses, including hysteresis and ratcheting, with fewer parameters than recent models. Numerical simulations using the proposed model are compared with both experimental data and results from existing models. The comparisons demonstrate that the present model can accurately reproduce the nonlinear behavior of glassy polymers under various loading conditions. Its simplicity and predictive capability make it a promising tool for designing and analyzing polymeric materials in engineering applications.

# RECENT DEVELOPMENT ON LINEPIPE FOR HYDROGEN TRANSPORTATION

**Muhammad Arafin**

**Orion Steel, 71 S Wacker Dive., Chicago, IL, 60606. muhammad.arafin@orionsteel.com**

**ABSTRACT-** The safe and reliable transportation of hydrogen via pipelines is essential to achieving key decarbonization goals. However, several scientific and engineering challenges must be addressed to make this vision a reality. This presentation will explore critical topics, including: the dissociation behavior of hydrogen on steel surfaces, interactions between hydrogen and steel microstructures, optimization of welding procedures for enhanced hydrogen performance, and ongoing efforts to improve existing testing methods and develop new standards. Recent developments comparing standard linepipe grades with specially engineered hydrogen grades will also be presented. These findings highlight the pivotal role of microstructure in enhancing resistance to hydrogen embrittlement and improving overall pipeline performance.

# USING HIGH-RESOLUTION SYNCHROTRON X-RAY DIFFRACTION TO CHARACTERIZE DISLOCATION CELLS IN ADDITIVELY MANUFACTURES HASTELLOY-X

**Levente Balogh, Lucas Ravkov, Thalles Lucas, Shengze Yin, Arash Nikniazi, Vahid Fallah**

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**ABSTRACT-** This study introduces a novel high-resolution synchrotron X-ray diffraction methodology to quantitatively characterize dislocation cell microstructures in additively manufactured (AM) Hastelloy X. By directly analyzing diffraction patterns, we differentiate between two distinct regions: cell walls (29% ± 11% of the microstructure), defined by elevated dislocation density and micro-segregation, and cell interiors (71% ± 11%), which exhibit reduced defect densities. These distributions were validated via electron backscatter diffraction (EBSD). Using Diffraction Line Profile Analysis (DLPA) we further quantified key microstructural parameters: the weighted average dislocation density in fully dense specimens reached $(8.6 \pm 2.3)\times10^{14}$ $mm^{-2}$, while cell walls displayed a 0.16% tensile lattice strain relative to cell interiors. This strain partitioning suggests localized deformation mechanisms inherent to AM processing. Furthermore, the demonstrated DLPA technique establishes a foundation for in-situ monitoring of microstructural evolution during manufacturing, enabling real-time process control to optimize mechanical performance. This work also advances the integration of microstructure-informed design in additive manufacturing.

# OBSERVING CO-ORDINATED BURSTS OF PLASTICITY IN BULK MAGNESIUM ALLOYS

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**ABSTRACT-** A modified Synchrotron transmission X-ray Laue diffraction method was used to track grain rotations for the first 1% of tensile strain in a magnesium alloy, over 4400 time-steps. 33 grains were indexed. The magnitude and frequency of intermittent bursts of grain rotation were quantified. Bursts of rotation are interpreted as bursts of plastic deformation. These events were seen to be highly coordinated amongst nearby grains. Twinning and slip events were distinguished by analysis of Laue peak intensity change. For orientations favorable for twinning, 7 out of the 10 indexed grains showed significant drops in diffracted intensity due to twin induced re-orientation. For other orientations, 20 out of 23 grains displayed bursts of deformation attributable to lattice dislocation glide. Slip and twinning events are seen to co-ordinate. The results are discussed in terms of the dominating mechanisms and the prospects of the technique.

# EVOLUTION OF POLYCRYSTALLINE TEXTURES WITH MINIMAL STATE CELL RNN

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**ABSTRACT-** Predicting the evolution of polycrystalline textures is critical for materials design, yet numerical simulations with Crystal Plasticity (CP) constitutive models are often prohibitively computationally expensive. In this work, we introduce a data-driven surrogate framework designed to replace full CP-based finite element and Fast Fourier Transform (FFT) simulations, focusing on predicting texture dynamics subjected to arbitrary plane-stress strain paths. The proposed architecture combines a spatio-temporal approach by leveraging a convolutional neural network for spatial feature extraction with a Minimal State Cell recurrent neural network for history-dependent state evolution. The latter ensures resolution invariance and stationarity during the state update. Training data are generated from extensive CPFFT simulations of a synthetic 2D representative volume element featuring 46 grains, subjected to 10,000 non-monotonic strain paths. The training targets the minimization of the mean squared error loss, and values of 6.2E-4 are reported after 1000 epochs. The model achieves a spatially averaged prediction accuracy of 96%, with errors of less than 4% reported in the orientation distribution function of the worst prediction. Furthermore, the model is also fine-tuned on 10 different RVEs, not seen during training, and found to achieve comparable performance.

# MINIMAL STATE CELL RNN SURROGATE MODEL FOR ELASTOPLASTIC POROUS DUCTILE SOLIDS

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**ABSTRACT-** Ever since its inception, the Gurson-Tveergaard-Needleman (GTN) model has been the *de facto* benchmark for the yielding of ductile porous solids, accounting for their known pressure-dependent behavior. In this work, we introduce a data-driven framework relying on the Minimal State Cell (MSC) recurrent neural network (RNN) architecture, trained and tested in complex non-monotonic loading paths with bounded deviatoric and volumetric strain components, and loading and unloading along randomly sampled directions. Data is generated through finite element simulations of an isotropic cubic representative volume element, featuring 20 randomly distributed spherical voids totaling 1% void volume fraction. The MSC surrogate model with about 5,000 trainable parameters and 7 internal state variables is shown to generalize well across different strain increment norms, outperforming the GTN model by an order of magnitude, particularly when stress triaxialities or large hydrostatic stresses are involved. The reduced number of state variables also allows for explicit interpretation of their physical meaning. The model is, at last, embedded into an explicit finite element code and achieves competitive computational performance.

# FUNDAMENTAL PROPERTY EFFECTS ON CRITICAL RESOLVED SHEAR STRESSES IN REFRACTORY MULTI-PRINCIPAL ELEMENT ALLOYS

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**ABSTRACT –** Refractory multi-principal element alloys (RMPEAs) have gained increased interest over the last decade as a potential materials solution to the growing need for alloys that can operate under extreme environmental conditions. To realize the full potential of the unusually high chemical disorder of this relatively new class of alloys, atomic-scale computational techniques are employed to estimate characteristic stresses to move dislocations in different parts of the alloys. In this presentation, we will discuss the statistical distribution of critical stresses to move screw and edge dislocations in a wide range of RMPEA compositions. As the chemical disorder can encourage multiple slip pathways, the analysis will include critical stresses on three possible glide planes: {110}, {112}, and {123}. We will examine the role of fundamental properties, such as elastic anisotropy, composition, and lattice distortion, on these critical stresses as well as edge/screw and slip-plane selection.

# ON THE DIRECTION-DEPENDENT FORMABILITY OF AN ULTRA-THIN COMMERCIALLY PURE TITANIUM SHEET

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**ABSTRACT –** In this work, the formability of a 0.1 mm-thick commercially pure titanium (CP-Ti) sheet, developed for use as a metallic bipolar plate in proton exchange membrane fuel cells, was systematically investigated. During the forming of metallic bipolar plates, the major strain direction may vary depending on the microchannel geometry; therefore, it is essential to evaluate the forming limit diagrams (FLDs) under different orientations. The standard ISO 12004-2 procedure, which employs a 100 mm-diameter punch, was found to be unsuitable for such ultra-thin sheets because of pronounced size effects and the significantly higher formability observed when the major loading axis is aligned with the transverse direction. To overcome this limitation, a miniature Nakajima test utilizing a 20 mm-diameter punch was developed with the aid of finite element simulations that accounted for the experimentally observed strong planar anisotropy and differential hardening behavior. The experimental results revealed a strong anisotropy in formability and distinct differences in the FLD profiles corresponding to the major loading directions. Complementary crystal plasticity finite-element simulations were performed to elucidate the dominant deformation mechanisms responsible for the observed anisotropy in terms of the formability. Furthermore, detailed fractographic analyses clarified the fracture characteristics associated with each deformation mode.

# DEEP LEARNING BASED SURROGATE MODELING FOR CRYSTAL-PLASTICITY DRIVEN PREDICTION OF ALUMINUM ALLOY FRACTURE SURFACES

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**ABSTRACT-** A key utility of micromechanical models is as calibration tools for more computationally efficient phenomenological counterparts. This paradigm is primarily driven by the high computational cost of running these micromechanical models. In this paper, a deep operator network was employed to act as an efficient surrogate of a micromechanical model to predict ductile fracture in arbitrary age-hardenable aluminum alloys. The micromechanical model was used to generate training data by evaluating the fracture behavior of randomly generated alloys considering variable hardening parameters and crystallographic texture. The operator network was intentionally designed to require only input data obtained from a uniaxial tension test and a volumetric texture measurement, such as by X-ray diffraction or electron backscatter diffraction. The surrogate model was able to predict full material fracture surfaces under proportional loading using these data. The surrogate model was also tested using four real aluminum alloys; AA6014-T4, AA6061, AA6082, and AA7075-T6, showing excellent prediction accuracy. The surrogate model also achieved a four-order-of-magnitude increase in computational speed relative to the reference micromechanical model.

# STATISTICAL THERMOMECHANICS OF DUCTILE DAMAGE FOR DYNAMIC LOADING CONDITIONS

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**ABSTRACT –** Metallic material, when exposed to varied environmental conditions and mechanical loading invoke physical responses that are tightly coupled to evolution of their structural and thermodynamic states. The imparted energy is generally considered to be partitioned into stored and dissipated forms. Stored energy is typically retained in permanent lattice distortion facilitated by atomic and micro-scale rearrangements of atoms. Deformation mechanisms such as dislocation slip, deformation twinning, and intergranular interaction are examples where inelastic structural evolution leads to "stored energy of cold work". This stored energy involves significant atomistic change in the material involving non-equilibrium processes such as dislocation multiplication, annihilation, dislocation sub-cell development, and deformation twin nucleation/propagation/growth. During dynamic loading of ductile materials, the power delivered to the material is very large and therefore the plastic power response and temperature increase in the material is accordingly large. Material structural and thermodynamic state evolves with continued deformation, and many times leads to ductile damage fields in the form of porosity and/or adiabatic shear banding.

Ductile damage within polycrystalline metallic materials is known to be strongly dependent upon microstructure. This is presumed to be dictated by spatially distributed stress conditions and defect pore nucleation strength due to the statistical aggregate nature of the material. During shock loading, in addition to pore nucleation and growth, the material deforms via finite elastic and plastic mechanisms. The power delivered to the material during shock loading is distributed to each deformation/damage mechanism as stored and dissipated power with change of temperature by both Thompson-Joule and plastic power dissipation effects. A new finite deformation statistical porosity-based ductile damage model for high triaxiality conditions is presented which represents pore nucleation by a new combined probability distribution for stress and pore nucleation strength distributions. A new isotropic plasticity model is also presented for both thermally activated and phonon-drag regimes of dislocation motion. This model accounts for both stored energy via an effective temperature measure and thermal energy via kinetic-vibrational temperature. This formulation also proposes an expression for the Taylor-Quinney factor which is guided by second-law restrictions. Porosity growth is represented by a thick-

walled sphere unit cell approach which allows for inertial resistance to growth and facilitated by plastic deformation. A governing equation for thick wall sphere growth due to applied external pressure is derived which also accounts for surface energy and kinetic energy. Simulation results will be presented and compared with plate-impact experiments conducted on high-purity tantalum.

For shear dominated dynamic loading, adiabatic shear bands are commonly observed. These shea r bands are localized regions of very large plastic deformation which can also experience a signifi cant temperature increase. In recent years, there has been increasing evidence to suggest that a for m of dynamic rotational recrystallization occurs and contributes an additional softening mechanis m. The new thermomechanical model described above is expanded to include the dynamic rotati onal recrystallization process. Both dislocation structure and recrystallization are represented as t hermodynamically competing mechanisms where elastic stored energy of dislocations is transferr ed to greater grain boundary energy and thereby reduced grain size. This recrystallization process is demonstrated with metallographic analysis of forced shear samples of martensitic steel. This m odel is implemented into a computational framework designed to alleviate systemic mesh sensiti vity in simulations of adiabatic shear banding. This framework embeds an adiabatic shear zone w ithin a computational element and represents distinct material evolution within and without the s hear region after localization nucleation. Simulation results are presented which describe both de velopment of adiabatic shear banding and also structural evolution during dynamic recrystallizati on and compared directly with forced shear experiments of a martensitic steel.

# HEATING RATE DEPENDENT RECOVERY AND RECRYSTALLIZATION OF ROLLED TITANIUM AND AM'ed Ti-6Al-4V

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**ABSTRACT –** Additive Manufacture offers reductions in cost and waste in the production of metallic components as well as the ability to create unique and optimized topologies that are not achievable through conventional manufacturing. AM Ti-6Al-4V (Ti64) has received considerable attention because of the high material cost and the innate ability of AM to minimize material waste. Originally, the Ti64 alloy was developed for casting applications which have very slow cooling rates into an equilibrium microstructure consisting of ~94% $\alpha$ (hexagonal close packed) and ~6% $\beta$ (body center cubic) with excellent mechanical properties. Its property combinations are still desired for AM built components, but the much higher cooling rates associated with AM drive distinct and metastable microstructures and, subsequently, distinct material properties compared to conventional components. A high-energy, metastable microstructure including $\alpha'$ martensite super-saturated with vanadium, high dislocation density, and large intergranular stresses results in material with an enhanced flow strength compared to conventionally produced Ti64. Following the initial solidification and quench, which is supposed to occur at cooling rates approaching $10^3$-$10^6$ C/sec, the newly deposited material experiences several rapid re-heat cycles as more material continues to be deposited on top of it. Recent developments in high energy X-ray detectors have enabled high resolution (in **q** and d-space) diffraction measurements to be collected at data rates of 1kHz. This corresponds to measurements during heating (or cooling) rates of roughly 10,000C/sec without significant broadening of the diffraction peaks. Thus, the measurement rates are now commensurate with the heating rates experienced following materials deposition. We report the results of in-situ high-energy X-ray diffraction (HEXRD) experiments carried out on the ID15 beamline at the European Synchrotron Radiation Facility during repeated heating (~1000K/sec) of Laser Powder Bed Fusion (LPBF) Ti-6Al-4V. We will present the evolution of the phase fraction, texture, internal stress, dislocation density and solute chemistry, and their heating rate dependence, during these processes.

# UNDERSTANDING THE ROLE OF HYDROGEN ON THE DEFORMATION MECHANISMS AND DISLOCATION STRUCTURE EVOLUTION IN HIGH MN AUSTENITIC STEELS THROUGH NEUTRON DIFFRACTION LINE PROFILE ANALYSIS

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**Abstract -** Stacking fault energy was used as a design parameter to achieve hydrogen embrittlement (HE)-resistant high manganese austenitic alloys as economical alloy alternatives for hydrogen storage and transport applications. In this work, the role of hydrogen on the deformation mechanisms of high manganese austenitic steels with different stacking fault energies (29-49 $mJ/m^2$) was evaluated using *in-situ* neutron diffraction during tensile loading, combined with diffraction line profile analysis. The neutron diffraction data indicated that hydrogen pre-charging resulted in significant changes in lattice parameters, lattice strains, dislocation properties, and defect densities. An austenitic alloy with a relatively low stacking fault energy (29 $mJ/m^2$) exhibited a higher probability of stacking fault formation during tensile straining, and hydrogen pre-charging further promoted planar slip deformation. This alloy showed a higher sensitivity to HE than an austenitic alloy with higher SFE (49 $mJ/m^2$), which had a lower probability of stacking fault formation in both the non-charged and hydrogen-charged conditions. These observations are consistent with a hypothesis in the literature that planar slip behavior is strongly correlated with the HE sensitivity of stable austenitic alloys. The HE mechanisms are also discussed in the context of the influence of stacking fault energy on the hydrogen-defect interactions in these alloys.

# HYDROGEN EFFECT ON DISLOCATION MOBILITY IN SINGLE CRYSTAL NICKEL

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**ABSTRACT-** Hydrogen embrittlement (HE) is a longstanding challenge in structural materials. The presence of hydrogen can drastically reduce the ductility and toughness of metals, leading to their premature failure under mechanical loading. Despite decades of research, the underlying mechanisms of HE in face-centered cubic (FCC) metals remain incompletely understood, hindering the development of effective mitigation strategies for next-generation alloys. In this work, we use molecular dynamics (MD) simulations to understand the effects of hydrogen on dislocation mobility in single-crystal nickel, as a model material for nickel-based alloys. Our comprehensive study includes the effects of hydrogen concentration, temperature, applied stress, and dislocation character angles. Hydrogen is found to reduce the dislocation velocity through a solute drag mechanism. This leads to a threshold stress behavior for dislocation motion, given a sufficient hydrogen concentration and when temperature is not too high. Our findings provide material input to mesoscale dislocation dynamics (DD) models, hence contribute to the predictive capability of multiscale simulations for HE, paving the way for the development of hydrogen-resistant materials.

# TRANSFORMATION-ASSISTED TWIN NUCLEATION IN METALS

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**ABSTRACT –** Though twinning plays an equally vital role to that of dislocation slips in accommodating deformation in the many metals and alloys, its atomic-level nucleation mechanism has long been under debate. Accordingly, there is a critical need to rigorously understand the atomic mechanism of twin nucleation. We performed large-scale molecular dynamics simulations to study the deformation process in bcc and hcp metals. We found the nucleation of various deformation twins through reversible martensitic phase transformations, via evanescent intermediate phases. Furthermore, the findings are applied to rationalize the role of mechanical loading and anomalous temperature dependence of the activation of different twinning modes in both hcp and bcc metals.

# CORRELATING DISLOCATION WAVINESS AND STRENGTH WITH COMPOSITIONAL HETEROGENEITY VIA CONTINUOUS DISLOCATION DYNAMICS WITH SUB-CORE RESOLUTION

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**ABSTRACT –** Dislocations in complex concentrated alloys (CCAs) undulate morphologically due to fluctuating stacking fault energy (SFE) landscape, leading to elevated slip resistance. Simulative reproduction of such behavior with explicit dislocation core delineation is however limited to very few approaches. Here, a novel "intensive" continuous dislocation dynamics (CDD) method integrating Peierls-Nabarro type dislocation core description and chemical heterogeneity is devised for the dynamic simulation of wavy dislocations at sub-core resolution. A variety of idealized or randomized fluctuations are assigned to the desired dislocation core width w in the lattice misfit stress to represent SFE heterogeneity. Results reveal that increased w fluctuations amplify both dislocation waviness and critical resolved shear stress (CRSS), while the CRSS peaks at a critical correlation length of ordering suggesting competing mechanistic effects at play as short-range order increases in the alloy structure. Unidirectional w fluctuations highlight a non-linear relation between CRSS and w gradient in the gliding direction (X) $\partial w/\partial x$. Variations in $\partial w/\partial x$ or $\partial \gamma_{usf}/\partial x$ ($\gamma_{usf}$ = unstable SFE) along the dislocation direction (Y) emerge as the driver of local dislocation curvature, leading to the discovery of a factor $\partial^2 \gamma_{usf}/\partial y \partial x$ governing dislocation configuration and intrinsic strengthening given the positive intercorrelation among $\partial^2 \gamma_{usf}/\partial y \partial x$, waviness, and CRSS. Machine-learning analysis of molecular dynamics data confirms the significance of the second-derivative term. Intensive CDD serves as a powerful analytical tool to unfold core-related mechanisms of dislocations in CCAs.

# CROSS-SLIP AND EASY-GLIDE CRSS DETERMINATION IN TITANIUM: THEORETICAL PREDICTIONS AND IN-SITU EXPERIMENTAL MEASUREMENTS

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**ABSTRACT-**This study investigates the mechanics of prismatic and pyramidal-I $\langle a \rangle$ slip in titanium, elucidating the physics of easy glide and cross-slip through a combination of theory and experiments. Screw-character prismatic dislocations in titanium are of particular interest due to their complex core-structures which exhibit both stable and unstable configurations leading to different activation pathways involving cross-slip and planar glide. To investigate these mechanisms, site-specific micro tensile samples were prepared using focused ion beam (FIB) milling and mounted on a push-to-pull (PTP) device for in situ transmission electron microscopy (TEM) tensile testing. The in situ experiments provide direct observations of the onset of dislocation motion and the precise determination of the CRSS for the activated mechanisms, and its evolution with cycling. A comprehensive theory has been developed to predict the CRSS values for dislocation glide, cross-slip, and multiplication. The predicted critical stresses for pyramidal to prismatic and prismatic to pyramidal cross-slip show close agreement with the experimental measurements. The latter cross-slip stress is a factor of two higher compared to unobstructed planar slip. The model explicitly accounts for overlapping dislocation cores and employs a Wigner-Seitz based cell to evaluate misfit energies. By integrating ab-initio density functional theory (DFT) with anisotropic elasticity, the framework determines minimum energy pathways for dislocation glide. Overall, this study explores key critical stress parameters essential for informing higher-scale simulations of plasticity in titanium.

# GRAIN BOUNDARY SEGREGATION IN NANOCRYSTALLINE ALLOYS

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**ABSTRACT-** Segregation of solute atoms to grain boundaries (GBs) in metallic alloys can often impart thermomechanical stability of nanocrystalline microstructures. This, in turn, can lead to desirable mechanical properties including increased hardness and corrosion resistance. While some efforts have been made to understand the propensity for GB segregation through thermodynamic and atomistic modelling, a detailed understanding of the general relationships between elements that lead to segregation is still lacking. We present the results of simulations of GB segregation using EAM-X, a newly developed atomistic model for metals that enables systematic studies of the links between elemental properties and structure. We show how the differences between the elements (e.g. difference in atomic radius, enthalpy of mixing, etc.) result in segregation using 35 GBs, including symmetric tilt, asymmetric tilt and symmetric twist boundaries. Our results are coupled with machine learning to both accurately predict the propensity for segregation as well as to identify the key properties with the strongest influence. We also examine the effects of segregation on GB mobility in order to develop an understanding of nanocrystalline stability in these alloys.

# ROOM-TEMPERATURE PRECIPITATION STRENGTHENING IN AL-2.5MG-0.4FE SHEET INDUCED BY CYCLIC SEVERE PLASTICITY DEFORMATION

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**ABSTRACT –** A remarkable room-temperature precipitation strengthening method is proposed in this work, which significantly enhances the strength of conventionally un-heat-treatable Al-2.5Mg-0.4Fe sheet. It is found that the combination of severe plastic deformation and cyclic loading triggers the precipitation of abundant ultrafine-grained $Al_{13}Fe_4$ phases at room temperature. With increasing strain of 0.8 and loading cycles of 2000, the Al-2.5Mg-0.4Fe alloy exhibits excellent tensile strength of 480 MPa, far exceeding that by conventional strengthening method. Quantitative analysis indicates that both grain refinement strengthening and precipitation strengthening become more pronounced as plastic strain and cyclic loading increase, dominating the mechanical enhancement. Although the high stacking fault (SF) energy of aluminum alloy, cyclic severe plastic deformation (CSPD) introduces numerous SFs by high-density dislocation network and Fe atom segregation, which are confirmed by molecular dynamics analysis to promote structural transformation and subsequent precipitation at room temperature. Moreover, a new precipitation strengthening mechanism is revealed during CSPD that through twin refinement and lattice rotation, precipitates not only act as strong dislocation barriers to dislocation motion, but also as plasticity carriers to actively coordinate matrix deformation, achieving a superior strength-ductility synergy. This study presents a simple but effective room-temperature strengthening strategy for non-heat-treatable alloys.

# MACHINE LEARNING FRAMEWORK TO PREDICT THE COARSE GRAIN FORMATION DURING HOT WORKING

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**ABSTRACT –** Accurately predicting the formation and potential locations of coarse grains in the mixed grain structure has plagued scientists for over a century. The major bottleneck in the exploration of this phenomenon has been the lack of a robust computational tool that can predict structure heredity during the whole hot working. This work developed an interpretable machine learning (ML) framework based on automatic hyperparameter optimization to predict the occurrence of coarse grains. The multidimensional mapping dataset is constructed based on finite element simulation, large-area montage technique, grain category recognition algorithm and image annotation technology. The hyperparameter optimization were carried out hyperparameter optimization to obtain optimal ML model with high prediction accuracy. Our results demonstrate that ML framework based on dataset of small-sized specimens can even effectively predict structure heredity of large-sized components. Furthermore, we provide a new perspective on abnormal grain growth of steels during hot working based on lab-based X-ray diffraction contrast tomography.

# AN ANISOTROPIC CONSTITUTIVE MODEL FOR CARBON FABRIC-REINFORCED SHAPE MEMORY POLYMER COMPOSITES BASED ON PHASE TRANSITION CONCEPT

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**ABSTRACT –** Based on phase transition concept, this study develops a novel anisotropic constitutive model for carbon fabric-reinforced shape memory polymer composites (SMPCs) to address the inability of existing models to capture viscoelastic yield behavior and to rationally interpret the shape memory mechanism. A new dual-phase decomposition strategy is proposed, wherein the rubbery phase is described as a coupling of the SMP's hyperelastic response and the fabric's orthotropic behavior, while the glassy phase combines SMP viscoelasticity with fabric kinematic constraints. Each phase is independently modeled to capture distinct thermomechanical characteristics. The nonlinear behavior of the SMP matrix is characterized using the Mooney-Rivlin free energy formulation, and the anisotropic hyperelastic response of the fabric reinforcement is described by a polynomial constitutive function. A modified Eyring model and the viscous flow rule are used to describe the yield point and softening behavior of glassy phase of SMP matrix. To quantify shape memory effects of SMPCs, the storage strain concept is integrated into the thermodynamic framework. Through energy decomposition, the constitutive equations are rigorously derived based on the Clausius inequality and Helmholtz free energy principles, with temperature-independent phase effectiveness factors incorporated to account for non-ideal behaviors. The model is validated against comprehensive thermomechanical and shape memory experiments on SMPCs with various fiber orientations. Good agreement is achieved between simulations and experimental results, confirming the model's capability to predict anisotropic mechanical behavior and shape memory performance. Moreover, several orientation-dependent phenomena are identified and discussed. The validated framework offers new insights into strain storage mechanisms during phase transitions and provides practical guidance for the design and optimization of SMPC-based structural systems.

# MODELING OF INTERFACIAL FRACTURE IN STACKED THIN FILMS WITH STRAIN-RATE AND HYGROTHERMAL EFFECTS

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**ABSTRACT –** Fracture in stacked thin films with low interfacial strength not only occurs within the interfaces but, in some cases, can also deviate into the film bulk, posing challenges for conventional phase-field models (PFM). Results from double cantilever beam (DCB) tests indicate that higher loading rates generally enhance interfacial strength while promoting bulk microcracks and other inelastic contributions; in contrast, hygrothermal preconditioning significantly reduces interfacial strength. These observations suggest that fracture in stacked thin films is inherently hybrid in nature, with non-negligible inelastic dissipation, highlighting the limitations of conventional linear elastic fracture mechanics-based models. To address these challenges, a phase-field cohesive zone model (PF-CZM) is developed, which integrates a cohesive zone model (CZM) at the interfaces within a phase-field framework and is implemented in the finite element platform via user-defined elements (UEL) in Abaqus. The PF-CZM can simulate crack propagation and deflection along vertical or inclined interfaces under Mode-I fracture, successfully capturing fracture patterns under different material and interfacial properties. Inelastic energy dissipation within both the film bulk and interfaces is computed separately through the phase-field model and CZM, with viscous contributions and rate-dependent dissipation incorporated to account for loading rate effects. Hygrothermal effects are reflected through variations in interfacial fracture energy and bulk stress distribution. The predicted crack paths and energy dissipation trends are in close agreement with DCB experimental observations, demonstrating that the model reliably captures variations in interfacial energy release rate and crack propagation patterns under different loading rates and environmental conditions. Moreover, the PF CZM offers a practical and versatile framework for the design and optimization of multilayer thin-film systems with improved interfacial reliability.

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# INVAR 36 ALLOY ULTRA-THIN STRIP ROLLING PROCESS AND THE INFLUENCE MECHANISM OF SURFACE DEFECTS ON THE HOLE FORMATION RATE

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**ABSTRACT –** Invar 36 alloy is widely used in the electronics industry due to its extremely low expansion coefficient. Invar 36 alloy is a key material for making fine metal masks, and the quality of its hole formation directly affects the pixels of OLED displays. However, the mechanism by which the surface defects on the ultra-thin strip of invar 36 alloy affect the hole formation rate of the fine metal masks is still unclear, and high-quality ultra-thin strip of invar 36 alloy are not easily obtainable. Based on the existing production processes for fine metal masks, this report studies the mechanisms of the influence of surface morphology and microstructure on the hole formation rate of fine metal masks, providing theoretical basis and references for avoiding abnormal holes during etching and improving the product yield of fine metal masks from the source. Starting from the raw material of the ultra-thin strip of invar 36 alloy, a high-quality production process for these strips is proposed. By using a 280 mm twenty-roll rolling mill, the thickness of 40 μm strips of Invar 36 alloy was successfully cold rolled to 25 μm, providing a solid theoretical and technical foundation for the high-quality production of 4J36 iridium alloy strips.

# MONITORING PHASE TRANSITION DURING HIGH-RATE PLASTIC DEFORMATION

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**ABSTRACT –** For materials in impact applications, the plastic-deformation can be a critical aspect in their impact energy dissipation capacity. To understand the mechanisms of energy absorption, it is desired to track the microstructural evolution in real time during the dynamic plastic deformation of the specimens, which was not possible due to the lack of experimental tools. In the research presented, we integrated the high-speed X-ray imaging and diffraction capabilities present at the Advanced Photon Source beamline 32 ID-B (Argonne National Laboratory, Argonne, IL, USA) with the high-rate loading offered by a Kolsky compression/tension bar. High-speed X-ray images and full-ring X-ray diffraction, as well as temperature field and full strain field, can be obtained simultaneously. The effectiveness of these new experimental capabilities is verified via impact on various material systems, demonstrating in-situ image analysis inside of the material systems during loading rates commonly encountered in high-rate deformation environments.

# ON THE INVESTIGATION OF STRENGTHENING AND IRRADIATION DAMAGE IN MULTI-PRINCIPAL ELEMENT ALLOYS: MULTISCALE DISLOCATIONS DYNAMICS SIMULATIONS

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**ABSTRACT –** In multi-principal element alloys (MPEAs), their intrinsic features, such as significant lattice distortion, compositional fluctuations, and local short-range order, lead to unusual dislocation motion, resulting in exceptional strength and outstanding radiation resistance. The intrinsic characteristics of MPEAs depend on atomic species and spatial arrangement information. Therefore, it is necessary to develop atomic-information-informed dislocation dynamics simulation methods to investigate the collective motion of large-scale dislocations in MPEAs and their effects on strength and radiation performance. This study proposes: by incorporating experimentally measured lattice strain fields in MPEAs, we develop an atomic-lattice-distortion-dependent discrete dislocation dynamics framework consisting of random field theory and a phenomenological dislocation model to investigate the fundamental deformation mechanisms underlying massive dislocation motions in MPEAs. i) The heterogeneous lattice strain causes unusual dislocation behaviors (e.g., multiple kinks/jogs and bidirectional cross-slips), leading to strengthening mechanisms that underpin the strength-ductility synergy; ii) The heterogeneous lattice strain field induces unique dislocation turbulent behavior and forms a special dislocation structure that acts as both a source and a trap at vortex points, significantly enhancing both strength and ductility; iii) The lattice strain reduces radiation-induced hardening, which aligns with recent experimental observations of superior radiation hardening resistance in high-entropy alloys (HEAs). This reveals a new cross-slip mechanism formed through collinear reactions between dislocations and rhombus-shaped perfect loops, leading to strong radiation resistance due to numerous narrow defect-free channels under relatively random strain localization.

# COUPLING OPTIMIZED SOLIDIFICATION AND HEAT TREATMENT ENABLES SUPERIOR STRENGTH-DUCTILITY SYNERGY IN ADDITIVE MANUFACTURED NiTi ALLOYS

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**ABSTRACT –** NiTi alloys exhibit excellent mechanical properties and unique shape memory effects. Complex NiTi structures fabricated by laser powder bed fusion (LPBF) are highly attractive for biomedical and aerospace applications. However, their ductility remains unsatisfactory, reaching at most ~23% in either the as-fabricated or heat-treated states, far below the ~50% achieved by conventionally counterparts. Here, we propose an integrated strategy of optimized solidification and heat treatment to substantially improve the strength–ductility synergy. Optimized solidification enables the as-fabricated samples to achieve a tensile strength of 682.7MPa and elongation of 22.7%, comparable to the best reported values. Subsequent heat treatment further raises tensile strength to 823.5MPa and elongation to 45.8%, more than twice the as-fabricated ductility and approaching the conventional benchmark. Microstructural analyses combined with in-situ tensile testing reveal the underlying mechanisms. Modified solidification suppresses forming of cellular structures, thereby eliminating elongated Ti2NiOx precipitates along cell boundaries. The martensite fraction is markedly reduced simultaneously, shifting the stress-induced martensitic transformation from a growth-dominated to a nucleation-growth mode. Heat treatment induces recrystallization and grain coarsening, converting the disordered fine grains into homogeneous coarse grains with significantly fewer grain boundaries. These combined effects extend both the phase transformation plateau and plastic deformation stage, resulting in substantial enhancement of strength–ductility synergy. The results advance our capabilities in fabricating high-performance complex NiTi structures through LPBF.

# CONTRIBUTION OF LATTICE ROTATION AND RECRYSTALLIZATION MECHANISM TO THE TRANSFORMATION OF ORIENTATION PREFERENCE IN ALUMINUM SINGLE CRYSTAL DURING ECAP

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**ABSTRACT –** The optimization of mechanical properties and formability is critical for aluminum alloys, and tailoring texture through equal channel angular pressing (ECAP) is an effective way for property enhancement. In our study, the microstructural evolution and orientation transformation of aluminum single crystals (ASCs) was systematically investigated during ECAP. According to the well-defined shear characteristics of ECAP and the orientation sensitivity of ASCs, the synergistic effect of initial orientation and loading direction on texture evolution was analyzed in detail. The results show that the lattice rotation is the primarily transformation mechanism of initial orientation toward preferred orientations during the low-strain deformation, and its evolution path is controlled by the distribution of initial slip systems. The position of preferred orientation is predetermined by the external loading direction, where slip system is approximately parallel to the applied shear direction. As the deformation increases, the orientation transformation is mainly achieved by dynamic recrystallization (DRX), and its mechanism depends on the misorientation between the deformed matrix and preferred orientation. For the larger misorientation, the orientation transformation is primarily by the discontinuous dynamic recrystallization (DDRX), while it mainly via continuous dynamic recrystallization (CDRX) when the misorientation is small. The above research highlights the potential to tailor textures by control of the initial texture and the ECAP processing parameters.

# HYDROGEN EMBRITTLEMENT UNDER EQUIVALENT HYDROGEN FUGACITY: A COMPARISON OF HYDROGEN CHARGING METHODS

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**ABSTRACT** − The hydrogen embrittlement of metallic materials poses a significant challenge to the safety of hydrogen transportation infrastructure. Mechanical testing in hydrogen-containing environments directly compares mechanical behaviors among various materials. Current experimental approaches primarily utilize a high-pressure gaseous hydrogen environment or electrochemical hydrogen charging. While the high-pressure environment is similar to the service conditions for gaseous hydrogen transportation, it presents limitations such as high costs and significant safety risks. In contrast, using low-concentration electrolytes, electrochemical charging enables hydrogen permeation without high pressure. However, the equivalence between electrochemical charging and high-pressure hydrogen environments remains questionable. The differing influences of these two charging methods on mechanical behaviors bring challenges in translating laboratory findings to engineering applications. Therefore, we investigated X52 and X60 pipeline steels to examine the effects of hydrogen charging methods. The mechanical behaviors of two steels are tested with the equivalent hydrogen fugacity. First, we conducted electrochemical and gaseous hydrogen charging experiments, accompanied by thermal desorption spectroscopy (TDS) analyses, and established an equivalent relationship for hydrogen fugacity between the two charging methods. The activation energy of hydrogen traps in both steels was determined, and energy level analysis proved that grain boundaries and dislocations serve as the primary reversible hydrogen trap sites. Subsequently, slow strain rate tensile tests were conducted under equivalent hydrogen fugacity conditions based on the hydrogen equivalence theory. The results indicate that both steels experienced minimal changes in yield strength and tensile strength under either type of hydrogen charging. The higher hydrogen fugacity significantly reduced the elongation and area reduction. Fractographic analysis revealed that the kind of hydrogen charging affected the damage mechanisms of the pipeline steel: gaseous hydrogen primarily resulted in brittle fracture surfaces, whereas electrochemical hydrogen charging led to a mixed ductile-brittle fracture characteristic.

# INVESTIGATION OF THE MECHANISM FOR EDGE CRACK REDUCTION AND ANALYSIS OF THE EFFECT OF MAJOR PROCESS VARIABLES IN EQUAL-SPEED ASYMMETRIC ROLLING

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**ABSTRACT –** This study investigates the mechanisms of edge crack reduction in equal-speed asymmetric rolling, a specific form of asymmetric rolling, and systematically analyzes the influence of key process parameters on crack formation. To this end, a stress-based fracture model incorporating a yield function, hardening behavior, and strain-rate effects was developed and implemented within a three-dimensional finite element model to accurately simulate material behavior during rolling. A comparative analysis revealed that equal-speed asymmetric rolling suppresses edge crack formation through the combined effects of an increased strain rate, the induction of simple shear stress, and a reduction in the forward slip zone. Furthermore, the influence of upper roll radius, friction coefficient, and tension on edge crack initiation was examined. The results indicate that edge cracking is mitigated by decreasing the upper roll radius, friction coefficient, and tension.

These findings provide a fundamental mechanistic understanding of edge crack mitigation in equal-speed asymmetric rolling and are expected to serve as a valuable basis for future process design and optimization aimed at minimizing edge cracks.

# STATISTICAL INFERENCE AND UNCERTAINTY QUANTIFICATION FOR MODELING OF BODY-CENTERED-CUBIC SINGLE CRYSTALS

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**ABSTRACT-** Predictive modeling of bcc materials remains challenging due to the complex nature of slip activity, patterns and interactions. Additionally, the high-dimensional space of material parameters with significant uncertainties poses a challenge to the further development of continuum constitutive models especially at the single crystal level. In this work, we aim to identify key physical assumptions and the associated uncertainties for the predictive modeling of bcc single crystal molybdenum under quasi-static to shock loading conditions. To this end, we employ two representative physics-based bcc single crystal plasticity models taken from our previous work (Nguyen et al., Int J Plasticity 139 (2021) 102940; Lee et al., Int J. Plasticity 163 (2023) 103529), each prioritizing different key deformation mechanisms. First, the Bayesian model calibration (BMC) is used for probabilistic estimates of parameters in both models using the same experimental data spanning diverse strain rates, temperatures, and crystallographic orientations. In conjunction with the BMC procedure, the global sensitivity analysis is conducted to quantify the impact of uncertainties in the model parameters on the key simulation results of quasi-static to shock responses. The global sensitivity analysis of uniaxial stress responses at various strain rates and temperatures shows that the influence of individual parameters is strongly correlated with loading conditions. The sensitivity indices at various loading conditions clearly illustrate the physical basis underlying the predictive capabilities of the two distinct bcc models for the rate- and temperature-dependence. Then, both of the physics-based bcc crystal plasticity models are further validated at extreme shock loading conditions beyond the calibration regime. By assessing the predictive capabilities of the two calibrated bcc models for plate impact experiments, we further identify critical physical mechanisms that govern the elastic-plastic transition in single crystal molybdenum under shock loading.

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# ANISOTROPIC COMPRESSION BEHAVIOR OF 316L STAINLESS STEEL AT CRYOGENIC TEMPERATURE

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**ABSTRACT-** This study investigates the microstructural evolution and deformation behavior of 316L stainless steel (SS) fabricated by direct energy deposition (DED) under compressive loading at room temperature (RT) and cryogenic temperature (CT), along the scanning (SD) and transverse (TD) directions. Electron backscatter diffraction (EBSD), transmission electron microscopy (TEM), and electron channeling contrast imaging (ECCI), combined with dislocation-based crystal plasticity simulations, were employed. The as-fabricated microstructure exhibited columnar grains with cellular substructures, and δ-ferrite at cell boundaries enriched in Cr and Mo due to segregation. At RT, SD samples deformed via dislocation glide and twinning in [001]-oriented grains, gradually reorienting toward the less favorable [110] direction. TD samples predominantly deformed by slip. At CT, yield strength differed significantly between SD and TD samples, indicating mechanical anisotropy arising from grain morphology, local stress heterogeneities, and martensitic transformations ($\gamma \rightarrow \varepsilon \rightarrow \alpha'$ and $\gamma \rightarrow \alpha'$). Simulations incorporating twinning- and transformation-induced plasticity (TWIP and TRIP) showed that [110]- and [111]-oriented grains relative to the loading direction exhibited higher resistance to deformation, consistent with lower twinning and martensite formation. Overall, deformation mechanisms varied with temperature. At RT, twinning and screw dislocation glide were dominant, while at CT, anisotropy was governed by the interaction between hard and soft phases, with martensite variant selection playing a central role. The activation of TWIP and TRIP was strongly dependent on crystallographic orientation, with [001]-oriented grains showing greater deformation tendency.

# MICROMECHANICAL RESPONSE OF AN ADDITIVELY MANUFACTURED NEAR-α Ti-6242 ALLOY UNDER CYCLIC LOADING: INSIGHTS FROM EXPERIMENTS AND CRYSTAL PLASTICITY SIMULATIONS

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**ABSTRACT** –Additive manufacturing of Ti alloys is emerging rapidly for the design of complicated structures suitable for aerospace applications. Near-α Ti6242 (Ti-6Al-2Sn-4Zr2Mo) alloy is used in the compressor section of the jet engine up to the temperature of 540ºC. The current study investigates the behaviour of the directed energy deposited near-α Ti6242 alloy under cyclic loading conditions. A post-printing heat treatment was utilized to convert the non-equilibrium martensitic α′ into an equilibrium α+β microstructure. Load-controlled cyclic tests were performed at an R ratio of 0.1. However, the alloy in as-printed conditions showed a poor fatigue response. Post-printing heat treatment resulted in improved fatigue life. A microstructural investigation was carried out, coupled with the EBSD analysis by scanning electron microscope, on fatigued specimens, to understand the localized slip behaviour and crack nucleation process. Furthermore, full-field crystal plasticity simulations using the opensource DAMASK package were performed to understand the local plasticity and evolution of different field quantities in the different microstructural constituents. Crystal plasticity simulation results were well in agreement with the experimental findings.

# FE-CNN FRAMEWORK FOR NON-DESTRUCTIVE CHARACTERIZATION OF RESIDUAL STRESS VIA SPHERICAL INDENTATION

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**ABSTRACT-** This study introduces a Finite Element – Convolutional Neural Network (FE-CNN) framework for simultaneously predicting plastic properties and in-plane non-equibiaxial residual stress near the surface based on spherical indentation plastometry. Conventional residual stress evaluation methods are often destructive or require reference conditions, and the proposed framework provides a practical and non-destructive alternative. Validated FE simulations of spherical indentation were used to systematically construct a large database representing a wide range of material properties. Sensitivity analyses identified the optimal indenter size and penetration depth that ensures sufficiently large plastic deformation, enabling reliable residual stress characterization. The CNN model effectively captured spatial information from both the load-displacement curve and the three-directional indentation profile, thereby allowing directional residual stress prediction. Its performance was validated against other model architectures, including Multi-Layer Perceptron and Vision Transformer, and demonstrated superior predictive accuracy. Furthermore, the robustness of the developed model was examined using noise-augmented data that mimic experimental conditions. The predictive capability of the framework was verified through applications to OFHC copper samples with known residual stresses and additively manufactured samples, by comparing the predictions with the applied stresses and neutron diffraction measurements, respectively. Overall, the FE-CNN framework offers a practical, non-destructive, and robust platform for comprehensive material characterization through spherical indentation.

# OVERCOMING LIMITATIONS IN PREDICTING BIAXIAL TENSION OF ANISOTROPIC ALUMINUM ALLOY TUBES USING BARLAT89 YIELD CRITERION

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**ABSTRACT –** Applying anisotropic constitutive models to tube materials is crucial for achieving precise simulation of forming thin-walled tubular components. However, it is challenging to obtain the tube's anisotropic parameters due to their semi-closed structure, which leads to the inability to model the tube plasticity accurately. In this paper, a novel pyramid-segment ring expansion test (PRET) was developed based on digital image correlation (DIC) technology, in which the stress state can be analyzed quantitatively. The PERT method achieves the accurate determination of the circumferential stress-strain curve of tubes for the first time. Meanwhile, a new hybrid calibration strategy of the Barlat89 yield criterion was formulated for thin-walled tubes. The coefficients $a$ and $c$ are solved using the axial and circumferential $r$ values ($r_0$ and $r_{90}$), while the coefficient $h$ is solved using the axial and circumferential flow stress ($\sigma_0$ and $\sigma_{90}$), without the demand for the equi-biaxial tensile parameters. Subsequently, the deformation data of 6061 aluminum alloy tubes under uniaxial and biaxial stress states were acquired using the PRET, controllable biaxial tension test, and hydro-bulging test. The subsequent yield loci and plastic flow directions in the biaxial tensile strain zone were quantified and predicted. The results indicate that the Barlat89 yield criterion under the hybrid calibration strategy exhibits extremely high prediction accuracy for the anisotropic hardening and flow behaviors, with a prediction error of 0.8% for hardening and 2.1° for flow. Thus, combining the PRET method with the hybrid calibration strategy enables accurate modeling of the biaxial tension of aluminum alloy tubes within the associated flow rule framework by utilizing the Barlat89 yield criterion. Ultimately, an efficient modeling and evaluation approach was established for aluminum alloy tube materials. It not only avoids the adoption of complex models that reduce efficiency and convenience but also significantly reduces the experimental cost for calibration, thus having potential for application in both academia and industry.

# DATA-DRIVEN MULTISCALE MODELING OF HETEROGENEITY EFFECTS ON ALLOY STRENGTH AND FATIGUE

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**ABSTRACT-**Despite the widespread use of complex alloys in engineering applications, how nanoscale compositional heterogeneity and microscale microsctructure heterogeneity governs macroscopic mechanical properties remains an open question. This talk presents our recently developed data-driven multiscale mechanics framework that integrates data-driven modeling, high-throughput molecular dynamics (MD), discrete dislocation dynamics (DDD), kinetic Monte Carlo (KMC), and crystal plasticity (CP) theory to elucidate how compositional and microsctructure heterogeneity mediates strength and fatigue behavior across multiple scales.

# IN SITU HIGH THROUGHPUT CHARACTERIZATION AND ANALYSIS OF ALUMINUM ALLOYS

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**ABSTRACT –** The lightweight development of next-generation aerospace equipment requires advanced materials that combine high strength with complex formability. Aluminum alloys, owing to their low density, high specific strength, and good processability, are currently the most widely used lightweight structural materials. This study systematically investigates the service failure behavior of aluminum alloys by integrating multi-scale in-situ characterization with high-throughput machine learning algorithms. For forged aluminum alloys, it elucidates the mapping relationship between crack initiation/propagation and grain boundaries as well as grain orientations, proposing a criterion for crack propagation prediction. For additively manufactured aluminum alloys, it reveals for the first time that a three-dimensional micro-nano dual-phase network structure can inhibit fatigue crack initiation, with an intrinsic fatigue strength exceeding 85% of the tensile strength. This breakthrough overcomes the fatigue strength limitations of metallic materials and provides important theoretical support for theapplication of aluminum alloys in aerospace equipment.

# CRACK INITIATION OF HYDROGEN-CHARGED 304 STAINLESS STEELS UNDER MONOTONIC AND CYCLIC LOADING

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**ABSTRACT –** Hydrogen embrittlement (HE) is a critical challenge in the design and application of structural materials in hydrogen-rich environments. This study investigates the mechanical behavior and fracture mechanisms of electrochemically charged 304 stainless steels under monotonic and cyclic loading conditions. Our results reveal that hydrogen-charged specimens exhibit increased yield strength but reduced ductility, with distinct microstructural changes facilitating microcrack initiation and propagation. Post mortem analyses highlight the influence of crystallographic slip systems and grain boundary interactions on fracture behavior. Complementary crystal plasticity simulations elucidate the mechanisms of slip activation and stress redistribution, linking these phenomena to crack growth pathways. These findings not only deepen our understanding of hydrogen-induced material degradation but also provide critical insights for the development of high-performance materials in hydrogen-centric applications.

# THERMODYNAMICALLY CONSISTENT CRYSTAL PLASTICITY MOD EL COUPLING MARTENSITIC TRANSFORMATION AND DAMAGE EVOLUTION IN QP STEELS

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**ABSTRACT –** Quenching and Partitioning (QP) steels achieve their superior strength–ductility balance through transformation-induced plasticity (TRIP), in which retained austenite (RA) progressively transforms to martensite during deformation. While the TRIP effect provides additional hardening and delays necking, the accompanying transformation could also lead to a redistribution of local stress and strain inhomogeneities that can accelerate void nucleation and growth, ultimately controlling failure. Existing transformation-based crystal plasticity models successfully capture rate- and temperature dependent martensitic transformation, but they do not explicitly account for the coupled role of TRIP in damage initiation and evolution. In this work, a novel thermodynamically consistent crystal plasticity framework is developed that incorporates martensitic transformation kinetics, rate and temperature sensitivity, and transformation-modulated damage evolution. The model introduces transformation rate as a direct state variable influencing void nucleation, growth, and shape evolution. Void evolution is formulated as a function of stress triaxiality and Lode parameter, enabling predictions of anisotropic damage resistance under multiaxial strain paths. The framework captures the dual role of martensitic transformation: providing further hardening while simultaneously promoting damage evolution, all within a unified constitutive law. The proposed model is applied to QP1180 and QP980 steel across a wide range of strain rates and temperatures relevant to forming and crash loading. Results demonstrate that accelerated martensitic transformation at higher strain rates enhances hardening while simultaneously increasing rate of damage evolution under triaxial loading. Predicted phase fraction evolution, damage progression, and failure strain trends are validated against experimental observations, including EBSD-based RA fraction measurements and macroscopic stress strain curves. This work represents the first attempt to explicitly couple strain-rate- and temperature-dependent TRIP with void-mediated damage in a micromechanical crystal plasticity framework. The model provides new insights into how transformation affects damage and failure in QP steels and establishes a pathway toward predictive design of advanced high strength steels for forming and crashworthiness applications.

# LOCAL FAILURE STRAIN AND REDUCTION OF AREA PROVIDE EARLY METRICS FOR HYDROGEN EMBRITTLEMENT IN MICROSCALE TENSILE SPECIMENS

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**ABSTRACT –** Hydrogen embrittlement is the phenomenon by which a metal loses ductility and strength due to the presence of hydrogen atoms within the lattice. In this paper, we studied hydrogen embrittlement in microscale austenitic steel specimens (AISI 303, 316L, and 316Ti) during tensile testing as a function of charging conditions. In particular, microstructure, hydrogen content, global and local mechanical properties, and failure modes were investigated through scanning electron microscopy, thermal desorption spectroscopy, microscale tensile tests, and fractography. The microstructural and hydrogen desorption measurements showed that the hydrogen content was relatively invariant of microstructure with a 2× change between the low-pressure and high-pressure conditions. The micromechanical tests and fractographic images revealed negligible changes in global properties (tensile strength, global failure strain), but significant changes in local properties (local failure strain, reduction of area), with embrittlement. The extent of embrittlement increased as hydrogen content increased and microstructural stability decreased. Similar to results on macroscale tensile specimens, the results from microscale tensile specimens showed reduction of area provided a reliable measure for embrittlement. Local failure strain confirmed these trends. Moreover, the microscale method facilitated a significant decrease in time for hydrogen saturation and material for specimen fabrication, enabling testing of small components or local properties in large components.

# VISUALIZING THERMOMECHANICAL WEAKENING OF MUSCOVITE MICA VIA MICROSCALE SHEAR TESTING

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**ABSTRACT –** Micas are a group of hydrous aluminum silicate minerals with laminated structure that can be split on basal cleavage planes into films that are transparent, flexible, elastic, tough, and waterproof and have outstanding dielectric and insulating properties. This rare combination of structure and properties makes micas ideal materials in different application areas, most notably as geological, technological, and metrological materials. In this paper, we studied the thermomechanical weakening of muscovite mica subjected to mechanical loading. Rectangular pillars were created from high-quality V-1 muscovite mica using focused ion beam (FIB) milling. The structure and chemistry were measured via transmission electron microscopy (STEM) and energy dispersive spectroscopy (EDS). In-situ and ex-situ microscale shear testing were used to assess failure force as a function of pillar size, loading position, and test temperature, and finite element analysis was used to convert the resulting failure forces to fracture toughnesses $K_{IC}$. STEM images showed a base mica layer with an interlayer spacing of about 1 nm, but also detected the presence of a damaged, amorphous layer on the surface. EDS spectra showed three distinct regions in the damaged area: (1) a layer with low K, no Ga, and thickness of 15 nm, (2) a layer with moderate Ga and thickness of 10 nm, and (3) a layer with high Ga and thickness of 20 nm. In-situ shear testing showed $K_{IC}$ was dependent on pillar size and loading position while ex-situ testing showed $K_{IC}$ decreased as temperature increased. The results from the ex-situ shear testing were compared to those from high-temperature nanoindentation. The trends in $K_{IC}$ with pillar size and loading position were analyzed in light of the damage layer, whereas the trends in $K_{IC}$ with temperature were interpreted via structural changes as observed in Raman spectroscopy and molecular dynamics simulations.

# INVESTIGATION INTO THE EFFECT OF CRYOGENIC TEMPERATURES ON WEAR BEHAVIORS OF EUTECTIC ALCOCRFENI$_{2.1}$ HIGH ENTROPY ALLOY

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**ABSTRACT-** This study systematically investigates the wear behavior of AlCoCrFeNi$_{2.1}$ EHEA (Eutectic High Entropy Alloy) under different cryogenic temperatures. The semi-coherent interface of the EHEA, with its excellent phase matching, enables effective stress transfer between the two phases, preventing rapid delamination caused by stress concentration. Furthermore, the hard phase can effectively withstand frictional stress, preventing plastic deformation at lower stress levels and exhibiting superior wear resistance due to work hardening at higher stress levels. At cryogenic temperatures, as the alloy's strength increases, it is able to endure higher frictional stresses, significantly reducing the affected stress area. This reduction in the stress-affected region leads to less plastic deformation and fatigue wear during friction, resulting in excellent wear resistance at low temperatures. The unique soft-hard dual-lamella microstructure of the eutectic alloy maintains strong interfacial bonding under low temperatures, while its outstanding stress transfer capability enables the alloy to exhibit excellent wear resistance even under extreme cold and high-load conditions.

# ON THE CONNECTION BETWEEN MECHANICAL RELAXATION AND EQUILIBRATION KINETICS IN A HIGH-ENTROPY METALLIC GLASS

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**ABSTRACT –** The slow transition from an out-of-equilibrium glass towards a supercooled liquid is a complex relaxation phenomenon which involves a wide range of time scales. In this study, we aimed to establish the correlation between mechanical relaxation and the equilibration kinetics of a $Pd_{20}Pt_{20}Cu_{20}Ni_{20}P_{20}$ high-entropy alloy. The evolution of stress relaxation with aging time was obtained experimentally with an unprecedented detail for metallic glasses, allowing us to pinpoint new interesting features. The long structural relaxation towards equilibrium contains a wide distribution of activation energies instead of being just associated to the β relaxation as commonly accepted. In addition, within the studied aging-time window, we observe a decrease of microstructural heterogeneity which contrasts with an increase of dynamic heterogeneity. This gradual broadening of the time distribution of relaxation modes, at the same time that aging homogenizes the spatial fluctuation of mechanical properties, has been observed before but it is not yet explained by a microscopic model. These results significantly enhance our insight of the interplay between relaxation dynamics and thermodynamics in metallic glasses.

# MACHINE LEARNING-AUGMENTED MODELING ON THE FORMATION OF NON-CONVENTIONAL NANO-PRECIPITATES IN FAST SOLIDIFIED AL ALLOYS

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**ABSTRACT –** The mechanical behaviors of Al alloys are dictated by the precipitates formed during processing and/or heat treatment. Recent experiments have shown that Al-Si-Mg alloys solidified under high cooling rates contain Si-enriched clusters that are remarkably different from the Mg-Si co-clusters (e.g. β□ particles) in conventionally cast alloys. However, the responsible mechanism remains unknown. Here by integrating energy landscape sampling within complex local chemistry, machine learning techniques, and a kMC framework, we discovered that the actual vacancy-Si migration barriers are much lower than those assumed in the classic linear interpolation approximation, and we further uncovered new microstructural evolution pathways leading to the formation of non-conventional nanoscale precipitates. Our findings help explain the experiments in Al alloys processed via high-pressure die casting or selective laser melting. These results may have important implications for the strengthening mechanisms in hardenable Al alloys, particularly through the lens of nanoscale structural evolution and non-equilibrium processing pathways.

# A NOVEL CONSTITUTIVE MODEL FOR ALUMINUM ALLOYS UNDER COMPRESSION & SHEAR COUPLED DEFORMATION

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**ABSTRACT –** Constitutive model is key to determine the accuracy of the finite element simulation for spring-back prediction of formed components, especially for component experiencing coupled deformation during hot forming processes. However, current constitutive models concentrate on describing hot flow behaviors under uniaxial deformation, one could quantitatively describe the viscoplastic behaviors and the microstructure evolutions under coupled deformation are lacking, leading to low prediction accuracy. This work for the first time introduces a set of constitutive equations, which quantitatively describes the effect of compression & shear coupled deformation on the viscoplastic behavior of AA6061, by introducing a compression-to-equivalent strain ratio α (i.e. $\varepsilon_c/\varepsilon_E$). Effects of α on both the microstructure evolutions (i.e. accumulation and recovery of dislocations, recrystallization and evolution of the material damage) and the viscoplastic behaviors are formulated into the introduced equations based on the underlying mechanisms during compression & shear coupled deformation. Such set of equations are further verified by compression & shear combined experiments at different temperatures and equivalent strain rates. Good agreements are achieved compared to the predicted and experimental results. Such model is expected to significantly improve the accuracy for any future prediction of the hot forming process of aluminum alloys under compression & shear coupled deformation, e.g. differential velocity extrusion, etc.

# EFFECT OF HIGH TEMPERATURE QUENCHING TEMPERATURE ON THE WEAR PERFORMANCE OF AVIATION GEAR STEEL 15Cr14Co12Mo5Ni2

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**ABSTRACT** –15Cr14Co12Mo5Ni2 is a high-performance alloy structural steel with high strength, good toughness and anti-fatigue properties, which is widely used in the field of gear transmission system of aero engine. In order to meet the wear resistance of the material under extreme service conditions, the high temperature quenching heat treatment process of aviation gear steel 15Cr14Co12Mo5Ni2 was carried out at quenching temperatures of 1020°C, 1050°C, and 1080°C and friction, and wear test experiments under different quenching temperatures were performed at room temperature and high temperature using a pin-on-disk wear testing machine, also the influence of quenching temperature on the friction and wear behavior of aviation gear steel was investigated in this paper. The wear morphology of the samples is observed using OM, the wear rate is calculated, and the friction and wear performance of the samples at different quenching temperatures is compared and analyzed. The results show that the wear rate and the friction coefficient of the samples significantly reduced after high temperature quenching. The wear rate decreases as the quenching temperature increases from 1020°C to 1080°C, and their values are $1.55\times10^{-5}$ $mm^3/Nm$, $1.46\times10^{-5}$ $mm^3/Nm$ and $0.74\times10^{-5}$ $mm^3/Nm$ at room temperature. The friction coefficient at room temperature increase firstly then decrease with the increasing the quenching temperature from 1020°C to 1080°C, and the material exhibits the smallest friction coefficient of 0.51 at quenching temperature of 1080°C. Compared to room temperature, the friction coefficient at high temperature of 300 ℃ is smaller and it is the smallest at quenching temperature of 1020°C. The wear rate at high temperatures is significantly higher than that at room temperature and it is the smallest at quenching temperature of 1080°C. The main wear mechanism is abrasive wear at quenching temperature of 1080°C, while the samples primarily exhibit abrasive wear and fatigue wear and at quenching temperature of 1020°C and 1050°C.

# INFLUENCE OF INTERFACE ROUGHNESS AND ORIENTATION ON TH E DEFORMATION MECHANISMS OF AL–Ti BIMETALS

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**ABSTRACT-** The microstructural characteristics and morphology of interfaces in metals are crucial in governing deformation and failure mechanisms under extreme conditions. At high strain rates or during shock deformation, these interfaces significantly influence the evolution of dislocations and twinning, directly impacting the material's overall strength and failure. Despite this importance, a substantial knowledge gap remains between the observed material behavior and the effects of interface roughness and orientation, limiting the ability to design robust, high-performance components used in sectors such as defense, energy, aerospace, and infrastructure. To address this, we performed large-scale Molecular Dynamics (MD) simulations of various Al–Ti bimetal interfaces to explore their role in deformation mechanisms. This study investigates how interface roughness (flat vs. waveform interfaces) and orientation affect material behavior under high-strain-rate uniaxial stress compression loading. Atomistic simulations indicate that interface roughness reduces the critical stress for dislocation nucleation. Furthermore, by rotating these interfaces relative to the loading direction, we clarify how orientation influences deformation mechanisms, providing valuable insights for optimizing bimetal microstructures. Under shock loading, microstructures with flat interfaces and varying fractions of Al and Ti revealed that while the percentage of Ti and Al has minimal influence on peak compressive stress, it significantly affects spall strength. The introduction of waveform interfaces reduces peak tensile stress compared to flat interfaces. Additionally, we propose a novel approach to model oblique shock, allowing us to examine the role of interface orientation relative to the loading direction. This sheds light on how oblique shock affects deformation mechanisms, offering valuable insights for optimizing bimetal microstructures.

# MULTI-PHYSICS AND MULTI-DOMAIN SIMULATIONS OF COUPLED PROCESSES IN POROUS MEDIA

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**ABSTRACT –** The simulation of multiple physical processes in porous media, such as fluid flow, poromechanics, fault activation, thermal flow, and chemical reactions, that can take place simultaneously with multiple time and space scales, play a crucial role for a proper management of underground resources. The present communication focusses on the development of GReS, a novel open-source modular platform specifically designed with the aim at contributing to the design and testing of numerical algorithms for fully coupled multi-physics multi-domain poromechanical applications. The idea is to partition the overall computational domain into possibly non-conforming subdomains where different physics and discretization schemes can be used. The code is based on a high-level programming platform (MATLAB) that should lower the entry barrier for new users and developers, as well as the effort for implementing and testing innovative numerical algorithms. Moreover, the modular structure of the code encourages contributions from different developers at variable levels, from the implementation of new physics and discretization schemes to specific algorithms to accelerate the linear and non-linear solver.

In the present communication, we will introduce the GReS concept and its current development state, including advances to the mortar algorithm used to transfer the information among non-conforming subdomains with independent meshes. Basic benchmarks will be presented to show the current code's potentials, along with the projects for future developments.

# A MULTISCALE FINITE ELEMENT ANALYSIS OF THE DYNAMIC FRAGMENTATION OF ADDITIVELY MANUFACTURED POROUS METAL RINGS

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**ABSTRACT –** Dynamic fracture of additively manufactured porous metals under high loading rates is strongly influenced by the microstructural void morphology. This fact underscores the importance of integrating internal void information into large-scale simulations to accurately predict the energy absorption capacity of printed structures under impulsive loadings. However, this process presents challenges, as explicitly resolving the porous microstructure of the entire specimen is computationally prohibitive and most existing mesoscale damage models do not account for microstructure-specific information. This has motivated the development of a computational homogenization method which incorporates the size and spatial distribution of voids, measured from experimental tomography analysis, into microstructure-informed finite element models of additively manufactured $AlSi_{10}Mg$ rings subjected to rapid radial expansion and fragmentation. The central feature of the simulation model is an upscaling approach that converts microstructural morphology into a single initial porosity variable which changes spatially across the ring-shaped specimen to reflect the material's microstructural heterogeneity. The mechanical behavior of the porous aggregate is described using the Gurson-Tvergaard plasticity model, where fracture is assumed to occur when a critical porosity threshold is reached. Finite element calculations performed using ABAQUS/Explicit (2019) are compared with the ring expansion tests reported by Nieto-Fuentes et al. (2023b) and Kumar et al. (2025). The observed qualitative agreement, along with a reasonable quantitative correlation between the simulation results and the experimental fragmentation statistics for high strain rates (7,900 $s^{-1}$ to 15,400 $s^{-1}$), lends support to the validity of the developed computational homogenization approach. This simulation model offers a significant reduction in computational time compared to calculations that resolve the porous microstructure, while capturing the effects of the spatial distribution of porosity defects on fragment size—an aspect overlooked by simulation models assuming spatially homogeneous porosity. This makes it suitable for rapid preliminary evaluations in engineering design and swift prediction of dynamic fracture in printed structures. The computational efficiency of the method has enabled an extensive parametric analysis which investigates the effects of void spatial distribution, intervoid distance, spatial porosity variability, and fracture porosity on the resulting fragment size distribution. The analysis of parameter space variations reveals key porous microstructure factors influencing dynamic fragmentation of metal

rings, offering valuable guidance for optimizing the performance of printed structures in impact-resistant applications.

# DAMAGE AND FRACTURE IN THE DEFORMATION OF MATERIALS

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**Abstract –** Deformation of materials is one of the most practical engineering activities involved in deformation-based manufacturing and product service. Deformation-based manufacturing is widely used to fabricate net- or near-net-shape parts through plastic deformation, while the service of products is the ultimate goal of manufacturing. These activities need to consider damage and fracture. In this talk, scientific insights into damage and fracture, along with an in-depth understanding of their behaviors, are presented. The mechanisms of void initiation, coalescence, and growth during material deformation, as well as the formation and occurrence of damage and fracture, will be presented from the perspective of the current state of the art in damage and fracture research. Additionally, the behaviors and prediction of damage and fracture, as well as their avoidance through experimentation and simulation, will also be discussed.

# COUPLED STRENGTHENING MECHANISMS IN TI/AL CLADDING TUBES WITH DUAL HETEROGENEOUS STRUCTURES FABRICATED BY THREE-ROLL SKEW ROLLING

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**ABSTRACT –** This study presents a novel approach for fabricating Ti/Al clad tubes with a dual heterostructure using the three-roll skew rolling (TRSR) process and investigates the sequentially activated multistage strengthening behavior induced by this hierarchical architecture. Unlike conventional solid-state bonding techniques such as cold drawing and extrusion, the TRSR process employs a unique three-dimensional shear deformation mode, which enables the simultaneous realization of interfacial metallurgical bonding and microstructural reconstruction within the titanium layer during the forming of Ti/Al clad tubes. Through this process, a robust metallurgical interface is achieved, while a bimodal grain structure develops within the hard Ti layer, where the fine-grained region has an average grain size of approximately 500 nm, and the coarse-grained region exhibits an average grain size of about 15 μm. The coexistence of the bimodal grain structure in the Ti layer and the heterogeneous interface between Ti and Al together constitutes the dual heterostructure of the clad tube. The formation of this dual heterostructure is attributed to the nonuniform large plastic deformation occurring during the TRSR process. The heterogeneous strain field within the titanium layer simultaneously activates continuous and discontinuous dynamic recrystallization (CDRX and DDRX), leading to the development of a bimodal grain structure. Meanwhile, the interfacial heterogeneity arises from the shear-induced fracture of the oxide layer and the subsequent exposure of fresh metallic surfaces, which promote metallurgical bonding. Furthermore, the coupling strengthening effect of the dual heterostructure was analyzed, revealing that the Ti/Al heterogeneous interface and the bimodal grain structure in the Ti layer respectively induce hetero-deformation-induced (HDI) strengthening at different stages of tensile deformation. In summary, this study highlights the unique capability of the TRSR process to simultaneously construct and activate multiscale heterogeneity, offering a simplified and scalable route for producing lightweight, high-strength clad tubes with an outstanding strength–ductility synergy.

# MULTISCALE PLASTICITY SIMULATION OF POLYLACTIC ACID SPHERULITES USING THREE-DIMENSIONAL LAMINATE THEORY INCORPORATING CRYSTALLINITY AND MICROSTRUCTURE

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**ABSTRACT –** Additive manufacturing of Ti alloys is emerging rapidly for the design of complicated structures suitable for aerospace applications. Near-α Ti6242 (Ti-6Al-2Sn-4Zr2Mo) alloy is used in the compressor section of the jet engine up to the temperature of 540ºC. The current study investigates the behaviour of the directed energy deposited near-α Ti6242 alloy under cyclic loading conditions. A post-printing heat treatment was utilized to convert the non-equilibrium martensitic α′ into an equilibrium α+β microstructure. Load-controlled cyclic tests were performed at an R ratio of 0.1. However, the alloy in as-printed conditions showed a poor fatigue response. Post-printing heat treatment resulted in improved fatigue life. A microstructural investigation was carried out, coupled with the EBSD analysis by scanning electron microscope, on fatigued specimens, to understand the localized slip behaviour and crack nucleation process. Furthermore, full-field crystal plasticity simulations using the opensource DAMASK package were performed to understand the local plasticity and evolution of different field quantities in the different microstructural constituents. Crystal plasticity simulation results were well in agreement with the experimental findings.

# EXPLORING EXTREME CHEMISTRY AND EARTH PROCESSES WITH NEXT-GENERATION PORTABLE LARGE VOLUME HIGH P-T-STRESS SYNCHROTRON CELLS

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**ABSTRACT-** Synchrotron X-ray microtomography has emerged as a reference technique for non-destructive, high-resolution 3D imaging and microanalysis. It enables detailed characterization of a broad range of physical and chemical properties — including morphology, density, chemical composition, oxidation states, structural evolution, and crystallographic perfection — with exceptional spatial resolution and sensitivity. This versatility makes it an indispensable tool in both fundamental and applied research across the disciplines of Materials science, Earth sciences, and Condensed Matter Physics.

However, extending microtomography to multi-extreme environments — involving the combination of high pressures, high temperatures, mechanical stress fields, and non-conventional sintering methods such as Spark Plasma Sintering (SPS) — presents significant technological challenges. These include the necessity for devices that combine large sample volume, mechanical stability, X-ray transparency, and compatibility with tomography scanning and multi-modal analysis at synchrotron facilities.

In order to address this issue, a new suite of portable, large-volume, high-pressure high temperature (HPHT) devices capable of applying torsional deformation, and thus inducing severe plastic deformation, has been developed. These devices are derived from the Paris–Edinburgh press design and have been successfully implemented at major synchrotron facilities: ID27 at the ESRF (France), PSICHE at SOLEIL (France), and I12 at DIAMOND Light Source (UK), etc.

In this presentation, a detailed overview of these novel HPHT devices will be provided, outlining their conceptual design, technical capabilities and operational flexibility. I will also illustrate their scientific potential through a series of our recent in situ experiments addressing key questions in both Earth sciences — such as time resolved 3-D imaging of melt migration under extreme conditions — and materials science, including deformation mechanisms of hard materials ($B_4C$) or the densification of advanced ceramics (nano-$B_4C$, BP, etc.).

# A RELAXATION-BASED APPROACH TO DAMAGE MODELING

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**ABSTRACT –** Material models exhibiting softening effects due to damage or localization share the problem of leading to ill-posed boundary-value problems producing physically meaningless, mesh-dependent finite element results. It is thus necessary to apply regularization techniques that couple local behavior, described e.g. by internal variables, at a spatial level. The common way to do this is to account for higher gradients of the field variables thus introducing an internal length scale.

In this presentation we suggest a different approach to regularization that does not make use of any nonlocal enhancement like the inclusion of higher gradients or integration over local subdomains nor of any classical viscous effects. Instead, we perform an appropriate relaxation of the (condensed) free energy in a time-incremental setting which leads to a modified potential that is coercive and satisfies quasiconvexity in an approximate way. Thus, in every time-increment a regular boundary-value problem is solved. The proposed approach holds the same advantage as other methods, but with less numerical effort. We start with a theoretical derivation, discuss a rate-independent version of the proposed model and its relation to classical fracture mechanics and present details of the numerical treatment. Finally, we give finite element results that demonstrate the efficiency of this new approach.

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# EVALUATING SHEAR STRAIN UNDER NONIDEAL SIMPLE SHEAR DEFORMATION

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**ABSTRACT –** Simple shear tests are extensively adopted to reveal the stress-state-dependent mechanisms of material microstructure evolution with their corresponding mechanical properties, to develop sophisticated constitutive models capturing complex mechanical behaviors, and to precisely characterize the failure limits for shear-dominated or large-strain deformation processes. It has become a topic of growing interest because of its various distinctive capacities. In the current stage, the community lacks a widely-accepted and standardized procedure to conduct tests and to evaluate results, which makes the interpretation and comparation on experimental results to be indirect and difficult. Shear strain is commonly used to characterize the degree of deformation, but the method to estimate shear strain in experimental mechanics is often different from one to another, and uncertainties will appear due to the inconsistence. In this work, some representative methods to evaluate shear strain will be compared analytically and numerically. The influence of nonideal simple shear deformation (that is, the emergence of normal strain and rotation in ideal simple shear deformation, which is common in experiments due to the difficulty to reproduce ideal simple shear experimentally) will be investigated, and it was indicated that some specific shear strain estimations will lead to a certain degree of error at large deformation levels. The results provided are expected to enhance the understanding of experimental mechanics of simple shear test.

# TOWARD AN INTEGRATED MODELING FRAMEWORK FOR RECRYSTALLIZATION-DRIVEN MICROSTRUCTURE CONTROL

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**ABSTRACT** – This paper presents an integrated perspective on recent advances in static recrystallization modeling aimed at enhancing the mechanical performance of metallic materials. First, a coupled crystal plasticity (CP)–phase-field (PF) modeling framework was developed for ultra-low carbon steels, enabling the simultaneous prediction of recrystallization texture evolution and anisotropic mechanical properties. Second, in grain-oriented electrical steels, the nucleation mechanism of Goss {110}<001> grains during primary recrystallization was elucidated through the integrated CP–PF framework, demonstrating the critical role of shear bands as preferential nucleation sites. Third, building on these modeling insights, a particle-assisted texture engineering strategy was introduced for Cu–Ni–Si alloys, where finely dispersed precipitates directed the recrystallization texture by accelerating the nucleation of favorable orientations while suppressing unfavorable ones, thereby overcoming the typical trade-off between strength and formability in high-performance Cu alloys.

Together, these studies build toward an integrated modeling framework of recrystallization, offering a comprehensive roadmap for recrystallization-driven microstructure control and property optimization in metallic systems. The proposed approaches not only deepen our fundamental understanding of recrystallization but also furnish versatile tools for designing next-generation structural and functional alloys.

# RELATIVE MOBILITY OF SCREW VERSUS EEDGE DISLOCATIONS CONTROLS THE DUCTILE-TO-BRITTLE TRANSITION IN METALS

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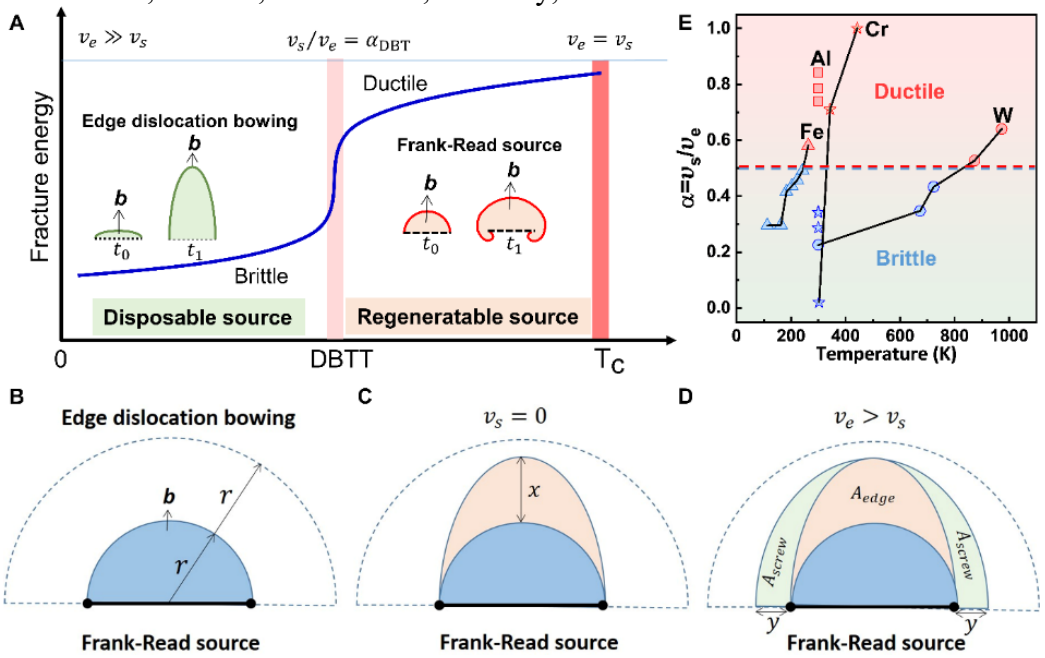
**ABSTRACT–** Body-centered-cubic metals including steels and refractory metals suffer from an abrupt ductile-to-brittle transition (DBT) at a critical temperature, hampering their performance and applications. Temperature-dependent dislocation mobility and dislocation nucleation have been proposed as the potential factors responsible for the DBT. However, the origin of this sudden switch from toughness to brittleness still remains a mystery. Here, we discover that the ratio of screw dislocation velocity to edge dislocation velocity is a controlling factor responsible for the DBT. A physical model was conceived to correlate the efficiency of Frank-Read dislocation source with the relative mobility of screw versus edge dislocations. A sufficiently high relative mobility is a pre-requisite for the coordinated movement of screw and edge segments to sustain dislocation multiplication (see Figure below). Nanoindentation experiments found that DBT in chromium requires a critical mobility ratio of 0.7, above which the dislocation sources transition from disposable to regeneratable ones. The proposed model is also supported by the experimental results of iron, tungsten and aluminum.

**Keywords:** Brittle; Ductile; Dislocation; Mobility; Metal.

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# EVADING STRENGTH-DUCTILITY TRADE-OFF IN EUTECTIC HIGH ENTROPY ALLOYS THROUGH HETERIGENEOUS STRUCTURE INDUCED MARTENSITIC TRANSFOAMATION

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**ABSTRACT-** The synergistic activation of multiple strengthening mechanisms during deformation plays a pivotal role in overcoming the longstanding strength-ductility trade-off in structural materials. The introduction of the heterostructures enables effective control of strain partitioning during deformation to unlock additional strengthening mechanisms unattainable in homogeneous state. In this work, we designed a hierarchical heterostructured (HH) $Al_{19}Co_{20}Fe_{20}Ni_{41}$ eutectic high entropy alloy featuring alternating equiaxed-grain region (EGR) and lamellar-grain region (LGR). The HH alloy achieved an exceptional ultimate tensile strength of 1510 MPa and uniform elongation of 22.45%, which is significantly exceeding the homogeneous state. Superior strength-ductility synergy originates from the sustained effective work-hardening rate assisted by deformation-induced martensitic transformation (DIMT) in EGR. Systematic μ-DIC analysis reveals multiscale strain-partitioning behaviors during early plastic deformation in the HH alloy, which amplifies the heterogeneous deformation between FCC and B2 phases in EGR regions. The disruption of K-S interfaces generates intense dislocation pile-up to induce long-range internal stresses that activate DIMT in the B2 phase. The synchrotron X-ray diffraction analysis confirmed that the enhanced strength and work-hardening rate from DIMT originates from more pronounced dislocation strengthening of the martensite. This work demonstrates that heterostructure design not only provides additional hetero-deformation strengthening, but also activates novel deformation mechanisms through elevated internal stresses, offering a new paradigm to overcome the strength-ductility trade-off in EHEAs.

# HIGH-RESOLUTION CRYSTAL-PLASTICITY SIMULATIONS OF INNER YIELD SURFACES AFTER PRE-DEFORMATION

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**ABSTRACT –** In a polycrystal the innermost yield surface is given by that slip occurs on at least one slip system in at least one of the grains. During an elastic-plastic transition, slip occurs in more of the grains. When reaching the conventional yield surface, corresponding to Rp0.2, all grains respond plastic with slip activities. Between these two, yield surfaces can be calculated for yielding at intermediate levels of plastic strain or plastic work. After predeformation, inner yield surfaces are small and located inside the stress point before unloading from the predeformation, e.g. full unloading involves plastic slip activity. The inner yield surface is important for understanding limitations of the continuum plasticity theory related to strain-path changes during plastic instabilities, A novel rate-independent finite-element implementation of a user subroutine in Abaqus has been made and enables a novel determination of inner yield surfaces for representative volume elements for a polycrystal structure, with or without prestrain, and with very low probing strains. The spectral crystal plasticity code, DAMASK, has been used to investigate how yield surfaces, with a probing strain relevant for experimental conditions, depend on the texture and work hardening.

# A NOVEL HILL48 YIELD CRITERION FRAMEWORK USING STRESS ADJUSTMENT TO CAPTURE STRESS-STATE-DEPENDENT PLASTIC ANISOTROPY

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**ABSTRACT-** The stress-state-dependent plastic anisotropy of sheet metals has recently attracted significant attention. However, existing phenomenological plasticity models still exhibit limitations in characterizing the stress state dependence of anisotropic yield strength and plastic flow under a wide range of stress state spanning from equi-biaxial compression (EBC) to equi-biaxial tension (EBT). To address this issue, we proposed a modified Hill48 yield criterion framework with enhanced flexibility by coupling the classic Hill48 yield function with stress adjustment factors (SAFs), referred to as M-Hill48-SAF. A continuous interpolation method based on a sixth-order polynomial were proposed to define the anisotropic SAF as a function of stress triaxiality, which can analytically describe the yield strength ranging from EBC to EBT. Using artificial materials, the adaptability and enhanced flexibility of the proposed model in capturing stress state dependence was systematically validated. The predicted yield locus offers advantages — it can be independently adjusted and customized at a specific stress state without influencing the others. Moreover, the model accurately captures yield evolution behavior under arbitrary loading directions across all seven stress states. The proposed model was further applied to several representative sheet metals, including high-strength steel (DP980), aluminum alloy (AA5754-O), magnesium alloy (AZ31), and titanium alloy (Ti-6Al-4V). Comparative analysis with several recently developed yield criteria confirms that the proposed model enhances the prediction accuracy of strength characteristics across various stress states. Finally, the flexibility and customizability of the proposed model were discussed in relation to the availability of stress-state and loading-direction data, and their effects on the yield surface shape and convexity.

# A TEMPERATURE-EXPLICIT CRYSTAL PLASTICITY FRAMEWORK FOR PREDICTING MECHANICAL BEHAVIOR OF QP1500

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**ABSTRACT –** The third-generation advanced high-strength steel (G3-AHSS), quenching and partitioning steel with a tensile strength of 1500 MPa (QP1500), has been developed and utilized as a structural material due to its superior strength and ductility. During both forming and service, this steel is exposed to a wide range of temperatures, making it crucial to predict how thermal conditions influence the microstructural evolution and formability. In particular, temperature affects not only the intrinsic mechanical properties of each phase, namely martensite and austenite, but also the mechanical stability of retained austenite (RA), thereby altering transformation kinetics and consequently the macroscopic mechanical response. In this study, a temperature-explicit crystal plasticity model was proposed to predict the mechanical behavior of QP1500. The modeling framework incorporates the TRIP effect based on the phenomenological theory of martensite crystallography (PTMC) and couples it with a temperature-dependent deformation-induced martensitic transformation (DIMT) kinetics. The material parameters were calibrated using uniaxial tensile tests at −40 °C, room temperature (25 °C), and 100 °C, together with microstructural measurements of RA transformation kinetics from XRD and phase-resolved mechanical properties obtained via nanoindentation. The model is subsequently applied to the three-point tight bending (VDA) test to evaluate its predictive capability under multiaxial loading. This temperature-explicit CP-TRIP framework advances the quantitative understanding and prediction of QP1500 performance in diverse thermal environments, supporting both fundamental research and industrial application.

# AN EXTENDED ANISOTROPIC DISTORTIONAL HARDENING MODEL FOR THE FLEXIBLE BAUSCHINGER EFFECT UNDER NONLINEAR STRAIN PATHS

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**ABSTRACT -** To control the curvature of yield loci, an extended anisotropic distortional hardening (E-ADH) model are developed based on the framework for Bauschinger effect prediction in ADH2022 model (Hu and Yoon, 2022) and G-ADH model (Hu et al., 2025). For the proposed E-ADH model, the second order of the normalized third invariant $\xi$ is introduced into the ADH2022 model. Through analyzing the convex range of the E-ADH model, the relationship between two variables before $\xi$ and $\xi^2$ is determined. The parameter $\beta$ in the E-ADH model will control the curvature of yield loci. If $\beta = 0$, the E-ADH model will reduce to the ADH2022 model. To verify the effectiveness of the proposed model, the complex loading tests for AA1100-O are conducted. Through comparing with G-ADH model, it's found that the proposed E-ADH model processes the same ability as G-ADH model to describe the flow curves under different stress states except the biaxial tension with the pre-strain along the rolling direction. For the G-ADH model, only the transformed first stress invariant is used for the Bauschinger effect, while for E-ADH model, both of the transformed first and third stress invariants are used. Compared with the G-ADH model, the E-ADH model is more flexible to describe the Bauschinger effect around biaxial tension after uniaxial tension.

# PHYSICS-INFORMED MACHINE LEARNING OF THERMAL STABILITY IN GRADIENT NANOCRYSTALLINE 316L STAINLESS STEEL

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**ABSTRACT-** Nanocrystalline (NC) metal and alloys offer exceptional strength but are limited by thermal instability. Here we engineer a USP-driven gradient nanostructured layer in bulk 316L stainless steel, with nanograined surface layer transitioning smoothly to a coarse-grained core. Nanoindentation and micropillar compression tests report 6.2 GPa nanohardness and 2.1 GPa yield strength, approaching an order-of-magnitude gain over coarse-grained counterparts. Stability is achieved by uniformly dispersed nanoscale precipitates that pin boundaries and interfaces at nanoscale, suppressing coarsening while retaining deformation capacity. To interrogate and generalize these behaviors, we develop a physics-informed neural network (PINN) that jointly predicts grain size, precipitate fraction, and nanohardness as functions of time-temperature-depth. The model embeds Arrhenius grain-growth kinetics and Avrami-type precipitation kinetics as differentiable constraints and is trained on depth-resolved hardness profiles together with TEM/EDS microstructure acquired at 773.15 K across holding times. The PINN reproduces the observed hardening despite slight grain coarsening by attributing it to precipitation-driven boundary pinning and dispersion strengthening and extrapolates to unseen temperatures to deliver process maps for design. This combined gradient architecture and precipitate-pinning strategy, coupled with mechanism-constrained AI, establishes a practical route to thermally robust, high-strength NC 316L stainless steel. Beyond advancing process-structure-property understanding, the framework enables data-efficient prediction and optimization for applications in advanced mechanical systems, biomedical devices, and radiation-tolerant components in the future.

# GRAIN BOUNDARY SEGREGATION-INDUCED TRANSITION OF DEFORMATION MECHANISMS IN FENICRCOCU HIGH-ENTROPY ALLOY

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**ABSTRACT-** High-entropy alloys (HEAs), characterized by severe compositional disorder, exhibit unique properties arising from lattice distortion, short-range order (SRO), and elemental segregation. Among these, segregation at grain boundaries (GBs) plays a critical role in modulating GB structure and plasticity, yet its effect on GB deformation mechanisms in HEAs remains elusive. Here, hybrid Monte Carlo/molecular dynamics (MC/MD) simulations were employed to investigate segregation-induced GB plasticity in a FeNiCrCoCu HEA, focusing on the Σ5 (210) [001] symmetric tilt grain boundary. The results reveal Cu enrichment at the GB and demonstrate a transition of deformation mechanism from GB migration to GB sliding with increasing segregation. In the random elemental state, GB migration occurs via the nucleation of step dislocations facilitated by structural unit (SU) adjustments. Segregation suppresses such adjustments, thereby reducing the migration distance and increasing the critical shear displacement required for migration. At higher segregation levels, GB sliding dominates, while SRO introduces additional energy barriers to both migration and slip. An energy model was further developed to quantify the segregation-dependent migration barrier, showing good agreement with simulations. These findings provide mechanistic insights into segregation-governed GB plasticity in HEAs and suggest strategies for tailoring mechanical performance through GB engineering.

# A MULTI-SCALE PHASE FIELD MODEL FOR AMORPHIZATION AS A DEFORMATION MECHANISM IN NANOCRYSTALLINE MATERIALS

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**ABSTRACT-** Stress-induced amorphization represents an emerging deformation mechanism in nanocrystalline materials under severe deformation, yet existing computational frameworks inadequately capture the coupling between conventional crystal plasticity and amorphization. This work presents a novel multi-scale phase field model that integrates finite-strain elasto-plasticity with thermodynamically consistent phase transformation kinetics to investigate how severe plastic deformation drives amorphization in nanocrystalline materials. The model introduces a deviatoric stress-dependent transformation strain tensor that enables stress-driven amorphous phase nucleation, coupling crystal plasticity in the parent phase with visco-plastic flow in the amorphous phase through a unified free energy functional. Numerical investigations reveal several key findings relevant to the plasticity and fracture communities: amorphization exhibits avalanche-like dynamics during phase transformation, representing a critical-like process triggered by elastic instability in the crystalline phase; the Hall-Petch effect emerges naturally from the competition between plastic deformation and phase transformation, with smaller grains exhibiting higher yield strength but increased susceptibility to stress-induced amorphization; amorphous phases preferentially nucleate at surfaces and stress concentrators, forming localized regions that can accommodate additional plastic strain when conventional slip mechanisms are exhausted. The model successfully reproduces experimental observations including shear band formation, grain size effects, and surface amorphization in nanocrystalline alloys. By treating amorphization as a stress-driven phase transformation that fundamentally alters the local plasticity response, this framework provides new insights into how phase transformations influence the overall plastic deformation capacity and failure mechanisms of nanostructured materials under extreme loading conditions.

# MESOSCALE INVESTIGATION OF DISLOCATION-GRAIN BOUNDARY INTERACTIONS IN METALS AND ALLOYS

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**ABSTRACT-** "Microstructure" refers to the large number of crystal grains and their corresponding boundaries that make up metals and alloys. A material's ability to accommodate stress induced through mechanical loads is dependent on the ease with which dislocations can move through the microstructure to relieve accumulated stress. Grain boundaries (GBs) are the largest impediment to this motion – this is true to some extent regardless of the grain size. The GB structure defines whether a dislocation can transmit across a GB, be partially absorbed at the GB, or glide along the GB and re-emit, altering the GB structure. For poor alignment between grains, dislocations can pile-up against GBs, building localized internal stress regions that work harden the material. This preferential localization of strains and plastic deformation at specific microstructural sites are precursors to damage nucleation. Thus, understanding and predicting dislocation-grain boundary interactions are key for capturing mechanical response, but they are also incredibly complex in part due to the vast number of possible grain boundaries and corresponding dislocation interactions. This talk will focus on recent multiscale modeling efforts addressing dislocation-grain boundary interactions, with particular focus on a mesoscale approach called phase field dislocation dynamics. Connections to atomistic efforts will also be discussed, along with methods/approaches that can be used to scale information.

# ADVANCES IN MACHINE LEARNING-BASED MICROMECHANICS: TOWARDS GENERALIZABLE MODELS FOR CRYSTAL PLASTICITY

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**ABSTRACT -** Machine learning methods have shown good potential in constitutive modeling for single/poly crystals with notable computational efficiency. However, existing machine learning-based constitutive models often lack generalizability, limiting their application across diverse boundary-value problems, textures, and material parameters. While various models demonstrate some generalizability in predicting stress-strain responses, most rely on homogenization approaches and thus can't account for microstructure-level stress/strain partitioning. In this talk, two separate machine learning models that demonstrate great promise towards generalizable frameworks are presented. The first model is based on a thermodynamics-informed artificial neural network formulation to accelerate Fast Fourier transform simulations for cross-scale deformation behaviors of polycrystals under complex loading. To address local effects within each grain, this model also employs K-means clustering to group Gauss points within the microstructure. This reduces the number of nonlinear problems to solve, with cluster responses propagated throughout each group. The thermodynamics-based artificial neural network-extracted features are further processed using local material state clusters to account for history-dependent deformation and evolving microstructures. The second model, the so-called U-PolyConformer, is a spatiotemporal machine learning framework that combines U-Net convolutional neural networks with transformer layers, capable of capturing the full-field evolution of stress and strain under monotonic and random-walk loading conditions. Trained on a large dataset of crystal plasticity finite element method (CPFEM) simulations, the model accurately captures complex phenomena, including strain localization and stress unloading. U-PolyConformer achieves a 7,900x speed-up over the ground-truth CPFEM simulations while producing high-fidelity results in both interpolative and extrapolative regimes. Comprehensive evaluations are presented for both models to demonstrate their capacity to generalize beyond the training distribution to novel microstructures, loading conditions, and strain-hardening behaviours. Finally, to highlight the potential of the proposed frameworks for microstructure optimization and to accelerate computational materials engineering workflows, a microstructure optimization framework based on static recrystallization is developed and used to improve forming limit strains for various strain paths.

# DEFECT-DRIVEN PLASTICITY IN IRRADIATED NANOTWINNED Cu

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**ABSTRACT-** A commonly accepted fact in materials science is that immobile crystallographic defects typically restrict plasticity in metallic materials as they impede the glide of dislocations, the primary plasticity carrier within the crystal lattice. Consequently, an increase in the number of such defects amplifies strength but sacrifices ductility- an undesired effect that undermines the stability of engineering systems operating under conditions that generate additional defects, such as irradiation. In this study, we present experimental evidence of defect-driven plasticity in proton-irradiated nanotwinned Cu through *in-situ* nano-tensile testing. Contrary to conventional radiation hardening, our results demonstrate that radiation-induced defects can facilitate softening and improve ductility. This is achieved by intentionally disturbing interfacial coherency through radiation-induced defects, where local lattice discontinuities serve as dislocation nucleation sites. Furthermore, these discontinuities are readily eliminated by partial dislocations gliding along twin boundaries, thereby limiting the extent of radiation hardening.

# A VARIABLE FLOW STRESS SLIP-LINE MODEL AND EXPERIMENTAL VALIDATION FOR MACHINING PROCESSES

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**Abstract -** Classical slip-line models and analyses of metal cutting have laid the groundwork for fundamental understanding of chip formation and tool–chip interaction, and the shear-zone effects impacting and stress and temperature fields in the primary and secondary deformation zones, primarily focusing on machining performance predictions in terms of tool-wear/tool-life, chip-form/chip breakability and power consumption in machining. These insights led to the development of mechanics-based predictive models for machining with cutting tools offering improved chip-control geometries, tool material grades and coatings. Subsequently developed updated slip-line models considered rounded cutting edge (or edge geometry) involving a tertiary deformation zone representing the rounded cutting-edge enabling prediction of tribological conditions around the rounded cutting edge and their effects on machining performance.

This study presents an updated slip-line model with experimental investigation to validate the updated slip-line model for machining with rounded cutting-edge restricted contact grooved tools and to quantify the effect of groove geometry under controlled orthogonal tests. The analytical framework of the proposed model accounts for varying flow stress properties to include the effects of strains, strain-rates, and temperatures in the predictive model. The model was first validated using the set of 20 orthogonal cutting tests to establish its predictive capability for resultant cutting forces. Complementary validation was then carried out through 3 controlled turning experiments, focusing on chip thickness and chip up-curl radius to assess the model's ability to capture chip geometry characteristics.

Overall, the experiments validate the updated slip-line model for machining with rounded cutting-edge restricted contact grooved tools for both qualitatively (trends in geometry and forces with edge radius) and quantitatively (low prediction errors for key outputs) and corroborate the predicted role of edge roundness and secondary rake features on chip flow and cutting mechanics. Future research should focus on extending the validated slip-line framework by integrating artificial intelligence (AI) techniques with traditional plasticity-based modeling. Combining mechanics-based slip-line plasticity theory with AI-assisted model calibration would enable hybrid predictive tools that retain the physical interpretability of slip-line fields while leveraging large experimental and simulation datasets. Such integration could also facilitate real-time adaptive modeling of chip formation, advancing both the scientific understanding and industrial application of machining process optimization.

# PLASTIC BEHAVIOR OF REFRACTORY HIGH ENTROPY ALLOYS FROM NANOSCALE PERSPECTIVE

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**ABSTRACT –** The plastic deformation of refractory high-entropy alloys (RHEAs) is characterized by an intriguing yet challenging dichotomy: exceptional high-temperature strength often coexists with limited room-temperature ductility. A significant challenge arises when RHEAs are subjected to high strain rate loadings, such as shock or explosive impacts. Many metallic materials experience a drastic reduction in ductility in these scenarios. This embrittlement not only compromises material performance but also poses serious risks to the safety and integrity of engineering systems during shock events. To ensure the reliability of RHEAs in extreme environments, this study investigates their shock response through molecular dynamics simulations. The research aims to elucidate the underlying deformation mechanisms and evaluate the shock strength of RHEAs under high-strain-rate loading. Additionally, the effects of elemental addition and concentration fluctuations on the material properties are systematically examined to provide insights into the composition-property relationships based on density functional theory. These findings contribute to a deeper understanding of the dynamic performance of RHEAs and offer guidance for the design of advanced materials suited for extreme conditions.

# MATAL FATIGUE AND CYCLIC PLASTICITY: FROM A MACROSCOPIC PERSPECTIVE

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**ABSTRACT –** Metal fatigue is undoubtfully related to cyclic plasticity or plastic strain energy but the relationship is not straightforward. The current talk will be limited to cyclic plastic deformation and fatigue at macroscopic continuum scale with a focus on multiaxial fatigue modeling of a metal with different microstructures. Fatigue behavior is sensitive to microstructures and an identical material with different microstructures will have different material constants in a fatigue model. As a result, a great effort is needed to experimentally determine the material constants for the engineering materials requiring various processes and heat treatments. An ideal fatigue parameter would have material constants dependent on the material with little or no dependence on its microstructures. To explore such a possibility, experimental observations were made on an oxygen-free high conductivity polycrystalline copper with various grain sizes and textures, a 1045 carbon steel after different heat treatments, and a 310S stainless steel with different microstructures under combined axial-torsion loading. Several multiaxial fatigue models developed and validated over the last 50 years will be discussed for their pros and cons in general and based on the experimental results. It is observed that a multiaxial fatigue parameter should include the plastic strain energy directly or indirectly in order to properly model the effect of microstructures of a material. Plastic deformation can be very small at high cycle fatigue and the sensitivity of fatigue life to small plastic deformation requires a reliable and accurate cyclic plasticity model. Discussion will be extended to the use of loading cycles as the measure of fatigue life for general variable amplitude multiaxial loading. Experiences in multiaxial fatigue modeling will be shared and discussed together with some unusual fatigue phenomena observed under pure shear loading.

# ON THE MECHANICAL PROPERTY DEGRADATION OF POST-IRRADIATED U-MO ALLOYS

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**ABSTRACT –**The four-point bending experimental results clearly demonstrate that the irradiated U-Mo alloy exhibits substantial reductions in both effective Young's modulus and strength. During irradiation, the continuous formation and accumulation of fission gas bubbles (FGBs) at the grain boundaries contribute significantly to this degradation. Moreover, irradiation-induced damage can lead to further weakening of the U-Mo alloy skeleton. In this study, a multiscale numerical modeling approach is employed to investigate the mechanical degradation behavior of post-irradiated U-Mo alloy. At the microscale, the representative volume element (RVE) models for post-irradiated U-10Mo fuels including the bubble-contained region and no-bubble region are established. Simulations based on Continuum Damage Mechanics (CDM) theory are performed to model tensile tests. The results highlight that the strength degradation and fracture strain reduction of the U-Mo alloy skeleton in the bubble-contained region play a critical role in the macroscale embrittlement and strength loss. At the macroscale, four-point bending finite element models are used to identify the Young's modulus and strength of the irradiated U-Mo alloy skeleton. Finally, this study proposes quantitative models for the Young's modulus and strength degradation of irradiated U-Mo alloy skeleton, providing a critical basis for the safety evaluation of fuel elements and assemblies.

# INTERPRETABLE MACHINE LEARNING FOR PREDICTING TENSILE TWINNING AND REVEALING MICROSTRUCTURAL INFLUENCES IN PURE MG

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**ABSTRACT –** Tensile twinning plays a pivotal role in the plastic deformation of magnesium alloys, and its nucleation is governed by the coupling of multiple microstructural factors. Focusing on pure Mg, we combine electron backscatter diffraction (EBSD) with machine learning to develop a predictive model that captures multivariate interactions controlling tensile twinning. Thirty-four microstructural descriptors were extracted, an Extreme Gradient Boosting (XGBoost) classifier was trained on 5669 grains strained to 1%, and the model was interpreted using Shapley Additive Explanations (SHAP). The analysis reveals that grain size, the Schmid factor (SF) for slip, grain morphology, and neighboring grain attributes significantly influence tensile twin nucleation. Twinning is favored in large, irregularly shaped grains and in grains located within neighborhoods that provide poor strain accommodation. Moreover, twinning in low-SF grains is not anomalous and can be explained by grain boundary complexity that elevates local strain and facilitates local stress accumulation, thereby promoting twinning nucleation. External validation on AZ31 and GW93 alloys confirms strong predictive performance and transferability across distinct Mg alloy systems. This study provides data-driven insight into the nucleation of tensile twins in Mg and establishes a practical framework for microstructure design and deformation control in the development of high-performance magnesium alloys.

# A NEURAL NETWORK FRAMEWORK FOR THERMOVISCOPLASTICITY

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**ABSTRACT –** Although much attention is given to isothermal, rate-independent models of plasticity, many high-consequence performance assessments involve viscoplastic processes that generate substantial heat. In fact the materials may transit from a nearly isothermal, rate-independent regime to viscous, temperature-dependent regime, which makes modeling more challenging. In this work we develop a machine learning framework for modeling general temperature-dependent, rate-dependent inelastic processes firmly based on physical principles including the second law of thermodynamics and coordinate equivariance. These embedded properties are enabled by a number of architectural innovations in the structure and training of the potential-based neural ordinary differential equation framework. The resulting neural network models are capable of representing a wide spectrum of rate and temperature-dependence ranging from isothermal, rate-independent elastic-plastic phenomenology to rate-dependent fully viscous inelastic behavior, as we demonstrate. We also show the framework is capable of modeling complex microstructural inelasticity and predicting the conversion of plastic work to heating when calibrated to stress-temperature observations.

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# EXPERIMENTAL AND THEORETICAL STUDY ON TEMPERATURE-DEPENDENT RATCHETTING-FATIGUE INTERACTION OF EXTRUDED AZ31 MAGNESIUM ALLOYM ALLOY

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**ABSTRACT –** In this presentation, a detailed experimental investigation on the uniaxial ratchetting-fatigue interaction of extruded AZ31 Mg alloy is first conducted, including the macroscopic tests at room and elevated temperatures (i.e., 25°C, 100°C, 150°C, 200°C and 250°C) and with various stress levels by addressing the activation of single or multiple plastic deformation mechanisms (i.e., dislocation slipping, twinning, and detwinning), and necessary microscopic observations supporting a mechanistic explanation for the complex ratchetting and corresponding fatigue failure of the alloy. Based on the microscopic and macroscopic experimental results, a new multi-mechanism damage-coupled constitutive model is then proposed to reproduce the whole-life ratchetting and predict the fatigue life of the AZ31 Mg alloy. During the construction of damage coupled constitutive model, a macroscopic multi-mechanism elastoplastic constitutive model is newly developed at first by considering the dislocation slipping and twinning/detwinning-induced plastic deformations, respectively, in the framework of small deformation; then, based on the observed characteristics of damage evolution at different temperatures and with various stress levels, a damage-coupled constitutive model is proposed by extending the developed multi-mechanism constitutive model within the framework of continuum damage mechanics, by considering pure fatigue damage and an additional ratchetting damage. This model gains a reasonable prediction to the whole-life ratchetting and fatigue life of the AZ31 Mg alloy at different temperatures, thus provides a theoretical guidance for the anti-fatigue design and safety assessment of Mg alloy components.

# THE EFFECT OF AN ATOMIC HYDROGEN ON THE KINK MIGRATION IN A <111>{110} SCREW DISLOCATION IN BCC TUNGSTEN: ATOMISTIC STUDY

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**ABSTRACT –** Tungsten (W) exhibits exceptional physical properties, including a high melting point, radiation resistance, and excellent thermal conductivity, making it a highly attractive plasma-facing material. However, concerns exist about hydrogen-rich environments of fusion reactors that can cause material degradation. As solute strengthening mechanism explains, hydrogen as a solute can hinder dislocation motion by dragging or pinning it. In contrast, hydrogen-induced softening can occur as a result of an increased dislocation nucleation rate or an enhanced kink migration rate. In this study, we investigate the kink migration energy barrier for different hydrogen positions around a single screw dislocation, varying applied stress, using molecular dynamics simulation. Notably, the minimum energy path results for each hydrogen location show that there are certain positions where the energy barrier of kink migration is reduced, while other spots show an increased energy barrier. These opposite behaviors are discussed from the perspective of hydrogen-enhanced localized plasticity.

# ATOMISTIC STUDIES OF CUMULATIVE IRRADIATION DAMAGES IN SINGLE-CRYSTILLINE TUNGSTEN AND EVOLUTION OF SECONDARY DEFECTS

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**ABSTRACT –** Tungsten is a leading candidate for the plasma facing material due to its outstanding thermal and irradiation tolerance, withstanding extreme environments in fusion divertors (e.g., T >1000 K, heat fluxes of 1–20 $MW \cdot m^{-2}$, and ~14 MeV neutrons). To investigate the irradiation defect behavior in tungsten, we invoked a series of recoil atoms cumulatively to mimic neutron irradiation to the plasma facing material using molecular dynamics simulations. As irradiation accumulated, it was observed that prismatic dislocation loops of several different types were created and the preferred types depend on the loop size and the defect source, either vacancies or interstitials. It was also prevalent to form complex sessile dislocation structures. This variation and population in dislocations was not observed when the sample was irradiated one time with the same amount of net excessive energy. The continuous irradiation with smaller amount of energy is more effective to generate various irradiation damages. We also suggest a rotation or realignment mechanism of a dislocation loop, which could unveil the discrepancy between simulations and experiments regarding the vacancy-loop character.

# FULL-FIELD ANALYSES OF PLASTICITY AND VOID GROWTH IN MATERIALS DEFORMING BY SLIP AND TWINNING

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**ABSTRACT –** This paper demonstrates the full-field finite element analyses of plasticity and void growth in metallic materials deforming by slip and twinning, specifically the effect of model geometry on the deformation response of single and multi-crystals. The simulations employ a rate-dependent crystal plasticity model that incorporates both slip and twinning deformation mechanisms. It accounts for the spatially non-uniform appearance of new twin-related orientation, hardening due to slip–twin interactions, and modified properties of the twinned crystal. We use a probabilistic twin-volume-consistent scheme allowing parent and twinned orientations to coexist within the twinning domain and accounting for the volume effect of twins in the simulations. The CPFE implementation, together with the reorientation scheme, is performed using the AceGen package—a tool of automatic differentiation enabling us to obtain the consistent tangent operator and computationally efficient code. Simulation results are compared with experimental data. Two examples are used. First, assuming deformation by slip only, we analyse a multicrystalline aluminum sample with four intentionally made cylindrical holes. The strain field obtained by DIC as well as lattice rotation found by EBSD are compared with CPFE predictions, to demonstrate the effect of a void on the microstructure evolution. The second example deconvolutes the interaction of slip, twinning, and notch on the deformation response of an austenitic manganese (Hadfield) steel [1]. Limited experiments on single-crystal dog-bone and single-edge notch specimens, with two crystal orientations, are conducted to aid the simulation. Several features of the experimental observations are accurately captured in the simulations including the observed orientation-dependent asymmetric deformation of the notch in single-edge notch specimen.

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**REFERENCE**
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# SEQUENTIAL DEEP OPERATOR NEURAL NETWORKS FOR PLASTIC AND THERMO-VISCOPLASTIC MATERIAL BEHAVIOR

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**ABSTRACT–**Deep Operator Networks (DeepONet) are among the most advanced artificial neural network architectures, which approximate linear and nonlinear solution operators by taking parametric functions (infinite-dimensional objects) as inputs and mapping them to full partial differential equation (PDE) solution fields on a computational grid without training or transfer learning. Building on this idea, the Sequential Deep Operator (S-DeepONet) and the newly introduced Sequential Neural Operator Transformer (S-NOT) are particularly effective for path-dependent plasticity and path and rate-dependent viscoplasticity driven by transient loadings. We present recent variants of these architectures that accurately predict full stress and plastic-strain fields for real-world problems—from highly nonlinear thermo-viscoplastic multiphysics in steel solidification within continuous-casting molds to plastic deformation in complex 2D and 3D domains. Once properly trained, the models can accurately predict multiple solution fields up to four orders of magnitude faster than conventional non-linear finite-element analyses, enabling rapid design iteration, optimization, inverse and sensitivity studies, uncertainty quantification, and online control with data assimilation. These capabilities position operator-learning surrogates as practical engines for digital twins and other iterative workflows across engineering and science.

# AI-ASSISTED UNVEILING MICROMECHANICAL FAILURE MECHANISMS IN METAL MATRIX COMPOSITE: IN SITU ACOUSIC EMISSION AND NEUTRON DIFFRACTION

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**ABSTRACT-** This study investigates the micromechanical damage evolution in a particle-reinforced $B_4C$/AA6061 composite through combined in situ acoustic emission (AE), neutron diffraction (NED), and scanning electron microscopy (SEM) during tensile loading. AE monitoring captured transient events that were classified through data-driven analysis of frequency–energy signatures, enabling distinction among matrix plasticity, interfacial decohesion, and particle fracture. NED measurements revealed phase-specific lattice strain evolution in both the aluminum matrix and the $B_4C$ reinforcement, while in situ SEM observations confirmed localized cracking and separation along particle–matrix interfaces. The concurrent interpretation of AE and NED data revealed that the onset of interfacial decohesion and particle rupture coincides with the relaxation of lattice strain in the $B_4C$ phase, demonstrating that stress redistribution originates from interfacial instability rather than matrix yielding alone. This coupling between microdamage and stress transfer indicates that progressive debonding and particle cracking relieve mechanical constraint on the matrix, facilitating strain localization and accelerating macroscopic fracture. These results provide direct mechanistic evidence that interface-driven stress redistribution governs plastic compatibility and damage accumulation in metallic systems with heterogeneous particle reinforcement.

# HYDROGEN AFFECTED FRACTURE TOUGHNESS OF X52 PIPELINE STEEL WITH ITS MECHANISM OF PLASTICITY DEGRADATION

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**ABSTRACT –** Hydrogen blended traditional oil and gas was considered to be a potential way to reduce the greenhouse emission. However, hydrogen absorption into pipeline steel will threaten the structural integrity due to the effect of hydrogen embrittlement, particularly in the presence of stress concentrations. This work investigated the hydrogen effect on the fracture toughness of X552 pipeline steel that was extracted from in-service pipeline system of Jemena WSGG in Australia. In-situ electrochemical hydrogen charging device was built to simulate the hydrogen adsorption into specimens during three-point bend tests that were conducted as per the ASTM E1820 standard. The specimens with different initial fatigue precrack lengths were used to determine the effect of constraint on the crack propagation in air and hydrogen. Fracture surface and crack tip plasticity were observed using a scanning electron microscope (SEM) and an electron backscattering diffraction (EBSD). Compared to the results in air, the presence of hydrogen remarkably decreased the peak force and accelerated the crack propagation, resulting in the decrease in fracture toughness i.e., crack tip open displacement. However, this degradation was not significantly influenced by the constraints of crack and the charging current density. The crack tip blunt phenomenon was absent in hydrogen and the fracture mode during crack propagation transited from ductile micro-voids coalescence to brittle quasi-cleavage fracture. The hydrogen notably limited the plastic deformation zone at crack tips mainly because of the hydrogen enhanced transgranular decohesion.

# DATA-DRIVEN APPROACH TO DISLOCATION MEDIATED PLASTICITY

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**ABSTRACT –** In this paper, a data-driven approach to dislocation-mediated plasticity is presented. Within a recently proposed thermodynamic dislocation theory incorporating configurational entropy and effective disorder temperature, we analyze mechanical test data for various metals under diverse loading conditions and use large scale least squares method to determine the parameters of the theory. This approach enables accurate predictions of stress-strain behavior and temperature evolution for fcc and bcc crystals under simple shear, tension/compression, and torsion over a broad range of strain rates and temperatures, where traditional crystal plasticity models fail. Furthermore, it captures size and Bauschinger effects, work hardening, and thermal softening. Next, we model notch-like defects to explore shear band instabilities, with predictions accurately matching Marchand and Duffy's experiments over a broad range of strain rates and temperatures. Finally, we apply this approach to the brittle-ductile transition, predicting fracture toughness in tungsten across a range of temperatures – consistent with the experimental findings of Gumbsch.

**Keywords:** Data-driven, Dislocations, Plasticity, Effective temperature, Strain rate

# COMBINATORIAL EXPERIMENTAL STUDY ON THE MECHANICAL BEHAVIOR OF Mo–Nb–Ti AND Ta–Nb–Ti COMPLEX-CONCENTRATED ALLOY THIN FILMS

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**ABSTRACT –** Refractory complex-concentrated alloys (RCCAs) exhibit diverse strengthening mechanisms arising from atomic size mismatch, electronic structure, and microstructural evolution. In this study, we employed a combinatorial experimental approach to systematically investigate Mo–Nb–Ti and Ta–Nb–Ti thin-film alloy libraries fabricated by magnetron co-sputtering at room temperature and 773 K. Composition-dependent X-ray diffraction and electron microscopy showed that Mo–Nb–Ti alloys retained ultrafine grain structures with minimal temperature sensitivity, whereas Ta–Nb–Ti alloys underwent significant grain coarsening at elevated temperatures. Nanoindentation mapping further revealed that Mo–Nb–Ti consistently exhibited higher hardness, stiffness, and resistance to plastic deformation, arising from the combined effects of suppressed grain growth and severe lattice distortion. To complement these experimental findings, molecular dynamics simulations were performed, which showed that Mo–Nb–Ti develops pronounced short-range order (SRO), while Ta–Nb–Ti exhibits only weak ordering, remaining close to a random distribution. This contrast in SRO provides a mechanistic explanation for the enhanced solid-solution strengthening observed in Mo–Nb–Ti compared to the grain-size-sensitive behavior of Ta–Nb–Ti. Taken together, this integrated experimental–computational framework links atomic descriptors, microstructural stability, and strengthening mechanisms, providing guidelines for the design of next-generation RCCAs with superior thermal and mechanical reliability.

# CONSTITUTIVE MODELING FOR MULTI-SCALE SIMULATION OF BUMPLESS HYBRID BONDING PROCESSES IN SEMICONDUCTOR DIE STACKING FOR HIGH-PERFORMANCE COMPUTING SYSTEM

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**ABSTRACT-** Semiconductors are playing a growing role in large-scale computing and data processing, driven by System-in-Package (SiP) technologies like chiplets, TSVs, interposers, and heterogeneous integration. Among these, bumpless hybrid bonding stands out by removing micro-bumps, enabling denser die stacking, more I/O, and better thermal diffusion. However, translating these designs into manufacturable products remains difficult, as optimal designs are often hard to fabricate. Thus, understanding how process parameters influence bonding is essential for robust implementation. A precise constitutive model describing Cu behavior is key. In hybrid bonding, Cu is surrounded by dielectrics, and thermal expansion brings Cu surfaces into contact. Surface roughness creates voids, which must be filled to ensure reliable bonding. Atomic flux, driven by potential differences, fills these voids and is influenced by Cu slip behavior. This study presents a constitutive model capturing thermal, mechanical, and chemical effects in the bonding process. Simulations show that interface bonding at the microscale is temperature-dependent, while void size at the nanoscale is more affected by potential difference, indicating scale-dependent factors. Cu grain orientation also strongly affects initial bonding formation. All results were experimentally validated using a crystal plasticity framework. Future work will explore post-bonding annealing effects.

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# UNDERSTANDING ANISOTROPIC PLASTICITY IN POLYCRYSTALLIN E METALS THROUGH MICROSTRUCTURE-PROPERTY RELATIONSHIPS

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**ABSTRACT –** The mechanical properties of metals are intrinsically governed by their microstructural characteristics, which evolve during thermo-mechanical processing. Therefore, understanding the interrelationships among processing, microstructure, and mechanical properties is essential for optimizing material design and enhancing the performance of final products in application. In this presentation, anisotropic plasticity—one of the key features of polycrystalline metals during deformation—is examined in relation to various microstructural characteristics, such as the interactions of dislocations with obstacles at both single-crystal and polycrystal scales. In particular, anisotropy in plastic deformation, often described by quadratic or non-quadratic anisotropic yield functions, is correlated with crystal plasticity through different homogenization schemes. Furthermore, path-dependent anisotropic hardening, typically formulated through kinematic or distortional hardening models, is interpreted using a simplified back stress model based on the concept of dislocation pile-up polarization. Finally, examples of complex plastic behavior under loading-path changes in steels and lightweight alloys are presented, demonstrating constitutive modeling approaches and finite element simulations.

# A HIGH-THROUGHPUT APPROACH TO ACQUIRE TENSILE AND COMPRESSIVE RESPONSES OF THIN FILMS AT ELEVATED TEMPERATURES

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**ABSTRACT-** Considering the numerous possibilities in creating alloy materials, alloy exploration persists as a notable subject of interest, driving efforts in the field to develop novel experimental methodologies with the aim to ensure their functionality. Following the progressive advancement in micro/nano technologies, a key breakthrough associated with testing at elevated temperatures remains in the pursuit of refining thin film characterization efficiency for alloy exploration. Although the high temperature (HT) nanoindentation experiment has been introduced, establishing techniques to attain recognition as the high-throughput tensile counterpart of the nanoindentation experiment persist as an underexplored area to date. Our work demonstrates a one-of-a-kind high-throughput approach to extract both tensile and compressive responses of thin film materials beyond room and into elevated temperatures. With the use of a single commercialized InSEM HT nanoindenter unit, HT membrane deflection experiments – a high-throughput technique developed for assessing thin film tensile responses – are conducted in conjunction with HT nanoindentation experiments. The potential of this high-throughput approach is highlighted through assessing the distinctive temperature and stress-dependent phase transformation behavior of shape memory alloy thin films. The prospective use of this methodology holds considerable promise for assessing the high temperature functionality of thin film materials such as high-temperature SMAs and high entropy alloys.

# ACHIEVING HIGH STRENGTH IN 6061 ALUMINUM ALLOY THIN FILMS THROUGH INTERSTITIAL CARBON INCORPORATION

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**ABSTRACT –** 6061 aluminum alloy (6061AA) is a heat-treatable Al-Mg-Si alloy known for its excellent formability, corrosion resistance, and moderate tensile strength. This study aims to enhance the strength of 6061AA while maintaining its inherent advantages by fabricating 6061AA-carbon (6061AA-C) thin films through co-sputter deposition of 6061AA and graphite targets. Microstructural analysis showed that the carbon atoms were uniformly distributed within the aluminum alloy matrix through this fabrication technique. Subsequently tensile tests were conducted using a custom-built micro-tensile tester. The 6061AA-C films exhibited an increased tensile strength while maintaining its failure strain compared to pure 6061AA films. However, it was demonstrated that excessive carbon content resulted in a decrease in both tensile strength and ductility. This result can be explained by the different strengthening mechanisms occurring in the co-sputtered 6061AA-C thin films: the aluminum alloy undergoes substitutional solid solution strengthening, while the carbon addition induces interstitial solid solution strengthening and grain refinement.

The annealing effect of 6061AA-C thin films was also investigated. Precipitate formation and microcrack annihilation were observed in the films annealed at 300℃, thereby overcoming the strength-ductility trade-off. Consequently, this study demonstrates that C incorporation into the 6061 aluminum alloy system effectively improves the mechanical properties.

# RECENT ADVANCES IN SEVERE PLASTIC DEFORMATIONS, STRAIN-INDUCED PHASE TRANSFORMATIONS, AND MICROSTRUCTURE EVOLUTION AT HIGH PRESSURE

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**ABSTRACT-** Plastic strain-induced phase transformations (PTs) during compression in diamond anvil cell (DAC) and torsion in rotational DAC (RDAC) require entirely different thermodynamic and kinetic treatments and experimental characterization [1] than pressure-induced PTs. Five topics will be covered.

1. It was found [2-4] for severely predeformed Zr that (a) crystallite size and dislocation density in both phases in a single-phase state, the minimum pressure for the strain-induced α-ω PT, and the pressure-dependent yield strength of ω-Zr are independent of plastic strain tensor $\boldsymbol{\varepsilon}_p$ and strain path $\boldsymbol{\varepsilon}_p^{path}$; (b) crystallite size and dislocation density in ω-Zr and (with some outliners) α-Zr during PT are independent of pressure, $\boldsymbol{\varepsilon}_p$ , and $\boldsymbol{\varepsilon}_p^{path}$, and depend on the volume fraction of the high-pressure phase only. Obtained results can be used to find economic ways of grain refinement during PT and obtain nanocomposite with optimal properties.

2. Coupled experimental-analytical-computational approaches, utilizing synchrotron X-ray diffraction, to solve an inverse problem and find fields of all components of stress and plastic strain tensors and friction rules before, during, and after α-ω PT in Zr, are developed [5,6]. The kinetics of strain-induced PT is described in the whole sample.

3. We revealed in situ various unexpected plastic strain-induced PT phenomena in Si [7]. Thus, for 100 nm Si, strain-induced PT Si-I→Si-II initiates at 0.3 GPa versus 16.2 GPa under hydrostatic conditions; for 30 nm Si, it is 6.1 GPa versus ∞ since it does not occur. For 100 nm Si-I→Si-III, it is 0.6 GPa vs. ∞. The predicted theoretical correlation between the direct and inverse Hall-Petch effect of the grain size on the yield strength and the minimum pressure for strain-induced PT is confirmed. Retaining Si-II at ambient pressure and obtaining reverse Si-II→Si-I PT are achieved for the first time. Retaining single-phase Si III is achieved at much more economic conditions than the currently known. Pressure in the small regions of Si II and III is 5-7 GPa higher than the applied pressure to Si I. All these results strongly support nucleation at the tip of dislocation pileup during strain-induced PTs, predicted theoretically.

4. A new theory is developed for the plastic strain-induced olivine-spinel PT in a shear band, which resolves multiple existing puzzles in the mechanism of deep-focus earthquakes [8]. Conceptual experimental confirmation is obtained [9].

5. The first real-time experimental results on the behavior of Fe-7%Mn alloy in the dynamic RDAC for the strain rates up to $2\times10^3$/s were obtained, and new rules are revealed.

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# A DISLOCATION DENSITY-BASED CP-MPF UNIFIED FRACTURE MODEL OF NBSX ACROSS WIDE TEMPERATURE RANGES

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**ABSTRACT -** Nickel-based single crystal superalloys (NBSX) are widely used in turbine blades of aero-engines, operating under complex service environments with large temperature variations. Their deformation and damage mechanisms vary significantly with temperature, while few models are capable of capturing their fracture behavior over a wide temperature range. In this work, a dislocation density-based crystal plasticity multi-phase field fracture model is proposed to describe the tensile fracture behavior of NBSX from room to high temperatures. Four {111} slip planes with corresponding γ/γ' two-phase configurations serve as the fundamental microstructural constituents in the damage model, each governed by distinct phase field variables. In the γ′ phase, phase field variables describe the damage associated with cleavage and shear, while in the γ phase they reflect the damage induced by void evolution and shear. Then, the constitutive equations of both phases are derived within the thermodynamic framework by incorporating dislocation mechanisms. A comprehensive dislocation density evolution framework is developed to address the temperature-dependent deformation and damage behaviors. Dislocation mechanisms such as Kear-Wilsdorf locks, anti-phase boundary shearing, stacking fault shearing, Orowan bypassing, dislocation-loop shearing, dislocation climb, and dislocation annihilation are all incorporated in the model. Different microdamage modes are governed by the distinct dislocation mechanisms. Cleavage in the γ′ phase is driven by cross-slip dislocation density; void damage in the γ phase is controlled by edge dislocation climb and dislocation loop density; shear damage in both phases is determined by their respective edge and screw dislocation densities. On this basis, a unified fracture model in terms of crystal plasticity multi-phase field method is developed. An explicit numerical scheme is implemented to simulate the damage evolution process, and the model successfully predicts the tensile fracture and crack propagation of NBSX with different crystallographic orientations over a wide temperature range. This work rigorously incorporates temperature-dependent dislocation-based deformation and damage mechanisms into a thermodynamically consistent framework, enabling accurate and physically meaningful predictions of NBSX failure. The model offers new insights into fracture modeling of NBSX and provides a foundation for studying temperature-dependent failure phenomena such as thermomechanical fatigue.

# NEURAL NETWORK BASED MESOSCALE PLASTICITY MODEL FOR HCP MATERIAL WITH SLIP AND TWINNING MECHANISMS

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**ABSTRACT-** Neural network shows significant advantages in the complex plastic deformation modelling, especially for the surrogate model development at mesoscale. However, the available neural network based method is only applied to the materials dominant by slip mechanism. In the current work, a new neural network based mesoscale model, Multi-Mechanisms recurrent neural network model (MM-RNN) is proposed considering multiple slip and twinning deformation mechanisms in HCP material for the first time. To consider the twinning activity loading/orientation dependence and enhance the neural network surrogate model's prediction ability, the MM-RNN's architecture is designed with several subnetworks for twinning volume fraction, deformation activities, stress and texture predictions, where the subnetworks are organized for information flow driven by the physical relations from the crystal plasticity. Specifically, the twinning-RNN subnetwork cooperates a classifier for the twinning polarity, and its prediction feeds into deformation activity-RNN and stress RNN. The current architecture design with multiple subnetworks not only captures the complex deformation behaviors from both the mechanisms and response levels but also enhance the interpolation and reduce the depth of the model. The proposed MM-RNN model is further applied to different textures predictions with transfer learning which also illustrates good generalization ability.

# CONSTITUTIVE MODELING OF SHAPE MEMORY POLYMERS

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**ABSTRACT –** This paper discusses the historical development of constitutive modeling for thermoset shape memory polymers (SMPs). Since the invention of SMPs in the 1980s, modeling approaches have evolved significantly—from simple rheological models to advanced physics-informed machine learning techniques. In the early stages, research primarily focused on phenomenological descriptions of the shape memory effect, with rheological and phase evolution law-based models being the most common. As understanding deepened, the shape memory effect was increasingly interpreted through the lens of structural relaxation, leading to the development of models grounded in visco-plasto-elasticity theory. With advances in computational power, molecular dynamics simulations emerged as a valuable tool for capturing the stress-strain behavior of thermoset SMPs at the molecular level. More recently, data-driven approaches, particularly those leveraging machine learning, have gained traction. The latest progression in this area is the integration of physics-informed machine learning models, which have significantly improved prediction accuracy. This presentation systematically discusses the evolution of these modeling approaches, compares their respective strengths and limitations, and offers insights into future research directions.

# MECHANICAL RESPONSE-MICROSTRUCTURE-CRACKING RELATION OF POWDER METALLURGY NI-BASED SUPERALLOYS UNDER LOW CYCLE FATIGUE

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**ABSTRACT-** Powder metallurgy superalloys are critical for aerospace turbine disks, with low cycle fatigue (LCF) as a primary failure mode. We first introduce the state-of-the-art of LCF of Powder metallurgy superalloys. It is found that previous LCF studies often overlooked grain boundary properties and crack path-microstructure links, while simulations focused on lifetime prediction disregarding stress/strain/energy field effects on cracking. Addressing this, LCF experiments under various strain amplitudes are studied in the present work. Hardening, softening, and tension-compression asymmetry during fatigue, as well as systematically characterization of dislocations, stacking faults, grains, boundaries, cracks, and fracture surfaces are analyzed. Crystal plasticity finite element (CPFE) simulations incorporating experimental microstructures revealed correlations between stress, strain, and energy fields and high-risk cracking locations, linking microstructure, damage, and mechanical response. Results show grain orientation stability with increasing strain amplitude, but recrystallization at initial twin boundaries significantly increased high-angle grain boundary (HAGB) length; Σ3 twin boundaries (mainly {111} coherent) constituted nearly half of HAGBs. Geometrically necessary dislocation (GND) density increased with strain amplitude. Cracks initiated at the surface; early main cracks propagated perpendicularly, while later branch cracks emerged at triple junctions along ordinary HAGBs. When encountering a parallel Σ3 twin boundary, branch crack tips tended to deflect or arrest. Fracture surface characteristics varied distinctively with strain amplitude in initiation, propagation, and final fracture zones. CPFE-simulated hysteresis loops matched experiments; cumulative plastic slip and plastic energy dissipation better captured crack paths than equivalent stress/strain. Observed hardening, softening, and reverse Bauschinger effects were attributed to twin-induced recrystallization, dislocation kinematic hardening, and isotropic hardening mechanisms.

# MULTISCALE DEFORMATION MECHANISMS IN HIGH-ENTROPY ALLOYS FOR ENHANCED STRENGTH AND DUCTILITY

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**ABSTRACT –** High-entropy alloys (HEAs), or multi-principal element alloys, exhibit an exceptional synergy of strength and ductility, attributed to their pronounced lattice distortion and diverse deformation mechanisms. Precise prediction and assessment of these mechanisms and the resulting mechanical properties necessitate the development of advanced modeling and simulation approaches that account for the distinctive intrinsic characteristics of HEAs. This study presents: i) a discrete dislocation dynamics framework, augmented with random field theory and calibrated using high-resolution transmission electron microscopy, to elucidate the role of heterogeneous lattice strain in mediating complex dislocation interactions; ii) a cohesive multiscale modeling strategy that integrates atomistic simulations, discrete dislocation dynamics, and crystal plasticity finite element methods, facilitating the analysis of strain hardening behavior and the influence of cross-scale factors on plastic deformation; iii) a machine learning-assisted multistage design strategy for accelerating the development of dual-phase HEAs with optimized strength and ductility through precise control of phase composition and fraction. The outstanding strength–ductility combination in HEAs stems from dynamic phase transformations, coordinated deformation processes, and a hierarchical structural design, establishing a new paradigm for alloy development based on integrated multiscale theoretical models.

# AN ATOMICALLY INFORMED FINITE ELEMENT FRAMEWORK FOR LATTICE-DISTORTION-INDUCED STRAIN HARDENING IN HIGH-ENTROPY ALLOYS

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**ABSTRACT-** High-entropy alloys exhibit remarkable strain hardening behavior in contrast to traditional alloys, yet the quantitative understanding of their mechanical origin remains elusive in the literature. In this study, an atomically informed finite element framework is developed to investigate lattice-distortion-induced strain hardening in HEAs. A three-dimensional fractal function is proposed to theoretically describe lattice distortions, which is validated by high-resolution transmission electron microscopy. The distortion-dependent stress field across multiple scales is quantified by varying the scan size, and its influence on dislocation evolution is captured through a modified Kocks–Mecking model. By coupling the micrometer-scale stress field with mechanism-based plasticity theory in finite element simulations, the predicted stress–strain responses agree well with experimental data, particularly in yield strength and the early stages of plastic deformation. The quantitative contributions of different mechanisms to yield strength and strain hardening are clarified, highlighting severe lattice distortion and deformation twinning as key origins of the enhanced strain-hardening behavior in HEAs. This work establishes a mechanistic framework connecting atomic-scale lattice distortion to macroscopic mechanical response, thereby deepening the understanding of strain-hardening mechanisms in complex alloys.

# DETERMINING THE TAYLOR–QUINNEY COEFFICIENT AND ISOTHERMAL-TO-ADIABATIC TRANSITION FUNCTIONS FROM DYNAMIC IN-PLANE TORSION EXPERIMENTS

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**ABSTRACT –** Accurately quantifying the fraction of plastic work converted into heat is essential for reliable thermo-mechanical simulations of metallic components subjected to plastic deformation. In this study, experiments are carried out on DP800 sheet metal specimens at strain rates ranging from 0.001/s to 900/s. High strain rate in-plane torsion experiments are used for the first time to determine the Taylor-Quinney coefficient up to very large strains. To broaden the range of stress states and strain rates, additional uniaxial tension (UT), notched tension, as well as shear (SH) experiments are also performed. In all experiments, the surface strain fields are captured using a high-speed optical camera in conjunction with Digital Image Correlation (DIC). Simultaneously, the corresponding temperature fields are measured with an infrared high-speed camera. For torsion tests at the highest strain rate (900 $s^{-1}$) terminal surface temperatures up to 368°C are observed. A non-associated Hill'48 constitutive framework with modified Johnson Cook type of temperature and rate-dependent hardening law is used to perform coupled thermo-mechanical simulations. A novel strain rate, plastic strain and stress triaxiality dependent isothermal-to-adiabatic transition function is proposed to treat the temperature as an internal variable in purely mechanical simulations. This approach reduces computational cost by up to an order of magnitude compared to fully coupled thermo mechanical analyses, while maintaining a comparable level of accuracy.

# PATH-PLANNING FOR INDUCTION STRAIGHTENING PROCESS BASED ON REINFORCEMENT LEARNING APPROACH

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**ABSTRACT -** This paper presents an AI-driven methodology for optimizing the multi-energy fields (electro-thermal-mechanical) process of induction straightening. The method addresses the distinct challenges arising from the unique attributes of induction heating, notably its highly localized and transient temperature fields, which, while effective for distortion correction, can introduce complex and intense residual stress states. In industrial practice, a combined process—sequentially applying heating lines directly above the weld and on each flank—is commonly adopted. However, the optimal sequence and parameters for this combination lack a systematic design principle and are highly dependent on operator experience. To solve this, first, a physics-informed, fast sequential simulator is developed. It predicts the evolution of the stress-strain state at critical points by integrating material constitutive laws with thermal-mechanical analysis, while approximating angular distortion via a superposed inherent deformation approach. The model explicitly captures the distinct thermo-mechanical mechanisms of each mode: heating above the weld, while reducing distortion, tends to increase longitudinal tensile stress at the weld seam due to a secondary thermal cycle; conversely, heating on the flanks promotes stress release alongside its distortion-reduction effect. Second, the quest for an optimal heating sequence is formulated as a path-planning problem in a high-dimensional state space, defined by distortion metrics and residual stress values at various feature points. This problem is solved using a Deep Reinforcement Learning (DRL) algorithm, where the fast simulator serves as the environment for the agent to learn an optimal policy. The reward function is carefully designed to simultaneously minimize distortion and detrimental tensile stress. This approach effectively performs an inverse design of the subsurface thermal history, translating high-level performance goals (low stress, low distortion) back into an optimal sequence of induction heating parameters—the essential control variables governing the multi-physics process. Finally, the proposed methodology is validated through a case study on a T-shaped welded structure. The results demonstrate that this AI framework provides a principled method for designing multi-energy field forming processes, capable of discovering strategies that balance performance criteria more effectively than experiential trial-and-error methods.

# A THREE-DIMENSIONAL SHEAR TRANSFORMATION ZONE THEORY FOR GLASSY POLYMERS

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**ABSTRACT –** Developing constitutive models for the highly nonlinear behaviors of glassy polymers, such as yielding and strain hardening, is important for their engineering applications. Yielding is closely tied to nonequilibrium thermodynamics, often referred to as physical aging, while strain hardening is associated with the oriented microstructures of the polymer network, which further contribute to the Bauschinger effect in pre-deformed glassy polymers. To capture these nonlinear mechanical responses, we have developed a three-dimensional viscoplastic model grounded in shear transformation zone (STZ) theory, linking the plastic flow to the STZ microdynamics. The collective behavior of STZs is characterized by two statistical variables: the density and orientation tensor, both governed by first-order evolution equations. We established a conceptual relationship between these STZ variables and the plastic flow tensor by incorporating a prefactor that combines the amplitude of chain stretching with the angle between the driven stress and STZ orientation. Additionally, an effective temperature model has been integrated to capture nonequilibrium thermodynamics. The model was applied to quantitatively describe the stress responses of glassy polymers in uniaxial deformation and plane strain tests. The simulation results demonstrate that the model quantitatively captures physical aging under various thermal and mechanical conditions, as well as the Bauschinger effect, reflected in distinct stress responses of pre-deformed glassy polymers in opposite loading directions. This work extends the STZ model to the finite deformation three-dimensional condition, bridging the gap between the intricate microscopic mechanisms governing STZ transformation and the complex constitutive behaviors of glassy polymers.

# MICROSTRUCTURE-SENSITIVE CRYSTAL PLASTICITY AND PHASE-FIELD MODELING OF PLASTIC DEFORMATION, FRACTURE, RECRYSTALLIZATION IN MG ALLOYS

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**ABSTRACT –** The mechanical behavior of Mg alloys is governed by their strong crystallographic anisotropy and complex microstructure evolution involving dislocation slip, deformation twinning, and dynamic recrystallization. Understanding the interactions among these mechanisms is essential for designing high-strength and ductile Mg alloys. In this study, we develop a microstructure-sensitive coupled crystal plasticity and phase-field model within a finite strain framework to simulate the plastic deformation, fracture, and recrystallization processes in hexagonal close-packed Mg alloys. A dislocation-density-based crystal plasticity model is employed to capture the slip activities as well as the associated stress and strain heterogeneity among grains. The model is coupled with a multi-phase-field formulation that describes deformation twins, microcrack initiation, propagation, and recrystallization nucleation driven by stored energy and local stress concentration. By integrating these two frameworks, the model enables concurrent simulation of dislocation evolution, twin-twin interaction, damage accumulation, and grain structure refinement under monotonic and cyclic loading conditions. This study provides a unified modeling framework that bridges the microscale deformation mechanisms with macroscopic mechanical response. The insights obtained offer guidance for microstructure design strategies aimed at optimizing the strength–ductility balance and damage tolerance of Mg alloys.

# MESOSCALE MODELING ON IRRADITION HARDENING OF METALLIC MATERIALS

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**ABSTRACT –** Under the extreme multi-field coupling conditions involving complex stress, high temperature, and intense neutron irradiation, structural materials in nuclear reactors undergo mechanical property degradation such as irradiation hardening, creep, and embrittlement, which directly compromise the service life of reactors. At the microscopic level, the degradation of post-irradiation mechanical properties stems from the interactions between irradiation-induced defects (e.g., voids and dislocation loops) and intrinsic defects such as dislocations and grain boundaries. Therefore, this study focuses on the mesoscale models that bridge the microstructural evolution and macroscopic behavior, with an emphasis on developing crystal plasticity models to simulate and predict irradiation hardening. Taking tungsten—a plasma-facing material in fusion reactors—as an example, we have developed a crystal plasticity finite element model that incorporates the synergistic hardening law of voids and dislocation loops, as derived from dislocation dynamics (DD) simulations. Notably, the synergistic hardening law contains no adjustable parameters and is entirely based on DD simulations that capture the dynamic interactions between high-density defects and dislocations. These DD models themselves are founded on dislocation theory and molecular dynamics simulations, which reveal the underlying mechanisms of defect-induced obstacles to dislocation motion. The predicted irradiation responses from these mesoscale models show good agreement with various neutron irradiation experimental data, validating the models. Such modelling efforts enables quick evaluation of irradiation hardening and creep of irradiated materials.

# TAILORING MARTENSITIC TRANSFORMATION KINETICS IN $Co_{36.8}Ni_{39.2}Al_{24}$ HYPEREUTECTIC MEDIUM ENTROPY ALLOY THROUGH HEAT TREATMENT

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**ABSTRACT-** The strength-ductility paradox in high-entropy alloys can be resolved through precise regulation of deformation-induced martensitic transformation. This investigation systematically examines the microstructure-property relationship in a $Co_{36.8}Ni_{39.2}Al_{24}$ hypereutectic medium-entropy alloy (HMEA) subjected to isothermal annealing across a temperature range of 650-950 °C. Annealing at 650-950 °C facilitates complete reverse transformation of pre-existing martensitic phases within the B2 matrix. Notably, 800 °C annealing generates a high density of nanoscale ordered $L1_2$ precipitates with semi-coherent interfaces, whereas higher temperature treatments result in coarsened disordered FCC precipitates with incoherent interfaces. The specimen annealed at 800 °C achieves strength-ductility synergy, attributed to the elimination of pre-existing martensite and controlled transformation kinetics enabled by the $L1_2$ precipitates. These finely dispersed precipitates effectively regulate the martensitic transformation sequence, maintaining sustained work hardening. In contrast, incoherent FCC precipitates accelerate transformation saturation, diminishing the TRIP effect. The findings provide fundamental insights into precipitate-mediated transformation control and offer a viable strategy for designing high-performance transformation-induced plasticity high-entropy alloys.

# MICROSTRUCTURE AND PROPERTY CONTROL OF METALLIC MATERIALS VIA THERMOMECHANICAL-COUPLED INCREMENTAL FORMING

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**ABSTRACT –** Overcoming the trade-off between strength and ductility in metallic materials remains a significant challenge. This work introduces a novel approach employing thermomechanical-coupled incremental forming to simultaneously engineer dual-gradient structure of grain size and dislocation density. In 316L stainless steel, this approach yields an exceptional combination of ultrahigh ultimate tensile strength (~960 MPa) and considerable uniform elongation (~37.5%). The key breakthrough lies in the in-situ fragmentation of the passivation film into nano-oxides during processing, which effectively stabilize the nano-grain through pinning grain boundary. Microstructural analysis reveals coordinated deformation across multiple structural zones, transforming the material into a self-reinforcing system that integrates nanoscale stability with macroscopic deformability. Remarkably, this "nanoparticle-mediated grain boundary stabilization" concept demonstrates exceptional universality. we further applied this nanoparticle stabilization strategy to an Al-Mg-Sc-Zr system, demonstrating the generality of the approach for designing high-performance gradient materials across alloy systems. This work provides not only fundamental insights into gradient material deformation mechanisms but also a versatile pathway for designing advanced high-performance materials across different alloy systems.

# SHEAR-TAILORED MACROSCOPIC HETEROGENEOUS STRUCTURE DELIVERS EXCEPTIONAL SUPERPLASTICITY IN DUAL-PHASE TITANIUM ALLOYS

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**ABSTRACT –** Superplasticity in metallic materials is typically achieved through ultrafine equiaxed microstructures, which are commonly processed by severe plastic deformation (SPD) techniques. However, the limited scalability of SPD restricts its broader industrial application. Shear-mediated microstructural heterogeneity offers an industrially feasible alternative for accelerating microstructural refinement and promoting the formation of heterogeneous structures. In this study, the strong shear field associated with asymmetric rolling establishes a macroscopic surface-core gradient, where the intense shear near the roll-sample traction zones produce fine equiaxed grains, while the low-shear core regions retain elongated α laths containing abundant substructures. This shear-tailored heterogeneous structure supports exceptional superplasticity, with an elongation of 1205% at 775 °C and 1×10–3 s–1. During early deformation ($\varepsilon < 1.3$), the accumulated shear-stored energy promotes the continuous dynamic recrystallization of the elongated α laths, progressively converting the low-shear core into a stabilized equiaxed structure that sustains grain boundary sliding at large strains. Geometrically necessary dislocation (GND) analysis further revealed that the β phase became the primary carrier of plastic deformation at large strains, sustaining strain accommodation and delaying cavity formation and failure. Moreover, the Burgers orientation relationship (BOR) was well preserved throughout deformation, indicating coordinated α/β co-rotation and stable interface compatibility. Through the cooperation of shear-band-assisted grain refinement, GND-driven restoration, and BOR-

stabilized phase co-deformation, the alloy exhibits stable high-strain flow and exceptional superplasticity. These findings highlight the key shear-governed mechanisms for designing heterogeneous titanium alloys with superior high-temperature formability.

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# LODE-DEPENDENT FUNCTION FOR CHARACTERIZATION OF ANISOTROPY, STRENGTH DIFFERENTIAL EFFECT AND YIELD SURFACE EVOLUTION

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**ABSTRACT –** It is very difficult to accurate characterize the complicated plastic deformation of anisotropy, strength differential effect, anisotropic hardening, etc for metals. To overcome the difficulty, this research proposes a frame to extend anisotropic yield functions into asymmetric ones by introducing a Lode-dependent function. The frame is applied to extend Hill48, Stoughton-Yoon2009, Yld91, pDrucker2020 and $I_1J_2J_3$'2022 functions to model anisotropy, strength differential effect, yield surface evolution and yield stress of seven different stress states. The Lode-dependent functions are applied to advanced strenght steels and aluminum alloys to evaluate the performance. Simulation with the Lode-dependent functions is also conducted to first verify the accuracy. The convexity of the Lode-dependent functions is analyzed by GINCA (geometry-inspired numerical convex analysis). The evaluation shows that the Lode-dependent frame has high potential and flexibility to improve the accuracy of conventional yield functions.

# ELECTRODE FRACTURE AND ITS EFFECT ON BATTERY PERFORMANCE

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**ABSTRACT –** Electrode-level cracks in a Li ion battery significantly impact its performance. We develop a crack-containing electrochemical model to reveal the mechanism and quantify the effect of crack geometrical characteristics on specific energy, specific capacity and cell impedance. We show that lithium ion transport, electrochemical intercalation and the overall cell impedance are sensitive to the crack characteristics and electrotype absorption on crack surfaces. A longer crack more parallel to the current collector reduces the specific energy and specific capacity more significantly, especially when the current density is high. By contrast, a crack perpendicular to the current collector has little impact. The study of crack position shows that a crack closer to the separator has a stronger negative impact, dramatically reducing capacity. Electrochemical impedance spectroscopy simulations show that the crack shape factors such as semi-axis ratio, crack angle and electrolyte wetting ratio primarily affect the ohmic resistance. A longer crack more parallel to the current collector increases the ohmic resistance, while more crack wetting reduces the ohmic resistance. By contrast, crack position significantly affects the charge transfer resistance but with little impact on the ohmic resistance. A crack closer to the separator increases the charge transfer resistance. The effect of connected cracks into an open or closed ring shape is also considered, which can partially isolate active materials from the electrode depending on the size and orientation of the opening. This work provides a comprehensive and fundamental understanding of how various crack parameters affect the electrochemical behavior, which can assist in evaluating the significance of cracking, allow comparison with other degradation mechanisms to identify the limiting factor, and provide guidance on battery design and application strategy.

# ANISOTROPIC MULTISCALE PLASTICITY BEHAVIORS OF ADDITIVELY MANUFACTURED SUPERALLOYS: SYNCHROTRON X-RAY DIFFRACTION AND DISLOCATION-BASED CRYSTAL PLASTICITY MODELING

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**ABSTRACT –** Understanding the mechanical performance of additively manufactured superalloys requires deciphering their microplasticity-macroplasticity coupling. Multiscale links among microstructure, dislocation dynamics, and macroscopic mechanical behaviors in an additive manufactured superalloy are studied through in-situ synchrotron X-ray diffraction, dislocation-density-based crystal plasticity modeling, and microstructural characterization. In-situ characterization reveals that build orientation dictates stress partitioning across crystallographic planes, with texture strongly influencing plane-specific elastic moduli and lattice strain evolution during tension. A novel micromechanical framework integrating crystal plasticity and representative volume element modeling bridges dislocation dynamics with macroscale behavior, requiring minimal empirical fitting. Computational analyses show build orientation governs lattice strain, texture evolution, and stress-strain partitioning. Further parameter study reveals that material texture, rather than $\gamma''$ volume fraction or grain aspect ratio, dominates lattice strain behavior. Strong $\langle 001 \rangle$ material texture enhances $\{200\}$ lattice strain due to single-crystal-like deformation behavior, suppressing grain rotation and altering elastic-plastic transitions. This work uncovers multi-scale deformation mechanisms in additive manufactured superalloys, providing insights for manufacturing process optimization and microstructure-sensitive design.

# MULTISCALE MODELING AND SIMULATION OF Γ PHASE DURING GRADIENT STRAIN AND TEMPERATURE OF GH4586 SUPERALLOY USING INTEGRATED FINITE ELEMENT AND PHASE-FIELD METHOD

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**Abstract** - In this present work, a phase field model coupling the effect of second phases, recrystallization and grain growth during hot deformation and heat treatment was established, which considering the influence of carbides on the recrystallization nucleation and the influence of γ′ precipitates on the grain boundary migration. Then, the model was applied to GH4586 superalloy and validated via comparing calculated and experimental values of the recrystallized volume fraction and average grain size. The results showed that the maximum relative error, minimum relative error and average relative error of the former were 7.74%, 0.96%, and 3.80%, respectively. And those of the latter were 16.50%, 1.27% and 7.01%, respectively. Furthermore, numerical simulation of macroscopic physical field information (strain and temperature, et al) at different regions of GH4586 superalloy during controlling strain deformation (CSD) and gradient temperature heat treatment (GTHT) was conducted; Meanwhile, the node information of specific regions was extracted from macroscopic physical field simulation results and input into phase field simulation as external field information. By this method, a coupling simulation method of finite element method and phase field method (FEM-PFM) was constructed to investigate the evolution of γ grain morphology in GH4586 superalloy during CSD and GTHT. The simulation results showed that, at the deformation temperature of 1050℃ and the furnace temperature of 1120℃, the low-strain and high-temperature (LS-HT) region was composed of coarse-grained structures and the high-strain and low-temperature (HS-LT) region was composed of a heterogeneous structure with bimodal distribution of grain size. At the deformation temperature of 1080℃ and the furnace temperature of 1140℃, the LS-HT region was composed of coarse-grained structures and the HS-LT region was composed of coarse-grained structures.

**Keywords**: GH4586 superalloy; Recrystallization; Gradient-temperature heat treatment; Gradient microstructure; Finite element simulation; Phase field simulation

# STUDY ON THE COUPLING MECHANISM OF DYNAMIC RELAXATION AND INELASTIC DEFORMATION IN METALLIC GLASSES

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**ABSTRACT-** Metallic glasses (MGs) are metastable amorphous materials far from equilibrium, exhibiting complex dynamic relaxation behaviors. This study establishes a theoretical model that couples dynamic relaxation with inelastic deformation, which is verified through dynamic mechanical analysis, stress relaxation, creep, and strain recovery experiments. The findings reveal that the deformation modes of MGs include elasticity, viscoelasticity caused by β-relaxation, viscoelasticity due to α-relaxation at low temperatures, and viscoplasticity resulting from α-relaxation at high temperatures. Dynamic mechanical spectra and stress relaxation spectra uncover the dynamic characteristics from the glassy state to the liquid state. Experimental results indicate that β-relaxation and α-relaxation play significant roles in inelastic deformation. Through the analysis of the quasi-point defect (QPD) model, an experimental method for identifying ultra-low-frequency dynamic relaxation is proposed. This research provides a new perspective for understanding the relaxation dynamics of glassy materials and establishes a connection between dynamic relaxation behavior and deformation mechanisms, laying a theoretical and experimental foundation for the wide application of MGs.

# INTEGRATED CRYSTAL PLASTICITY-PHASE FIELD FRAMEWORK FOR PREDICTING ELECTRICALLY INDUCED RECRYSTALLIZATION AND GRAIN GROWTH IN POLYCRYSTALLINE TITANIUM

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**ABSTRACT–** Modern manufacturing methods increasingly demand precise control over microstructural evolution to achieve the desired mechanical characteristics in metallic components. Although traditional annealing heat treatment offers recognized methods for material improvement, the incorporation of electrical treatment (ET) alongside advanced computational modelling creates advantageous prospects for precision microstructural engineering. Electrically assisted (EA) forming applies electrical current to TA1 titanium sheets, ferritic stainless steel, and other metallic materials, achieving exceptionally rapid and effective dislocation recovery, static recrystallization, and grain growth within one second. This demonstrates the broad applicability and efficiency of the electrical treatment approach compared to conventional thermal processing methods. This study presents a detailed multi-stage framework that systematically integrates crystal plasticity finite element analysis and electrical treatment simulation to predict and control the parameters used later in simulating recrystallization and grain growth kinetics via phase field modelling. The framework consists of four sequential phases: First, the pre-straining stage uses the crystal plasticity finite element method (CPFEM) to solve the inhomogeneous local deformation, deformation texture, and dislocation density in plastically deformed polycrystalline titanium. Second, state variables computed by CPFEM—stored-energy proxies from dislocation densities, local orientations/misorientations, and stress measures—are transferred by a Wigner–Seitz mapping that preserves spatial gradients while bridging the unstructured FE discretization and the phase field (PF) grid. Third, to study the temperature effects on ET-induced recovery, electrical treatment simulation was conducted, with careful control of current parameters to avoid excessive temperature rises. Both grain boundary and intragranular temperature fields are addressed by computational analysis, which reveals heterogeneous heating profiles that have a major impact on local recovery. Experimental validation employs a thermal infrared imager and represents the apparent ET temperature of the specimen to verify computational predictions, establishing a robust calibration framework for electrical parameter optimization. Fourth, the phase field (PF) model then predicts microstructure evolution and kinetics of static recrystallization (SRX) from crystal plasticity-informed dislocation density via electrical treatment. The coupled approach successfully predicts recrystallization texture development and grain size evolution, demonstrating the effectiveness of the integrated computational framework. Through targeted temperature raising at grain boundaries, the results show that electrical treatment enables precise spatial control over recrystallization processes. The different heating regimes control the kinetics of grain growth while promoting certain nucleation sites. Compared to conventional heat treatment methods, this integrated approach provides better microstructural control, opening up new possibilities for advanced manufacturing applications requiring distinctive material properties.

# FACET 2.0 – A NEURAL NETWORK-BASED YIELD SURFACE: A FLEXIBLE AND EFFICIENT CALIBRATIONS TO CRYSTAL PLASTICITY DATA

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**ABSTRACT -** Sharp crystallographic textures give highly anisotropic yield surfaces that existing yield surfaces fail to fit accurately. We introduce a flexible, polynomial-based representation of a yield surface with guaranteed convexity through smoothly regularizing a high-order faceted polytope. This formulation has been proposed earlier as a FACET method [1], however, with only limited fitting possibilities. It has recently been shown that the FACET yield surface can be expressed as a shallow dense feed-forward neural network [2]. Any fitting accuracy can be achieved just by adding more facets in the FACET yield surface and adjusting their regularization exponent. Efficient calibration of large parameter sets is enabled by using modern machine-learning optimizers (stochastic gradient methods, automatic differentiation). The FACET method is well-suited to capture yield surfaces with both low and high symmetries.
We demonstrate the applicability of these formulations by calibrating the full-stress yield surfaces computed via a crystal plasticity model and comparing them to conventional Yld20xx predictions. The results highlight that the FACET yield surface achieves orders-of-magnitude lower fitting errors than Yld20xx while being computationally efficient and straightforward to embed into finite-element workflows.

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# ENHANCING STRENGTH AND DUCTILITY OF HCP/BCC AND FCC/BCC NANOLAMINATES VIA THICK 3D INTERFACES

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**ABSTRACT –** Biphase metallic nanolaminates possess extremely high strength but suffer a concomitant loss in strain to failure. Physical vapor deposited thick "3D interfaces" have been shown to improve upon these properties. In this work, we investigate a wide range of Cu/Nb 3D interfaces and Ti/Nb interfaces. We show via in-situ micropillar compression, nanoindentation, post-mortem TEM, and phase field dislocation dynamics (PFDD) simulations that the benefits of these thick interfaces persist over large layer and interfacial thicknesses, but there is a length scale at which bulk behavior is observed. Larger interfacial thicknesses are found to push the system towards metallic glass-like behavior. Shear localization in these nanolaminates is found to be distinct from that in metallic glasses, and their differing morphology allows for sustained plasticity. We also see that slip transmission across a 3D interface and therefore strength is an asymmetric process. Our results emphasize the importance of controlling the constituent pure phase thickness versus interface thickness for improved performance in nanolaminates.

# IMAGE-BASED QUANTIFICATION OF FRAGMENT KINETIC ENERGY IN DYNAMIC FAILURE OF BRITTLE MATERIALS

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**ABSTRACT –** Dynamic fragmentation of brittle materials dissipates energy through the creation of new fracture surfaces, fragment kinetic energy, acoustic emissions, and frictional heating. At high strain rates, the kinetic-energy partition becomes increasingly significant but is often underestimated because high-velocity fine fragments fall outside the available temporal observation window or exceed spatial/temporal resolution. Here, we present a high-speed, image-based method to quantify the fragment kinetic-energy contribution during drop-weight tests of brittle materials. Contrary to common assumptions of a single characteristic velocity per size class, our results show that fragments of nominally identical size exhibit a broad velocity distribution, with dispersion increasing as fragment size decreases. Furthermore, comparing representative coarse and fine size classes indicates that the volumetric kinetic-energy density of fine fragments is approximately fivefold higher than that of coarse fragments. These findings emphasise the need to incorporate fine fragments into kinetic-energy evaluation, providing a more complete basis for understanding energy partitioning and dissipation during the dynamic failure of brittle materials.

# PROBING MICRON SCALE PLASTIC RESPONSE UNDER NON-PROPORTIONAL LOADING AND HYDROGEN CHARGING EFFECTS USING SMALL SCALE MECHANICAL TESTING

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**ABSTRACT:** Plastic deformation at small length scales, from sub-millimeter to micron, is relevant to various technological applications, e.g., metal microforming and adhesion of metal/ceramic interfaces. Deformation responses vary depending on the deformation geometry and the characteristic deformation length scale, exhibiting various mechanical size effects. Plasticity relevant to forming processes often involves significant strain gradients and non-proportional straining. Strain gradient plasticity (SGP) models are believed to be the best candidates for predicting outcomes of experiments involving micron-scale plastic deformation with significant strain gradients. At the present time, there are two main classes of SGP formulations: the non-incremental theory and the incremental theory. These SGP formulations lead to similar model outcomes when plastic straining is proportional, but different predictions arise when plastic straining is non-proportional.

In this talk, we will describe results of recent micron-scale mechanical tests on single crystal copper cantilevers in which the loading is distinctly non-proportional. The experimental results are correlated to strain gradient plasticity finite element simulations to illustrate the difference between non-incremental and incremental SGP model outputs. In addition, recent results of small-scale mechanical testing on uncharged and hydrogen-charged titanium-tungsten alloys will be described in light of hydrogen-induced structural transformations.

# HARNESSING ELECTRICAL ASSISTANCE IN FORMING OF ULTRA-THIN TITANIUM SHEETS

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**ABSTRACT –** In order to improve formability and geometric accuracy, we developed a multi-step forming process of ultra-thin pure titanium sheets with intermediate electrical treatment, where a short-duration electrical treatment (1-2 seconds) is applied in-between two room-temperature stamping steps. The electrical treatment significantly reduces the twin density and dislocation pile-up, and expedites the formation of equiaxed recrystallized grains in the pre-deformed pure titanium sheets. Further microstructural analysis reveals the accelerated restoration within 1-2 seconds by electrical treatment is primarily attributed to the promoted dislocation climb, the increased recrystallization nucleation sites, and enhanced grain boundary migration. Electrothermal-coupling finite element analysis, theoretical modeling and first-principles calculations were performed to elucidate the physical origins of the distinct microstructural evolution. The results indicate that the accelerated restoration process primarily arises from the synergistic contributions of selective heating, electrically enhanced diffusion, and the reduction in atomic bonding strength associated with the charge imbalance effect. This study advances the fundamental understanding of electrically assisted forming and establishes a scientific basis for extending electrical treatment to other metallic materials.

# EXPERIMENTAL CHARACTERIZATION OF GRAIN BOUNDARY STRENGTHENING IN POLYCRYSTALLINE MAGNESIUM ALLOYS

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**ABSTRACT –** The role of grain boundaries and solute elements in polycrystal plasticity of hexagonal closed packed (HCP) alloys is characterized using (i) in situ tensile testing in a scanning electron microscope (SEM) in conjunction with high-resolution electron backscatter diffraction (HR-EBSD) under load, and (ii) site specific instrumented indentation and HR-EBSD. Using model systems such as Mg-Y and Mg-Al, the evolution of geometrically necessary dislocation (GND) densities at specific grain boundaries as a function of applied strain was evaluated. The increase in GND density was correlated with (i) geometric compatibility between slip systems across grain boundaries, and (ii) plastic incompatibility. The grain boundary GND density evolution as a function of plastic strain was quantitatively expressed in terms of plastic incompatibility, from which uniaxial tensile stress-strain response of polycrystalline Mg-4Al were computed and compared with experimental measurement.

In Mg-Al alloy, basal slip systems were dominant whereas for Mg-Y, non-basal slip was also active. The role of quantitative, site-specific, in situ experiments in developing fundamental understanding and prediction of the measured stress-strain response, particularly, the interpretation of polycrystal strain hardening in terms of GND at grain boundaries is highlighted.

# TOWARDS IDENTIFYING DATA-DRIVEN CONSTITUTIVE MODELS FROM ROBOT-ASSISTED EXPERIMENTS: MINIMAL STATE CELL–BASED MODELING ENHANCED BY MULTI-TASK AND TRANSFER LEARNING

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**ABSTRACT-** We present a unified framework for data-driven constitutive modeling that combines a robust recurrent architecture with highly data-efficient multi-material training strategies. We start from the Extended Minimal State Cell (EMSC), a recurrent neural network architecture that guarantees self-consistent stress predictions under large deformations, even for rate- and temperature-dependent materials. The EMSC decouples the number of internal state variables from the number of fitting parameters, allowing compact models with a minimal, physically interpretable state space while retaining high expressivity. Trained and validated on 1D and 3D random-walk datasets generated from micromechanical composite models, rheological networks, advanced thermo-visco-plasticity, and anisotropic yield criteria (von Mises, Hill'48, Yld2000–3d), EMSC models with fewer than 25,000 parameters accurately reproduce the large-strain response of all considered materials. Building on this architecture, we investigate how to drastically reduce the experimental data needed for model identification. First, we show that training on rough random-walk strain paths yields significantly better generalization than the same number of smooth loading paths. Second, we exploit transfer learning across materials: initializing from a previously trained material accelerates convergence and lowers the number of required sequences. Extending this idea, we train multi-task models for families of elasto-plastic von Mises materials and identify a large, shared "common core" complemented by lightweight material-specific layers. Using ensemble transfer learning, we demonstrate that adding a new material to this multi-task model requires datasets that are two to three orders of magnitude smaller than training an RNN from scratch, while preserving or improving accuracy. Finally, we present the robot-assisted experimental methods and discuss the potential of calibrating machine-learning based constitutive models directly from experiments.

# MIXED FINITE ELEMENT METHOD FOR A SIMPLIFIED GRADIENT ELASTIC-PLASTIC MODEL: FORMULATION, IMPLEMENTATION, AND APPLICATION TO REPRESENTATIVE PROBLEMS

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**ABSTRACT –** We consider a simplified strain gradient elastic-plastic model that includes a dimensional dependence associated with the microstructure of an isotropic material. It is assumed that elastic strains and their gradients are described by the equations of the simplified strain gradient elasticity theory. The equations of plastic flow are determined using a dissipative function expressed in terms of plastic strain rates and their corresponding gradients. According to the adopted equations, the elastic-plastic model is enriched with elastic and plastic strain gradients, which extend the modeling capabilities by including the dimensional scale of the material's internal length associated with elasticity and plasticity-induced dissipation. An alternative approach is used, in which the equations of plastic flow are integrated over the loading stage to obtain the governing equations not for increments, but for the full components of stresses, strains, and their gradients. The peculiarity of the formulated equations is that they are formally similar in form to the equations of the deformation theory of plasticity. This simplifies the analysis of the correctness and application of the obtained equations to solve boundary value problems. The conditions under which the considered elastic-plastic model with a strain gradient does not contradict Drucker's postulate are determined. A variational formulation of the boundary value problem in a mixed form involving displacements, strains, stresses, and strain gradients is presented. This mixed finite element method was applied to solve the selected model problems. The mixed approximation for displacements, deformations, stresses, and their gradients used here has a principal difference from others available in the literature. It ensures the continuity of displacement, strain, and stress fields throughout the area occupied by the body. It satisfies the necessary and sufficient condition, which is formulated and provides the uniqueness of the solution and the stability of this approximation within the framework of strain gradient elastic-plastic theory. The results of solving the model problems of uniaxial tension in square plates with a narrow U-tip cutout and a central circular hole, within the strain gradient elastic-plastic theory, are presented. These simulations demonstrate the influence of strain gradient effects on localized deformation distributions and confirm the accuracy and stability of the proposed method.

# HYDROGEN ENHANCED CROSS SLIP (HECS): A NOVEL ATOMISTIC MECHANISM FOR HYDROGEN ASSISTED EMBRITTLEMENT IN NICKEL GRAIN BOUNDARIES

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**ABSTRACT –** Hydrogen embrittlement (HE) remains a critical reliability issue for high strength metallic components, especially in hydrogen rich environments such as fuel cell systems and offshore pipelines. While conventional HE mechanisms (hydrogen enhanced decohesion, hydrogen enhanced localized plasticity, and hydrogen enhanced strain induced vacancy formation) successfully explain many macroscopic observations, they do not capture the atomistic pathways by which hydrogen can directly promote dislocation motion across grain boundaries (GBs). Here we introduce the Hydrogen Enhanced Cross Slip (HECS) mechanism, a previously unreported process by which interstitial H atoms lower the energetic barrier for a screw dislocation to cross slip from its primary glide plane onto a secondary plane within a tilt GB in face centered cubic Ni. The HECS mechanism provides a direct atomistic link between hydrogen segregation and enhanced plastic flow across grain boundaries, complementing existing HE theories. By revealing how H induced eigenstrains modify the local stress state and promote cross slip, our work suggests new alloy design strategies (e.g., GB chemistry engineering) and processing routes (e.g., grain size optimization) to mitigate HE in Ni based alloys and related fcc metals. The analytical framework presented here can be extended to other GB characters and solute species, offering a versatile tool for predicting hydrogen affected plasticity at the mesoscale.

# DISLOCATIONS IN COMPLEX CONCENTRATED ALLOYS – STATISTICAL MECHANICS AND MACHINE LEARNING OF RESISTANCES

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**ABSTRACT –** In complex concentrated alloys (CCAs) with principal elements in nearly equal ratios, travelling dislocations encounter spatially fluctuating resistance landscapes, causing them to exhibit constantly wiggling shapes. As dislocation energy is proportional to line length, the self-energy of dislocations therefore fluctuates as they glide. The first part of this talk will show that the self-energy distribution of dislocations qualifies for a statistical mechanics description in both thermal and athermal conditions. From dislocation shapes observed by electron microscopy and simulated by molecular dynamics (MD) at different temperatures in different alloys, the Fourier harmonics of dislocation shapes are found to follow two trends: the energies of long wave-length harmonics obey power-law distributions characteristic of random-walk, self-similar shapes, and the energies of short-wavelength harmonics follow an exponential law corresponding to maximum entropy with mean energy comprising a thermal and an athermal component. Both components contribute to strength but the athermal component is dominating. In the second part of the talk, the origin of dislocation resistance is machine-learned from MD-generated dislocation velocity and core property data. It is found that the waviness and hence the main component of resistance of dislocations are determined by a second-order derivative of the unstable stacking-fault energy landscape on the glide plane. This paper shows that statistical mechanics is a bona fide theoretical framework for describing and understanding dislocation fluctuations and strength in CCAs.

# BRIDGING THE SCALES IN CONSTITUTIVE MODELLING OF GEOMATERIALS

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**ABSTRACT –** Predicting geomaterial failure at field scales (ranging from underground mines to Arctic ice flows) is critical for engineering design and risk mitigation, yet remains computationally demanding. High-fidelity simulations are not often feasible, as besides very high computational costs, there are many factors affecting the accuracy beyond material models and numerical algorithms. This presentation focusses on how to encapsulate more lower scale details in constitutive models of engineering materials for computational efficiency in parallel with better prediction of failure at larger scales. A strategy is developed to embed only key mechanisms and essential lower scale details in constitutive models for engineering materials (e.g. soils, rocks, concrete, composites) for a good balance between computational efficiency and accuracy in large scale modelling. The key focus is the introduction of meso scale details, associated with localised failure, which is usually missing in constitutive modelling, in a new constitutive structure. This provides a way to correctly connect micro/grain with macro scales, and to obtain stress and strain at the meso scale of the localisation band from standard tests. Models derived from the proposed approach naturally possess a length scale, and hence remove the need of ad hoc regularisation in the analysis of Boundary Value Problems involving localised failure. The key basis in connecting meso with macro scales will be presented first, followed by interconnected specific topics on different materials and responses as a result of this approach.

# FORMATION AND STRENGTEHNING MECHANISMS OF PLATE-SHAPED PRECIPITATES IN LIGHT ALLOYS

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**ABSTRACT –** In precipitation-hardened aluminium and magnesium alloys, nano-sized, plate-shaped precipitates frequently develop on rational crystallographic planes of the matrix. While it is well established that a high number density of these precipitates enhances alloy strength, the critical influence of their shape is less widely recognised. Minor alloying additions can modify the nucleation and growth processes, thereby altering the morphology and spatial distribution of precipitate plates. Yet, the precise mechanisms by which these elements promote plate formation and control morphology remain under active debate. This presentation will first examine the fundamental processes governing plate-shaped precipitate formation, with emphasis on the role of alloying elements. It will then introduce strengthening models that explicitly incorporate precipitate geometry, highlighting how their plate-like shape leads to strengthening effects not captured by conventional spherical-particle theories. Importantly, many such precipitates—often assumed to form solely by diffusional, non-displacive processes—actually involve a significant shear component during their formation. This shear contribution critically influences nucleation behaviour and, ultimately, the strengthening response. Finally, it will be shown that controlled lengthening of precipitate plates can deliver exceptional strengthening, well exceeding that achievable with spherical particles.

# EFFECT OF PULSED CURRENT ON THE DEFORMATION AND INTERFACIAL BONDING OF COPPER/STAINLESS STEEL STRIPS IN ROLLING

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**ABSTRACT –** This study investigated the electrically assisted (EA) rolling and ultrafast electric pulse treatment (EPT) of copper/stainless steel (Cu/SS) composite thin strips to mitigate deformation mismatch and enhance interfacial bonding. Owing to the large difference in physical properties, Cu and SS exhibited distinct deformation behaviors during EA rolling. A pulsed-current tensile test and flow stress model revealed that SS was significantly more sensitive to current than Cu. The analysis showed that unwinding tension altered metal flow and neutral plane position, thereby affecting deformation compatibility of the composite strip. To strengthen interfacial bonding, a specially designed fixture enabling ultrafast EPT with vertically misaligned electrodes was developed. The localized pulsed current accelerated atomic diffusion and promoted rapid metallurgical bonding within seconds, while avoiding excessive recrystallization in both matrices. After EPT at 18.3 A/mm$^2$ for 5 s, the peel strength reached 8.30 N/mm (21.3 times that of the as-rolled strip), and the tensile strength retained 86.6% of the original value. This approach demonstrated a feasible pathway to achieve deformation compatibility, strong metallurgical interfaces, and well-balanced strength and ductility in Cu/SS thin composites.

# ATOMISTIC MODELING OF HYDROGEN IMPACT ON DEFECT KINETICS IN MATALS

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**ABSTRACT –** The study of hydrogen's impact on defect kinetics in metals is essential for understanding hydrogen-induced damage accumulation and embrittlement, yet it remains insufficiently elucidated. Atomistic simulation emerges as a valuable tool for directly investigating hydrogen effects on defect kinetics; however, the reliability of such simulations largely depends on accurately describing atomic interactions within metal–hydrogen systems. Recent advancements include the development of artificial neural network (ANN) atomic interaction models for metal–hydrogen systems, trained on datasets derived from density functional theory (DFT) calculations of energies, forces, and atomic structures. These ANN-based potentials combine the computational efficiency of empirical models with the accuracy and transferability of DFT, enabling quantitative elucidation of various defect kinetics—such as vacancy migration, surface diffusion, and dislocation motion— in metals under constant hydrogen chemical potential, temperature, and stress conditions. In this presentation, we introduce a unified theoretical framework that describes the kinetics of defects in hydrogen environments based on atomistic modeling.

# CRYSTAL PLASTICITY – PHASE FIELD DAMAGE SIMULATION: INVESTIGATING DUCTILE FRACTURE BEHAVIOR INDUCED BY CRYSTALLOGRAPHIC ORIENTATION AND PRECIPITATED PARTICLE

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**ABSTRACT-** Accurate prediction of service life is critical for reducing the life-cycle costs of structural materials. Ductile fracture, which occurs through void nucleation, growth, and coalescence, is a primary factor in determining the serviceability limits of ductile materials. Conventional predictive approaches often rely on macroscopic indicators, such as stress triaxiality or hydrostatic stress, to describe void growth. However, recent experimental and computational studies indicate that microscopic material features, including crystal orientation and the presence of precipitated particles, strongly influence void evolution. To explore these effects, we apply the crystal plasticity-phase field damage simulation to a single crystal containing a precipitated particle, focusing on the local evolution of voids under mechanical loading. By systematically varying the crystal orientation relative to the loading direction, the simulations reveal how local mechanical anisotropy and microstructural heterogeneity affect void nucleation and growth. The results highlight the influence of microscopic properties on local stress and strain fields around particles, and their potential implications for ductile fracture behavior are discussed.

# A SIMPLE YET FLEXIBLE POLY6 YIELD CRITERION FOR PLASTIC ANISOTROPY IN SHEET METALS

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**ABSTRACT -** This study presents a simple yet versatile analytical sixth-order polynomial (Poly6) yield criterion to characterize the flow stress of sheet metals under four representative stress states: uniaxial tension (UT), equi-biaxial tension (EBT), plane strain tension (PST), and pure shear (SH). Despite its simplicity, the proposed model exhibits remarkable flexibility, capable of representing a wide variety of yield surface shapes across different materials compared with existing yield criteria. A non-negative curvature method is proposed to rigorously clarify the convexity condition of the isotropic Poly6 yield function within the normal plane with respect to stress state-dependent parameters. The analysis shows that convex yield surfaces can be consistently predicted under special boundary conditions, and their diverse geometrical features illustrate the high flexibility and adaptability of the Poly6 yield function. In combination with crystal plasticity simulations for single crystals as well as typical textures of BCC (body-centered cubic) and FCC (face-centered cubic) structures, the Poly6 yield criterion effectively reproduces the shapes of yield surface. To further account for plastic anisotropy, the isotropic Poly6 form is extended through three complementary approaches according to the desired accuracy: (1) direct incorporation of anisotropic parameters, (2) additive coupling with an anisotropic term, and (3) introduction of loading-angle–dependent anisotropy parameters. All anisotropic extensions retain analytically determined parameters, enabling straightforward reproduction of strain hardening behavior without resorting to complex numerical optimization or yield locus interpolation The proposed Poly6 yield criterion is validated against experimental data for high-strength steels and aluminum alloys. Results demonstrate that the model accurately captures evolving yield behavior across multiple stress states, confirming its capability as a versatile and computationally efficient tool for modeling the plasticity of sheet metals.

# ANISOTROPY PREDICTION OF SHEET METALS WITH A TEXTURE-BASED POTENTIAL MODEL

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**ABSTRACT –** Conventional yield models for metallic materials commonly introduce plastic anisotropy by calibrating phenomenological yield functions through mechanical testing under an associated flow framework. While this strategy can reproduce directional dependencies, it requires extensive experiments and multi-parameter fitting, which increases cost and limits the model's ability to embed physically meaningful microstructural information.

To overcome these limitations, this study proposes a physics-informed plastic potential model that directly incorporates crystallographic texture. A polycrystal homogenization scheme is employed, where discrete stress–strain response points are generated using the Visco-Plastic Self-Consistent (VPSC) approach to capture grain-level orientation effects. These data points are then interpolated using a third-order polynomial to construct a smooth plastic potential surface with $C^1$ continuity, ensuring numerical stability for finite element analysis.

To enable more flexible representation of macroscopic anisotropy, a non-associated flow rule is adopted, allowing independent definition of the yield function and plastic potential. This formulation improves the capability to describe complex anisotropic plastic flow beyond the inherent constraints of the associated flow assumption.

The proposed model is validated through finite element simulation of a cylindrical cup drawing process. The results confirm that the model accurately captures texture-driven anisotropy while reducing dependence on experimental calibration, demonstrating its potential as a computationally efficient and physically interpretable alternative for sheet metal forming applications.

# ELASTO-VISCOPLASTIC MODELING OF DEFORMATION IN DUAL PHASE STEELS: FROM MICROSTRUCTURES TO COMPONENTS

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**ABSTRACT –** This paper reviews new developments for materials characterization for constitutive and failure modeling, focusing on compressive fracture strain with bilinear strain paths, laminated aluminum pouch film properties, gradient properties in Al-Steel spot weld. First, the bilinear strain paths subjected to pre-tensile loading followed by compressive loading is capable of predicting the cut-off region for ductile fracture loci and is verified through experiment and numerical simulation. Second, Lithium-ion battery pouch film is composed of polypropylene, aluminum, PET, and nylon. The material properties of the four layers are characterized by the delamination behavior between the aluminum and polymer layers during tensile testing and the polymer properties through nano-indentation testing. Individual layer properties are optimized to satisfy the combined stress-strain curve The modelled properties were verified through wrinkling and forming behaviors. Finally, aluminum-steel resistance spot welding (Al-steel RSW) is considered. This study develops an inhomogeneous sample to extract the material properties for the fusion zone (FZ), heat-affected zone (HAZ), and intermetallic compound (IMC) layers with a single tensile test. The results from inhomogeneous specimen is compared to the ones from homogeneous samples. Fracture mechanisms of Al-steel RSW are examined using a miniature weld performance test and in-situ micro DIC.

# ROLE OF LATTICE RE-ORIENTATION IN THE FORMATION OF SHEAR BANDS DURING HIGH STRAIN-RATE DEFORMATION

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**ABSTRACT –** The crystallographic aspects of nucleation and propagation of shear bands (SB) in dynamically deformed metals remain a largely unresolved issue. This study analyses the effect of local crystal lattice re-orientation within SB regions on slip transfer through twin and grain boundaries. Rectangular single-crystal samples of pure Cu and Cu–14 at.% Al alloy, with (112)[11-1] (C) and (346)[63-5] (S) orientations, were compressed in a channel-die up to logarithmic strains of 0.9 at a strain rate of $4.7 \times 10^5$ $s^{-1}$, using explosive energy. Polycrystalline α-Ti hat-shaped samples were deformed using a drop hammer at a strain rate of $4.9 \times 10^3$ $s^{-1}$. Microstructures in the strain localisation regions were characterised using scanning (SEM) and transmission (TEM) electron microscopy, while texture evolution was analysed by X-ray diffraction and electron backscatter diffraction (EBSD) in SEM. SEM/EBSD measurements documented that very high strain rates promoted intense deformation twinning in both Cu and α-Ti. In single-crystal specimens, at strain levels of 0.9, deformation twinning facilitated the formation of SB. Nucleation of SB was associated with the instability of compact twin-matrix (T-M) clusters, leading to the development of kink-type bands. A strictly directed rigid-body rotation of the T-M platelets within the narrow SB regions, combined with deformation twinning in re-oriented primary matrix platelets, resulted in the dominance of texture components near the {110}<001> orientation. This local lattice re-orientation aligns one of the {111} plane and the <112> direction along the shear plane and direction, respectively. In polycrystalline α-Ti, SB nucleated due to severe shear generated by the displacement of the ‘cap’ into the ‘brim’ region. The crystal lattice within the SB region rotated through activation of slip systems on the basal {0002} and prismatic {1-100} planes. This rotation led to the formation of texture components in the strain-localisation region, markedly different from those in the less deformed matrix. The {0002} planes in the dominant grain fraction of the shear zone tended to align perpendicular to the shear plane and parallel to the loading axis, while one of the {1-100} planes aligned parallel to the shear plane. A <11-20> direction, common to both planes, was oriented parallel to the shear direction. This work proposes a crystallographic framework for explaining the formation of SB in Cu, Cu-Al alloy and α-Ti deformed at high strain rates, providing new insights into the mechanical behaviour of metals under dynamic loading.

# CONSTITUTIVE MODEL FOR CAPTURING PRE AND POST-LOCALISATION RESPONSES OF PARTIALLY SATURATED SOILS

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**ABSTRACT –** Partially saturated soils usually undergo localized failure in the form of shear bands, inducing localized deformation and saturation. Inelastic responses largely take place within the shear band, while the surrounding material exhibits recoverability with comparatively small deformation and saturation changes. These are usually not correctly captured by classical constitutive models for partially saturated soils due to their homogeneous assumptions. Accordingly, we formulate a thermodynamics-based model enriched with kinematic terms, allowing accurate representation of strong stress-strain and suction-saturation variations inside and outside the shear band. The interaction between these zones governs the overall hydromechanical response. The resulting model provides a size-dependent constitutive structure capable of describing the transition between pre-and post-location regimes. Promissing features of the proposed approach are elucidated through data from drained triaxial tests.

**Keywords:** Partially saturated soils, Bifurcation, Size-dependent, Localisation, Localisation band, Thermodynamics, Hydro-mechanical coupling, Constitutive modelling

# ELECTRICALLY ASSISTED SOLID-STATE SPOT JOINING OF A CAST A365 ALLOY: IMPROVEMENT OF JOINT PROPERTY BY LOCAL RAPID HEAT TREATMENT

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**ABSTRACT –** The solid-state joining of a cast A365 alloy for automotive structural applications is experimentally investigated. An electrically assisted pressure joining technique is employed in a spot configuration, referred to as electrically assisted solid-state spot joining (EASSJ). During the EASSJ process, two identical 3 mm-thick plates are joined under simultaneous compressive deformation and an electric current. The solid-state joint by EASSJ is successfully fabricated at approximately 360 ºC, with no macro-defects observed. The joint interface consists of a mixture of elongated grains and recrystallized grains, accompanied by partial fragmentation of the eutectic Si network. A localized and rapid heat treatment (RHT) is applied by introducing additional pulsed currents, which promote artificial aging. As a result, the eutectic Si network is broken, resulting in a uniform dispersion of eutectic Si particles. Consequently, the EASSJ+RHT joints exhibit higher microhardness at the joining region compared with the EASSJ-only joints. Moreover, the failure mode transitioned from interfacial to pull-out fracture after RHT, reflecting higher fracture load capacity. The present study confirms that the RHT process significantly enhances the microstructural and mechanical performance of the EASSJed joints, offering a promising solution for the reliable joining of cast Al alloys.

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# MICROMECHANICS OF PLASTICITY IN HIGH-TEMPERATURE MATERIALS

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**ABSTRACT –** This talk examines the mechanisms of plastic deformation in three high-temperature materials: tungsten (W), zirconium (Zr), and a novel refractory dual-phase high-entropy alloy (HEA). Tungsten, a leading candidate for first-wall and divertor components in fusion energy systems, operates across a wide temperature range—from room temperature up to approximately 1000 °C. Within this regime, its plastic response changes dramatically due to thermally activated dislocation processes characteristic of body-centered cubic (bcc) metals. We investigate the deformation of W micropillars between 300 K and 900 K through combined *in situ* micropillar compression experiments and discrete dislocation dynamics (DDD) simulations. Results show that while the flow stress decreases with increasing temperature, stress fluctuations become more pronounced. Distinct statistical behaviors emerge at low and high temperatures, reflecting differences in dislocation source activation and propagation mechanisms. A DDD-based model is developed to rationalize these observations.

Zirconium, widely used in nuclear fission applications, exhibits a unique irradiation-induced "growth" phenomenon—an isochoric shape change occurring without applied stress. We explore its origin using a newly developed multiscale model coupling discrete dislocation dynamics with spatially resolved cluster dynamics simulations. Complementary micropillar compression tests on Zr single crystals reveal an unexpected inverse temperature dependence of flow stress, a behavior that also manifests in a Zr-containing dual-phase HEA. *In situ* micromechanical testing, supported by detailed TEM and APT characterization, elucidates the underlying mechanisms driving this unconventional deformation behavior.

# ESTABLISHMENT OF A UNIFIED ELASTOPLASTIC CONSTITUTIVE MODEL FOR SiC/AL COMPOSITES AND THREE-DIMENSIONAL FINITE ELEMENT MODELING BASED ON MICROSTRUCTURE

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**ABSTRACT** - SiC/Al composites have complex meso structure, and the addition of particles ca n strengthen the metal matrix, which makes SiC/Al composites show complex deformation and f ailure behavior under thermal deformation. Considering the influence of thermal modulus misma tch and grain refinement on flow stress, a unified viscoplastic constitutive model of 25 vol.% SiC /2009Al composite based on internal variable evolution was developed. A meso model of compo sites was established to reflect the deformation behavior of metal matrix and particle damage. Th e deformation of matrix, the evolution of dislocation density and particle damage in SiC/Al comp osites were described. The simulation results show that the model can well predict the properties of composites and reveal the damage mechanism. The results of internal variable evolution revea l that the softening behavior of composites is driven by dynamic recovery, and the occurrence of dynamic recrystallization is highly correlated with the strain rate. The addition of particles leads t o a high strain gradient in the surrounding matrix, and the resulting stress concentration leads to particle fracture. Particle fracture is the main form of damage in composites, and the cumulative damage factor increases exponentially.

# INTEGRATED MULTISCALE MODEL FOR THE VISCOELASTIC BEHAVIOR AND MICROSTRUCTURAL EVOLUTION OF METALLIC GLASSES: INSIGHTS FROM CYCLIC LOADING, CREEP AND THERMO-MECHANICAL COUPLING

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**ABSTRACT-** Establishing quantitative correlations between microstructure and macroscopic properties in metallic glasses (MGs) is pivotal for elucidating the coupled mechanisms of cyclic loading, creep and dynamic relaxation. Our work integrates free volume theory and shear transformation zones dynamics into an enhanced Burgers constitutive framework, grounded in hierarchically correlated atomic theory, to systematically investigate the cyclic tensile and creep behaviors of MGs near the glass transition temperature. Under cyclic loading, ratchet strain is quantitatively coupled with defect concentration, revealing that plastic viscosity decreases with increasing temperature and increases with stress rate, and structural relaxation dominates over stress-driven rejuvenation. Creep experiments indicate that high/low correlated deformation units correspond to regions that are sensitive to annealing treatment and to atomic diffusion processes, respectively. Prolonged annealing transitions the creep curve from a three-stage to a two-stage pattern, with characteristic times and correlation factors mapping onto the "single peak-shoulder-excess wing" forms of β relaxation, thus allowing the inference of microstructural heterogeneity from macroscopic parameters. Furthermore, the stepped isothermal method combined with the time-temperature-stress superposition principle rapidly constructs long-term creep master curves and clarifies the decoupling mechanism of thermal activation (predominant at high temperature/low stress) from mechanical stimulation (predominant at low temperature/high stress). It is pointed out that β relaxation significantly influences the initiation of creep by reducing the local atomic rearrangement energy barriers. This multi-level model provides a unified theoretical foundation and an efficient experimental-predictive platform for modulating the mechanical properties of MGs through thermo-mechanical pathways.

# MACHINE LEARNING-ASSISTED NON-PARAMETRIC FULL-FIELD STRESS-STRAIN IDENTIFICATION FOR HIGH-THROUGHPUT DATA ACQUISITION OF SHEET METALS

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**ABSTRACT-** We introduce Manifold-Optimized Self-Balanced Data-Driven Identification (MOSBDDI), a non-parametric framework for high-throughput full-field stress–strain extraction from digital image correlation (DIC) and applied-load data. MOSBDDI couples K-means domain segmentation with a clusterwise self-balanced stress corrector to enforce global equilibrium and boundary conditions, while local manifold learning builds convex hulls from neighboring material states to synthesize intermediate, physically consistent stress–strain pairs. An overcomplete autoencoder then denoises and compresses high-dimensional material representations, improving robustness to measurement noise. This combination reduces undersampling artifacts common in large-strain elastoplastic identification and prevents spurious matches in sparse databases. We validate MOSBDDI on multiple numerical benchmarks (uniaxial tensile, shear, perforated dog-bone, RVE and architected metamaterials) and on experimental shear tests, benchmarking against classical DDI and the LCDDI variant. MOSBDDI consistently yields superior fidelity: mean and median identification errors remain below 1% even under large plastic deformation, compared with mean errors >19% for DDI and ~8% for LCDDI. Additional tests show mean absolute errors below 1 MPa in RVE reconstruction and ≈1.6% mean relative error for complex metamaterials. MOSBDDI therefore enables rapid, parameter-free recovery of macroscale and microscale constitutive data from a single experiment, offering a practical route to generate high-quality datasets for data-driven constitutive modeling and multiscale simulation.

**Keywords:** Self-balanced, Local-convexity, Non-parametric, Data-driven identification

# REAL-TIME IN-SITU X-RAY IMAGING OF PORE COMPACTION AND SPALL FRACTURE IN PLATE IMPACT TESTS ON ADDITIVELY MANUFACTURED METALS

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**ABSTRACT -** This work presents the first direct, in-situ, real-time X-ray observations of pore compaction and spall fracture in porous additively manufactured metals under high velocity loading. To this end, planar plate impact experiments were conducted using a mesoscale gas launcher at the ID19 beamline of the European Synchrotron Radiation Facility on disc-shaped Ti6Al4V and AlSi10Mg specimens produced by laser powder bed fusion. The two alloys exhibit markedly different mechanical properties and distinct void volume fractions, ranging from 0.04% to 0.77%, with broad pore size distributions extending from a few microns to over 90 μm. The cylindrical samples had a diameter of 6 mm and two thicknesses, 1.2 and 2 mm. These reduced dimensions were dictated by the combined constraints of the synchrotron-based impact setup and the X-ray diagnostics, ensuring compatibility with the gas launcher and sufficient transmission for highresolution X-ray radiography. The tests were performed at impact velocities ranging from 225 to 738 m/s, spanning the transition from the onset of damage to complete spall cavity formation. Three ultra-high-speed cameras operating in an alternating-frame mode enabled X-ray phase-contrast imaging of the porous microstructure with a temporal resolution of 160-175 ns and a spatial resolution of 16 μm/pixel, capturing pore collapse during the compressive wave followed by void growth and spall fracture under tensile loading. A photonic Doppler velocimetry system synchronized with the X-ray imaging established a direct correspondence between the specimen's free-surface velocity signal and the in-situ microstructural processes of pore collapse, pore re-opening, and spall fracture, enabling the microstructure to be resolved at key stages of the shock-loading response, including the Hugoniot elastic limit, the plastic shock front, the peak-velocity plateau, and the pullback velocity. In addition, the free-surface velocity record provided measurements of spall strength, which showed good agreement with literature data and validated the dedicated setup developed in this study for in-situ, real-time plate impact testing. Furthermore, systematic comparison of X-ray tomography scans on selected samples before and after testing enabled direct assessment of the pre- and post-mortem shape and size of individual voids, indicating that spall fracture involves large preexisting pores formed during printing, sub-micron pores below the resolution limit of the tomograms, and pores newly nucleated during dynamic loading. The tomography analysis also allowed reconstruction of the spallation patterns and highlighted the differences in fracture morphology between the two materials tested. The observations reported in this work establish a direct

connection between pore-scale mechanisms and the macroscopic fracture response of AlSi10Mg and Ti6Al4V, providing a robust experimental framework for investigating dynamic failure in additively manufactured metals.

# RATE-DEPENDENT DUCTILE FRACTURE OF DP-STEELS: STATIC AND DYNAMIC HIGH-THROUGHPUT EXPERIMENTS AND NEURAL NETWORK MODELING

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**ABSTRACT –** This study presents an extensive characterization of five dual-phase steel grades (DP590, DP780, DP980, DP1180, and DP1470) through tensile testing at low, intermediate and high strain rates with more than 650 specimens. To facilitate this large campaign, besides recently developed setups at low strain rates, a novel high-throughput Split-Hopkinson Pressure Bar (SHPB) system with a load inversion device is introduced. This enables rapid and repeatable high-strain-rate tensile testing of sheet materials. The system integrates automated specimen clamping, input bar and striker handling, as well as an efficient post-processing workflow, thereby significantly reducing the experimental overhead. A range of stress states are probed in up to seven in-plane orientations for each steel grade using different specimen types, including uniaxial, notched, central-hole, and shear. Optical high-speed photography and 2D digital image correlation are used to capture the surface strain evolution, while high-speed infrared thermography provides detailed surface temperature measurements during deformation. Coupled thermo mechanical finite element analysis (FEA) is used based on these data, enabling a hybrid experimental-numerical identification of the material behavior. The constitutive model incorporates a non-associated quadratic yield function with Swift–Voce strain hardening and a neural network-based strain rate and temperature formulation. The model demonstrates accurate predictions of the force-displacement curves, local strain fields, as well as the temperature measurements. A neural network-enhanced Hosford-Coulomb fracture initiation model is also calibrated, accurately capturing fracture behavior over a range of strain rates.

# PHASE TRANSFORMATION-MEDIATED TRANSITION FROM LOW- TO HIGH-CYCLE FATIGUE IN Ni-RICH NiTi THIN FILMS

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**ABSTRACT –** Shape memory alloys (SMAs) have garnered considerable interest owing to their distinctive ability to reversibly transform between austenite and martensite phases, thereby recovering their initial shape when subjected to thermal or mechanical stimuli. The growing demand for SMAs in miniaturized applications – such as micro-robotics, elastocaloric cooling systems, and biomedical devices – together with rapid progress in microfabrication technologies, has spurred intensive studies on their behavior at the micro- and nano-scales. As these applications expand, understanding their fatigue performance has become increasing crucial. Unlike conventional metallic materials, SMAs necessitate a specialized approach for fatigue evaluation because their deformation is governed by stress-induced phase transformation. In this work, the fatigue life and cyclic stability of superelastic Ni-rich Nickel-Titanium (NiTi) thin films were examined under various cyclic loading conditions. Stress-controlled fatigue tests were performed using a custom-built micro-mechanical tester. The resulting fatigue responses were systematically analyzed in relation to the microstructural characteristics of the films. The findings indicate that the applied stress ratio plays a critical role in fatigue life. Post-mortem transmission electron microscopy (TEM) analysis was conducted to elucidate the contributions of phase boundaries and dislocations under both low- and high-cycle fatigue regimes. Additionally, the grain size and morphology of semi-coherent $Ni_4Ti_3$ precipitates were identified as key factors influencing cyclic stability. Overall, this study underscores the necessity of precise control over loading conditions and microstructural features for the reliable design and application of SMA thin films in micro-scale devices.

# PHYSICS-INFORMED DISCOVERY OF YIELD FUNCTIONS IN PLASTICITY USING Physics-Informed NEURAL NETWORKS

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**ABSTRACT –** This study presents a physics-informed deep learning framework for discovering elasto-plastic yield functions directly from full-field displacement and reaction force data without using internal stress measurements. The yield function is represented by an input convex neural network (ICNN) that intrinsically satisfies convexity and positive homogeneity, ensuring consistency with rate-independent plasticity. The network is embedded within a finite element formulation and trained by minimizing equilibrium residuals computed from multiple loading scenarios. Validation using von Mises, Hill 1948, and Yld2000-2d models demonstrates that the proposed approach accurately reconstructs both isotropic and anisotropic yield surfaces with minimal data. To ensure compatibility with standard implicit solvers, the learned neural yield surface is further fitted to a smooth polynomial surrogate, enabling integration into conventional return-mapping algorithms. The proposed framework offers a robust and interpretable pathway for data-driven constitutive model discovery in computational plasticity.

# SIZE EFFECTS IN HIGH-STRAIN RATE BEHAVIOR OF SINGLE CRYSTAL ALUMINUM: A FINITE SIMILITUDE APPROACH

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**ABSTRACT-** Laser-induced microprojectile impact testing (LIPIT) offers a desktop- level framework for evaluating the high-strain-rate behavior of materials. However, inherent size effects in microprojectile impact testing—resulting from shallow indentation depths, small-diameter projectiles, and the non-scalability of strain rate effects—impede obtaining scale-independent material properties. This study explores these issues by applying finite-similitude scaling theory, which can potentially correlate the material responses of projectiles across different sizes and indentation depths. Focusing on the second-order finite similitude rule, this study introduces a three-scales scaling theory that integrates data from three distinct scales. This approach enables reliable reproduction of results at any specified indentation depth and projectile size, providing a systematic framework to connect macro and microprojectile impact testing. This multiscaled methodology effectively mitigates size effects arising from microstructural characteristics and different projectile diameters by targeting length as an invariant. Additionally, the method resolves the non-scalability of strain rate effects by establishing correlations among strain rates across multiple scales. Experimental validation is conducted on single-crystal aluminum samples with variable projectile velocities and diameters, revealing the high accuracy and potential of the proposed multiscaled methodology.

# MODELING POROUS/NON-POROUS MEDIA AT DIFFERENT SCALES FOR SUSTAINABLE APPLICATIONS

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**ABSTRACT –** Concrete materials can be conceptualized at the meso-scale as three-phase heterogeneous media comprising coarse aggregates, matrix, and the Interfacial Transition Zone (ITZ) between the matrix and inclusions. Meso-scale modeling necessitates accurate geometry reconstruction and adequately sophisticated material description. Generally, geometry can be acquired through industrial tomography or by means of specific random distribution algorithms capable of reproducing the correct grading curve. A visco-elasto-plasto-damage model is proposed to assess concrete materials under varying loading conditions, with different approaches to geometry reconstruction being applied.

The use of renewable energies is crucial and green hydrogen energy storage plays an essential role as a potent carbon-neutral energy source. Proton Exchange Membrane Water Electrolysis (PEMWE) stands out as a promising technology for producing high purity hydrogen and offers several advantages. Central to this methodology is the macroscopic modeling of multiphase and multilayer systems. The model captures the mechanical behavior of the membrane material, the water flux and pressure in the membrane nano-pores as well as the diffusion of protons through the membrane due to concentration and electric potential gradient, which are the key factors for the PEMWE process.

When accounting for cyclic mobility problems, repeated loading conditions might affect the computational cost. Therefore, the efficiency of finite elements represents a crucial aspect of speeding up the design process. Additive hypoelastic-based and multiplicative hyperelastic-based constitutive equations of the Extended Subloading Surface (ESS) model for three-dimensional finite elements adopting fully implicit integration schemes are considered. Particularly, the constitutive equations of the ESS theory are reformulated for shell and plane stress elements, aiming to obtain an efficient computational tool suitable for cyclic mobility problems. The numerical implementation considers isotropic hardening, kinematic hardening, and material anisotropy.

# ATOMISTICS INFORMED CONTINUUM STRAIN FIELD OF DISLOCATIONS

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**ABSTRACT –** We formulate a novel methodology called Regularized Green's Function Method for Dislocations (RGFMD) for determining the continuum elastic fields of dislocation at the lattice scales. RGFMD utilizes the Quantum Mechanical Force Density (QMFD) to represent atoms within the elastic media without creating any singularities in the elastic fields. QMFD is related to electron wavefunctions, which is a fundamental result of Density Function Theory (DFT) calculations. RGFMD solves the force equilibrium equation where QMFD is used to represent atomic displacements via computationally efficient Fourier Transforms. The quasi-periodic nature of dislocations is accounted for by introducing the periodic images of individual atoms along the dislocation line. The advantage of RGFMD over existing classical elasticity solutions and atomistic simulations for dislocations is threefold: Firstly, RGFMD guarantees to produce well-behaving bounded elastic fields, whereas classical elasticity frameworks diverge at the dislocation core. Secondly, classical elasticity frameworks are built upon the assumption of plane strain conditions, which limits their ability to realistically capture variations in the elastic fields along the dislocation line. RGFMD accurately accounts for the local atomic configuration and does not imply simplifying conditions such as plane strain. Thirdly, atomistic calculations can report elastic quantities such as displacements only at the lattice sites, which precludes their full integration with well-established continuum field theories. RGFMD bridges this gap between atomistic and continuum theories by mapping out continuum elastic fields using discrete displacement data provided by DFT calculations. Upon applying strain, Quantum Mechanical Stress Density (QMSD) can be obtained, which includes kinetic energy, exchange-correlation, and electrostatic interaction effects. We also establish the Quantum Mechanical Moduli Field (QMMF) by taking the derivative of QMSD in this work. RGFM and QMMF consequently result in accurate misfits in size and modulus gradients at atomic scales, providing crucial insights into solute strengthening in structural metals.

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# MOLTEN POOL SHAPE AND IN-SITU NANO (Nb,Ti)C PRECIPITATION ON MECHANICAL PROPERTIES IN LASER DIRECTED ENERGY DEPOSITED IN718/TICP COMPOSITE

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**ABSTRACT –** The microstructure and mechanical properties of laser directed energy deposited TiC strengthened IN718 composite were investigated by mixing IN718 and 1wt.%TiC powders. It is confirmed that the nano (Nb,Ti)C phase is uniformly in-situ precipitated during laser directed energy deposition process, with an average size of 56.85 nm and an aspect ratio of 4.12. The microstructure exhibits a weaker grain texture and 36% reduction in grain size, compared to that of the pure IN718. Specifically, the Laves phase presents a block-like distribution with an average size of 1.29μm within the inter-dendritic regions, contrasting with the chain-like distribution observed in pure IN718, which has an average size of 3.1μm. The weaker texture observed in the IN718/TiCp composite can be attributed to changes in the molten pool shape. And the incorporation of TiC promotes HAGBs proportion within the composite by enhancing the trend of columnar-to-equiaxed transition. The IN718/TiCp composite exhibits an increase of 32.2% in yield strength and an increase of 16.8% in ultimate tensile strength compared to the IN718 deposit. These improvements are primarily attributed to the dispersion strengthening and solution strengthening induced by in-situ precipitation of the nano (Nb,Ti)C phase.

# UNVEILING DEFORMATION MECHANISM OF METAL COMPOSITE USING COMBINED IN-SITU DIFFRACTION EXPEREIMENTS AND FULL-FIELD CRYSTAL PLASTICITY MODELING

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**ABSTRACT –** Diffraction experiments and full-field crystal plasticity modeling demonstrate efficient tools for analyzing the deformation mechanisms of dislocation slip, load transfer, and phase transformation. In this work, a novel high-entropy alloy (HEA) AlCoCrFeNi reinforced magnesium-based composite was fabricated using thixomolding technology. The AlCoCrFeNi/AZ91D composite achieves a well-balanced combination of mechanical properties, as the AlCoCrFeNi particles effectively bear the applied load without cracking or interface debonding. In-situ synchrotron X-ray diffraction reveals that the AlCoCrFeNi particles undergoes a tensile stress up to 418.75 MPa. Additionally, the AlCoCrFeNi particles accommodate matrix deformation through localized plastic slip at their edges. Full-field CPSM simulations reveal a higher von Mises stress, exceeding 1200 MPa at particle edges, while it is only about 700 MPa in the particle interior. This localized high stress, induced by deformation inhomogeneity, fundamentally drives plastic deformation. Further emphasis will be placed on the deformation mechanism of metals with phase transformation characteristics. Exploration of adding phase-transformable reinforcements into magnesium matrix to introduce new mechanisms in magnesium-based composites is ongoing. Considering the limitations in neutron diffraction data processing, we are developing a new method for aligning diffraction experiments and crystal plasticity simulation, which can directly compare Debye rings, differentiate edge and screw dislocations, avoiding the complex process of compressing Debye ring data and spectral fitting.

# A POLYCRYSTALLINE THERMO-ELASTO-PLASTIC CONSTITUTIVE MODEL BASED ON EULERIAN STRAIN FRAMEWORK: THEORY, NUMERICAL IMPLEMENTATION, AND APPLICATION FOR SHOCK AND QUASI-ISENTROPIC LOADING

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**ABSTRACT -** We developed a polycrystalline thermo-elasto-plastic constitutive model within a unified Eulerian strain framework, integrating the experimentally based pressure–volume–temperature equation of state with crystal plasticity theory to describe the response of crystalline materials under arbitrary dynamic high-pressure loading paths across a wide range of strain rates. The integration is theoretically grounded in a covariant Eulerian strain-based volumetric-deviatoric decoupling scheme within thermo-elasticity framework for an objective mathematical description of volumetric deformation energy, with attention paid to the push-forward/pull-back operations between configurations due to its unique covariant nature. Furthermore, the model fully incorporates temperature evolution resulting from both elastoplastic deformation and viscous dissipation. Its capability to capture deformation behavior over a broad range of strain rates stems from the coupling of a previously developed mobile dislocation density model, based on dislocation chain statistics, with a unified thermally activated–phonon drag dislocation motion model. To accurately describe the dynamic response in polycrystals and high-strain-gradient regions, the model also incorporates grain boundary resistance effects and a slip-based discrete strain gradient theory, extending the gradient theory's applicability to dynamic loading conditions. Systematic theoretical analysis and numerical simulations confirm the Eulerian strain framework's advantages in physical consistency and computational robustness. Analytical comparisons reveal that under large shear and compression deformations where traditional Green strain tends to lose stability, the Eulerian strain predicts the evolution of stress, energy, and temperature with superior physical performance and numerical stability. Finite element simulations of flyer-plate impact problems further validate the framework's engineering practicality, demonstrating better computational efficiency, mesh convergence, and numerical stability under extreme pressures compared to the Green strain-based model. Applying this Eulerian strain-based constitutive model, we systematically investigate the dynamic yield behavior of LY12 aluminum alloy under shock and quasi-isentropic loading paths. Through precise analysis of wave profiles during shock-reload/unload processes, it is clarified that existing self-consistent wave profile measurements actually capture the material's yield strength upon the arrival of the secondary stress wave, whereas direct measurement methods such as stress gauge techniques detect the initial yield strength upon the first wave arrival. A series of simulated plate-impact experiments with varying peak pressures elucidate the influences of loading path, microstructure evolution, grain boundary resistance, and strain gradient effects on

the secondary yield strength. This study provides a unified physical explanation for the path dependence of dynamic yield strength under high-pressure loading, clarifying experimental discrepancies and establishing a solid theoretical basis for predicting material dynamic strength.

# ANISOTROPIC YIELD LOCI AND INVERSE SWIFT EFFECT IN EXTRUDED AZ31 MG ALLOY

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**ABSTRACT-**The deformation mechanisms of Mg alloy under combined tensional/compressive and torsional loadings remains critically unclear, which is particularly significant in the case of the anisotropic evolution of yield loci and Swift-inverse Swift effect. In order to clarify the underlying deformation mechanisms, combined axial–torsional non-proportional loading paths are designed. The anisotropic evolution of the yield loci and Swift–inverse Swift effects in extruded AZ31 Mg alloys are investigated. The strong loading-path–dependent twinning activities and underlying deformation mechanisms are clarified. It is found that the inverse Swift effect during free rotational tension (FR_Ten) is attributed to the residual shear stress and initial texture heterogeneity, while the spontaneous macroscopic rotation during free rotational compression (FR_Com) originate from the heterogeneous local strain induced by the interactions of the {10-12} twins. Free end torsion (FE_Tor) pre-straining induces subsequent yield locus (SYL) rotation towards the positive $\tau$ axis and expansion along the negative $\sigma$ axis. The anisotropic Swift–inverse Swift effects are captured by the plastic strain-components on the yield loci. Tensile twinning and basal slip coordinate the plastic deformation under FR_Com-dominated loading paths, owing to the low twin favourability, and the relative activities of non-basal slips under FR_Ten-dominated loading paths are significantly improved. The evolutions of the Swift–inverse Swift effects are determined by elastic pre-loadings, resulting in loading–path-dependent anisotropic evolutions of mechanical responses.

# ALUMINUM-CARBON THIN FILMS WITH HIGH STRENGTH AND DUCTILITY

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**ABSTRACT-** Aluminum (Al) offers advantages such as low residual stress, corrosion resistance, and strong oxidation resistance. However, its relatively low strength necessitates enhancement through microstructural modification via alloying, deposition control, or heat treatment. One promising approach is alloying Al with strong carbon-based nanomaterials, such as carbon nanotubes and graphene. Nevertheless, homogeneous dispersion of these nanomaterials within the Al matrix remains challenging due to the poor solubility between Al and carbon (C).

In this study, we report the exceptional mechanical properties of aluminum–carbon (Al–C) thin films deposited by multi-source co-sputtering. A high-throughput combinatorial approach was employed to investigate the mechanical and electrical properties of compositionally graded Al–C films. Hardness increased with carbon addition, albeit at the expense of electrical conductivity. Rapid screening revealed that regions containing 6.4 at% C achieved a favorable balance between hardness (2.8 GPa) and conductivity (142 Ω·nm). Micro-tensile experiments on freestanding Al, Al–C 6.4 at%, and Al–C 10.3 at% films were conducted to evaluate tensile properties and elucidate the strengthening mechanism. Both Al–C 6.4 at% and 10.3 at% films exhibited markedly higher yield stresses exceeding 300 MPa while retaining ductility. In both cases, plastic flow initiated at an upper yield point, followed by a stress drop to a lower flow stress. The magnitude of the stress drop was ~5% for Al–C 6.4 at% and >10% for Al–C 10.3 at%. This distinct yield-drop behavior resembles that of low-carbon steel, where it is attributed to the formation of a “Cottrell atmosphere.” Uniaxial tensile tests with repeated unloading–aging–reloading cycles confirmed that the yield drop intensified with longer aging times and higher temperatures. Comprehensive microstructural analysis demonstrated that the formation of a Cottrell atmosphere is the primary deformation mechanism in Al–C thin films.

# GRAPHITE UNDER SEVERE SHEAR DEFORMATION-ENROUTE SYNTHESIS OF HEXAGONAL DIAMOND

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**ABSTRACT** - For over half a century, the existence of a hexagonal diamond allotrope(lonsdaleite) has been a subject of scientific controversy. We demonstrate a novel, room-temperature pathway to synthesize lonsdaleite by subjecting graphite nanoplatelets to severe shear plastic deformation under pressure in a rotational diamond anvil cell. Synchrotron X-ray diffraction, multi-wavelength Raman spectroscopy and scanning transmission electron microscopy analysis reveal that a specific combination of uniaxial compression and torsion directly induces a phase transformation from nano-graphite to hexagonal diamond. This mechanism provides a unique alternative to conventional high-pressure/high-temperature synthesis. We detail the transformation mechanism, establishing severe shear deformation as a critical and efficient driver for forming this ultra-hard material under ambient temperature conditions.

# UNIFIED LOW-CYCLE FATIGUE BEHAVIOR AND LIFE PREDICTION OF HIGH-MANGANESE TWIP STEELS UNDER COMPLEX LOADING CONDITIONS

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**ABSTRACT –** This study investigates the low-cycle fatigue behavior of high-manganese TWIP steel at specimen orientations of 0°, 22.5°, 45°, 67.5°, and 90° relative to the rolling direction, tested at temperatures of 295K and 449K. Fatigue tests covered a total strain amplitude range of 0.6% to 2.4%, under both pre-deformed (M-type, P-type) and non-pre-deformed (F-type) loading conditions. Results indicate that higher temperatures enhance ductility but decrease strength. Notably, severe pre-straining at 449K significantly reduces fatigue life, contrasting with the behavior at room temperature. The deformation mechanisms and fatigue responses are influenced considerably by loading orientation, strain amplitude, and temperature. A life-prediction model was developed to account for these varying mechanisms, successfully predicting fatigue lives across 77 different loadings, including five orientations, seven strain amplitudes, three loading modes, and two temperatures. All predicted results fall within a 2.5× error band, with 97.4% of predictions residing within a 2× error band. The comparison between experimental results and model predictions highlights the model's robust proficiency in accurately characterizing the fatigue life of high-Mn TWIP steel, thereby confirming its effectiveness in capturing complex fatigue behaviors under diverse conditions.

# FATIGUE-RESISTANT ALLOYS THROUGH DYNAMIC PLASTIC DEFORMATION DELOCALIZATION ACTIVATION

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**ABSTRACT –** The development of fatigue-resistant structural alloys requires not only enhanced monotonic strength but also the ability to mitigate damage initiation and propagation under cyclic loading. Conventional alloy design strategies often emphasize strengthening mechanisms such as solid-solution hardening, precipitation, or microstructure refinement. However, these approaches typically promote intense plastic deformation localization at the microstructural scale, which in turn accelerates fatigue crack initiation and propagation. As a result, a persistent tradeoff between strength and fatigue resistance efficiency is generally observed in metallic alloys. To overcome this limitation, it is critical to suppress intense plastic strain localization during deformation.

In this work, we reveal a previously unidentified mechanism of plasticity deformation delocalization that dynamically (during deformation) promotes the homogenization of deformation and prevents localized strain accumulation. This mechanism occurs within a narrow range of stacking fault energies and originates from the competition between nanoscale planar defects and dislocation slip. We refer to this phenomenon as *dynamic plastic deformation delocalization*, a concept that opens a new design space for engineering fatigue-resistant alloys. We demonstrate, in face-centered cubic solid solution–strengthened metallic alloys, that activation of this mechanism significantly enhances fatigue strength.

# APPLICATION OF DIGITAL IMAGE CORRELATION TECHNOLOGY FOR CHARACTERIZATION OF ELASTO-PLASTICITY, NECKING, AND FRACTURE PROPERTIES OF SHEET METAL

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**ABSTRACT-** This paper focuses on new developments in application of Digital Image Correlation (DIC) technology for calibration of constitutive and failure models of sheet metals. The paper presents results from a newly developed software application called DIC Database Manager, capable of automatically recognizing and processing data files created by commercial DIC programs. Processing includes the extraction and analysis of material properties and failure limits for the purpose of calibrating advanced material models. In addition to recognizing the data from both bulge tests and uniaxial tension tests pulled at any angle to the Rolling Direction (RD) of the sheet coil, the software automatically determines the range of data during elastic loading to determine the elastic properties, then automatically decomposes the strains into elastic and plastic components and uses the latter to determine the R values and stress-strain hardening function. In addition to these standard constitutive properties, the software also takes advantage of the DIC system data to determine variability in the properties across the dimension of each specimen. Finally, again taking advantage of DIC data, the software also automatically determines the onset of localized necking, if a neck is detected in the data, and a lower bound of the fracture limit, if the test has been run to the point of a detected fracture.

# STEADY-STATE ELASTIC PLASTIC SHOCK WAVES IN A LOW-SYMMETRY MOLECULAR CRYSTAL

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**ABSTRACT-** Large-scale non-equilibrium molecular dynamics simulations of RDX shocked along [100] reveal a steady-state regime of elastic-plastic shock wave propagation along slip-hindered directions of molecular crystals. For a shock with a particle velocity of 1 km/s, steady state is achieved after approximately 100 ps or 0.5 microns from the impact plane. The transient regime is characterized by a dynamic evolution of plasticity, which transitions from the simultaneous nucleation of a high density of shear bands to the growth of fewer shear bands, each resulting in significant localized shear strain and temperature. This evolution of the plastic wave leads to a significant attenuation of the elastic precursor, with a 20% drop in stress along the shock direction. This significant variation in the structure of the shock wave over distances larger than most atomistic simulations to date highlights the need for continuing efforts towards scalable molecular simulations and the challenges in multiscale modeling of dynamical properties.

# A PHYSICAL-BASED CRYSTAL PLASTICITY MODEL FOR HIGH-MANGANESE STEEL CONSIDERING γ-ε-α' MARTENSITIC TRANSFORMATION

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**ABSTRACT –** Micromechanical models are capable of accurately describing and simulating the characteristic plastic deformation behavior of high-manganese steels exhibiting twinning-induced plasticity (TWIP) and transformation-induced plasticity (TRIP) effects at the macro level. However, the uncertainty in describing the evolution of state variables based on crystal plasticity theory poses a great challenge in handling the complex plastic deformation with different deformation mechanisms, complicated interactions, and interplays at microscopic scale. Consequently, this work systematically investigates the plastic deformation mechanisms and evolution in a typical Fe-18Mn-1.6Al-0.6C high-manganese steel under multiple microscopic mechanisms. The slip and twin mechanism are studied from the dislocation point of view, and the phase transition path of γ-ε-α′ is considered in the TWIP phase transition at the same time. A physical-based crystal plastic finite element (CPFE) model considering γ-ε-α′ transformation is established, and the deformation behavior of Fe-18Mn-1.6Al-0.6C high-manganese steel is analyzed. Through crystal plastic finite element simulation, it is found that the formation of twin can obviously strengthen the hardening of the material. The γ-ε martensite transformation is only used as a strengthening phase to cut austenite grains to refine the grain, and ε-α' martensite transformation which is used as the subsequent deformation of γ-ε, acts on hardening by affecting the volume fraction of ε-martensite. At the same time, when martensite transformation occurs during plastic deformation, there is a strong variant selection. The model serves as a feasible approach to reflecting the micro deformation mechanisms during the plastic deformation process of high-manganese steel.

# CYCLIC TRANSFORMATION-INDUCED PLASTICITY, ELASTOCALORIC COOLING AND SYSTEM PERFORMANCE DEGRADATION

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**ABSTRACT –** Elastocaloric cooling/heating by harvesting latent heat from phase transition of shape memory alloys (SMAs) attracts considerable interest as a greenhouse gas-free alternative to conventional vapor-compression refrigeration. This talk reviews new developments in this SMA-based emerging technology. It focuses on cyclic phase transition induced dislocation accumulation and the resulting functional degradations at both material level and system level cooling performance. New material science research efforts in developing high performance fatigue-resistant SMAs by composition, processing and microstructure control are emphasized. So far, kilowatt-scale elastocaloric cooling prototypes have been built based on cyclic compressive phase transition of solid state NiTi SMA refrigerant. Large specific heat transfer area of NiTi tubular structure and heat transfer nano-fluid enables a large cooling power density of 12.3 W g-1, total cooling power of 1284 Watt, and a temperature lift of 75 K. These works have demonstrated great potential of this disruptive technology for space cooling and heating in the future. This talk also summarizes progress and challenging issues in SMA-based elastocaloric refrigeration technology based on our recent publications in Nature, Nature Energy, Nature Nanotechnology, Nature Communications, and Joule. Multidisciplinary interaction and collaborations among material science, solid mechanics, heat transfer, manufacturing and fluid mechanics in both theory, experiment and computation will be demonstrated. Some important aspects in design, manufacturing, characterization and scientific understanding in developing this disruptive technology will also be highlighted.

# A FULLY COUPLED MULTI-PHYSICS MULTI-PHASE FIELD CRYSTAL PLASTICITY FINITE ELEMENT MODEL (MPF-CPFEM) FOR PREDICTING MICROSTRUCTURE EVOLUTION AND THERMOMECHANICAL BEHAVIOR IN ADDITIVE MANUFACTURING

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**ABSTRACT -** In additive manufacturing (AM), the interactions between thermomechanical stress and microstructure evolution demonstrate complex coupling mechanisms due to the dynamic motion of the multi-physics molten pool, influencing residual stress prediction, defect control, and performance design. However, models incorporating the two-way coupling mechanisms in AM remain undeveloped. Therefore, this study proposes the first two-way fully coupled multi-physics multi-phase field crystal plasticity finite element model (MPF-CPFEM) simultaneously simulating microstructure evolution and thermomechanical coupling behavior in AM processes. Linking with the thermal-fluid flow model, the MPF-CPFEM model enables the dynamic coupling of multiple mechanisms, including heterogeneous deformation, dislocation density evolution, polycrystalline mechanical response, and microstructure evolution such as recrystallization, grain growth, and liquid-solid transformation. MPF and CPFEM utilize shared dynamic unstructured meshes to achieve simultaneous predictions of thermal stress, non-uniform plastic deformation, and microstructure evolution during AM processes, supported by a newly proposed element-free Galerkin-based finite difference method (EFG-FDM) to derive and solve nonlocal variables, such as phase fields and geometrically necessary dislocations, thereby reducing dependence on the selection of basis functions while maintaining both sufficient accuracy and efficiency. The material constitutive model comprehensively considers a wide temperature range (from room temperature to the melting point) and the rate-dependent stress response characteristics. The dynamic evolution and interactions among thermomechanical response (including residual stress), plastic deformation, dislocation density, and microstructure during a single-track laser powder bed fusion (LPBF) process are captured for the first time. The physical mechanisms underlying unconventional phenomena, such as the type of recrystallization in LPBF processes, are also uncovered. This two-way coupling model is expected to offer insights into microstructure regulation and process optimization in AM.

# MICROSTRUCTURAL ORIGIN OF DWELL-FATIGUE DEBIT IN NEAR-α TITANIUM ALLOYS

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**ABSTRACT –** Dwell fatigue in titanium alloys is a critical concern for aeroengine components, where stress held at ambient temperatures can severely reduce fatigue life. This work systematically investigates the role of crystallographic texture, micro-texture, and processing-induced microstructural variations on the dwell fatigue behaviour of near-α titanium alloys using a combination of experiments, electron backscatter diffraction (EBSD), and crystal plasticity fast Fourier transform (CPFFT) simulations.

Experiments reveal a significant anisotropy in the strain hardening when deformed along the rolling direction compared to the transverse direction which was attributed to the difference in texture which eventually led to the anisotropy of dwell fatigue life. The stress hotspots were identified and correlated with the initial texture. These findings establish texture as a primary driver of dwell fatigue anisotropy in a single-phase titanium system.

The results of cyclic and dwell fatigue tests reveal that the presence of micro-textured regions (MTR) in the forged billet reduces the fatigue life of the material, under dwell fatigue conditions. The microscopic observation of dwell fatigue crack initiation sites provides new insights into the three-dimensional arrangement of neighbouring grains and their role in facilitating stress transfer and crack propagation. By integrating experiments polycrystal modelling, this work provides mechanistic insight into stress localization, slip activity, and failure initiation, offering pathways toward microstructure-informed alloy design for improved dwell fatigue resistance.

**Keywords:** Titanium alloy, Dwell fatigue, Texture, Microstructure, Crystal plasticity simulation

# AN ELASTO-VISCOPLASTIC APPROACH TO POLYMER RHEOLOGY

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**ABSTRACT –** This presentation examines the rheology of polymer melts and solutions through a standard elasto-viscoplastic framework. Using the recoverable strain—a tensorial measure of elastic deformation stored in the material—as a central variable, we derive thermodynamically consistent evolution equations within the GENERIC (General Equation for Non-Equilibrium Reversible–Irreversible Coupling) formalism. From this basis, we propose a compact closed-form expression for the stress tensor that, despite its simplicity, captures essential nonlinear phenomena while requiring only linear viscoelastic input data.

Analytical solutions are provided for stationary states in common flow fields. A multimode extension is validated against experimental data for elongational, shear, and superposed flows of polymer melts, and benchmarked against established non-separable constitutive models, notably the Leonov model. Connections to the empirical Cox–Merz relation are discussed.

To broaden applicability, we introduce two optional nonlinear parameters to fine-tune material responses and outline thermodynamically consistent modifications, underscoring the model's flexibility. Overall, framing rheology in terms of recoverable strain enables accurate representation of strongly nonlinear effects—such as shear thinning and strain hardening—within a structure that relies solely on linear material input.

# HYDROGEN EMBRITTLEMENT IN ENERGY INDUSTRY: PERSPECTIVE ON MECHANISMS AND EMERGING CHALLENGES IN $H_2$ and $CO_2$ TRANSPORTATION

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**ABSTRACT –** The energy industry operates in environments that expose materials to hydrogen in service in upstream, midstream, and downstream operations. For instance, U/S pipelines and flow lines must endure a combination of mechanical loading and aggressive corrosive environment, while resisting environmental assisted cracking from high concentrations of hydrogen sulfide ($H_2S$) due to hydrogen-induced cracking (HIC) and sulfide stress cracking (SSC). Similarly, in refining and petrochemical processes, equipment is exposed to high pressure hydrogen in various hydrotreating processes. Recently, there is a strong interest in carbon capture and storage (CCS) and hydrogen as an alternative fuel to decarbonize "difficult to decarbonize industries".

In this presentation we discuss our work on the mechanisms of hydrogen embrittlement in high pressure H2 gas and under electrochemical charging conditions. Following that we discuss our efforts to enable the use of carbon steels in severe sour service as carbon steels are cost effective structural materials than specialized corrosion resistant alloys and corrosion-resistant claddings. We will then discuss the emerging challenges associated with transportation of hydrogen and CO2 through pipelines. Hydrogen infrastructure, for example, faces decreased fracture toughness of steels, which poses challenges for repurposing existing infrastructure for hydrogen service. For CCS, we will discuss the emerging challenge associated with dilute (~1 bar partial pressure) H2 as an impurity in CO2 pipelines, and approaches being taken to effectively manage this challenge using engineering and scientific insights. These challenges demand a multidisciplinary approach combining advanced materials design, mechanics, modeling and inspection to ensure structural integrity and reliability of assets.

# AB-INITIO INSIGHTS INTO THE INTERACTIONS OF HYDROGEN WITH METALS IN ELECTROCHEMICAL ENVIRONMENT

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**ABSTRACT –** Reactions of hydrogen with metal surfaces are intimately linked to material degradation phenomena such as corrosion and hydrogen-embrittlement. A detailed atomistic understanding of these interactions and the underlying reaction mechanisms is essential for developing strategies to mitigate such detrimental processes. Density-functional theory calculations and ab-initio molecular dynamics calculations, provide a powerful framework for probing hydrogen–metal interfaces at the electronic level. Together with our resent methodological advances of a efficient computational electrode and a thermopotentiostat for constant-potential simulations they enable unprecedented insight into H interactions with electrified solid/liquid interfaces, enabling us to quantify H uptake and identify reaction mechanisms under realistic electrochemical conditions. We employ these tools to (i) elucidate the mechanisms that render low-alloyed steels especially vulnerable to sour-gas ($H_2S$) corrosion, and (ii) resolve the long-standing puzzle of anomalous hydrogen evolution and the associated high corrosion rate observed on anodically polarized magnesium. The fully atomistic reaction pathways we present reconcile the experimental findings, while the underlying methodologies constitute a versatile framework for probing hydrogen interactions and uptake in electrochemical environments. This capability is directly relevant to a broad spectrum of bulk and surface degradation processes.

# NUMERICAL MODELING OF THERMAL HISTORY– AND STRAIN RATE– DEPEDENT DOUBLE YIELDING BEHAVIOR OF SEMI-CRYSTALLINE POLYMER

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**ABSTRACT** – The microstructure of a semi-crystalline polymer (SCP) is a two-phase composite consisting of crystalline and amorphous regions. Their distinct deformation mechanisms and interactions lead to complex viscoelastic–viscoplastic behavior, including double-yielding (DY). This DY behavior is strongly influenced by thermal history, as the crystallization of molecular chains depends on temperature [1]. In addition, the strain rate also affects DY behavior because the strain-rate dependence differs between the crystalline and amorphous phases. In this study, we experimentally evaluated and numerically modeled the effects of thermal history and strain rate on the DY behavior of SCPs.

In the experimental part, uniaxial tensile tests at different strain rates were performed on polyamide (PA) specimens prepared at various annealing temperatures. The first yield stress was governed solely by the strain rate, whereas the annealing temperature influenced only the second yield stress. These results indicate that the first and second yielding are primarily associated with the amorphous and crystalline phases, respectively.To reproduce the experimentally observed DY behavior under different thermal histories and strain rates, the viscoelastic–viscoplastic transient network model [2] was extended. The proposed approach requires more than 20 material parameters to capture the complexity of DY behavior. To identify parameters that accurately reproduce the experimental results, we introduced a machine-learning-supported fitting scheme. Finite element simulation results based on the parameters obtained with this method successfully reproduced the experimentally observed mechanical responses.

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# HYDROGEN-INDUCED FAST FRACTURE IN A 1.5 GPa DUAL-PHASE STEEL

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**ABSTRACT –** Developing high-strength steels for structural applications with a high strength-to-weight ratio is crucial for reducing the carbon footprint associated with both production and service. However, enhanced strength can result in an increase in susceptibility to hydrogen embrittlement (HE). The presence of hydrogen, even in quantities ~0.1 ppm, can render high-strength steels brittle, a phenomenon known as HE. This work explores the strategy of introducing ductile ferrite to mitigate HE in a 1.5 GPa ferrite-martensite dual-phase steel. Despite the presence of 25% ferrite, upon tensile loading an electrochemically hydrogen charged specimen (3.8 mass ppm diffusible H) at a strain rate of $10^{-4}$ $s^{-1}$, the DP steel fractured within the elastic limit at 900 MPa. Detailed fractographic analysis, along with site-specific transmission electron microscopy (TEM) analyses of the fracture surface, were performed to elucidate the underlying failure mechanisms:

1. Firstly, we present the limitation of fractography in understanding HE; while the uncharged sample exhibited predominantly brittle fracture, the pre-hydrogen-charged specimens displayed mixed-mode fracture characteristics, combining both ductile and brittle features.
2. The observed HE response is explained by the hydrogen-induced fast fracture (HIFF) model. We propose modifications to the crack nucleation mechanism described in the HIFF model.
3. The formation of the river pattern features on the {100} ferrite cleavage surface is explained based on TEM investigations.

# THE EFFECTS OF HYDROGEN TRAPPING AT GRAIN-BOUNDARIES AND PRECIPITATE INTERFACES ON MECHANICAL PROPERTIES: A MOLECULAR DYNAMICS STUDY

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**ABSTRACT –** The successful realization of a hydrogen economy is crucially dependent on a comprehensive understanding of the effects of hydrogen on the hydrogen infrastructure materials and the development of hydrogen compatible materials with long term reliability. An overview of a recent university-national laboratory-industry collaborative effort on understanding the effect of hydrogen on the mechanical properties of hydrogen-facing materials is presented. In particular, a molecular dynamics (MD)-based modeling framework is developed to understand hydrogen trapping by precipitates and their influence on dislocation-precipitate interactions in a model system with Fe matrix and Cu nano-precipitates. It is found that the interface regions (esp., incoherent interfaces) between the matrix and the precipitate serve as efficient hydrogen trapping sites. The hydrogen that is trapped at the precipitate-matrix interface increases the critical stress for dislocation movement. The critical stress for dislocation movement across precipitates depends on the nature of the interface, precipitate size, dislocation line lengths, and hydrogen concentration. Furthermore, MD simulations are invoked to study hydrogen trapping at ferrite-ferrite grain boundaries in pearlitic steels. It is observed that the ferrite grain boundary misorientation angle has a strong influence on hydrogen trapping and has a significant influence on its mechanical strength.

# THE EFFECT OF MICROSTRUCTURAL INERTIA ON PLASTIC LOCALIZATION AND VOID GROWTH IN POROUS SOLIDS

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**ABSTRACT –** We investigated the impact of microstructural inertia on plastic localization, void growth, and coalescence in ductile porous materials subjected to high strain rates. For that purpose, we have performed finite element calculations on a flat double-notched specimen subjected to dynamic plane strain tension. The simulations employ three distinct approaches to model the mechanical behavior of the porous aggregate: (1) discrete voids within a matrix material governed by von Mises plasticity; (2) homogenized porosity represented using standard quasi-static Gurson-Tvergaard plasticity; and (3) homogenized porosity described with Gurson-Tvergaard plasticity extended by Molinari and Mercier (2001) to account for microinertia effects. The porous microstructures used in the simulations are representative of additive manufactured metals, featuring initial void volume fractions varying between 0.5% and 4%, and pore diameters ranging from 30 μm to 150 μm. The applied tensile velocities ranged from 100 m/s to 1000 m/s, producing maximum strain rates between 105 s−1 and 106 s−1, and stress triaxiality values spanning from 4 to 30. The simulations with discrete voids validate the calculations performed using homogenized porosity and microinertia effects, demonstrating that higher strain rates and larger pore sizes lead to slower void growth and a delayed, regularized plastic localization. Conversely, the standard Gurson Tvergaard model shows notable mesh sensitivity and fails to describe the influence of the loading rate on plastic localization. Ultimately, the comparison between finite element models with discrete voids and those with homogenized porosity illustrates the stabilizing effects of porous microstructure and multiscale inertia on dynamic plastic flow, while also highlighting the strengths of the constitutive model introduced by Molinari and Mercier (2001) for simulating engineering problems involving porous ductile materials subjected to high-velocity impacts.

# HIGH-VELOCITY FRAGMENTATION AND SPALL FRACTURE OF STEEL AF9628

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**ABSTRACT –** This paper investigates the mechanics of high-velocity fragmentation and spall fracture of steel AF9628. An experimental campaign was conducted, comprising 25 ring expansion tests and 36 planar plate impact experiments using a single-stage light-gas gun. In the ring expansion tests, a conical-nosed cylindrical projectile impacts a thin walled tube over which the specimen is inserted, inducing multiple necks and fractures across the circumference of the ring as the tube expands. Two high-speed cameras captured the deformation and fracture processes, synchronized with photonic Doppler velocimetry to measure the radial expansion velocity of the ring, corresponding to strain rates of ≈ 8000 $s^{-1}$ to ≈ 15000 $s^{-1}$ at impact velocities of ≈ 240 m/s to ≈ 370 m/s. Fragments were soft-recovered, sized, weighed, and analyzed via scanning electron microscopy and X-ray tomography, revealing a mixture of equiaxed tensile dimples and elliptical shear dimples, with the number of necks and fragments increasing with expansion velocity. In the planar plate impact experiments, disc-like projectiles impacted stationary disc-like targets at velocities from ≈ 380 m/s to ≈ 780 m/s. The target thickness was twice that of the projectile, positioning the spall plane near the center. Photonic Doppler velocimetry measured axial free-surface velocity, providing data on shock pressure, Hugoniot elastic limit, spall strength, and strain rates ranging from ≈ 5 × 104 $s^{-1}$ to ≈ 1.7 × 105 $s^{-1}$. Soft-recovered targets were analyzed by scanning electron microscopy (SEM) and X-ray tomography, which allowed three-dimensional reconstruction of spallation and quantitative assessment of fracture size and volume evolution. SEM investigations showed void growth, coalescence, and intervoid cracking as dominant mechanisms, with no clear influence of microstructure on crack propagation paths.

# EXCELLENT CRYOGENIC-TEMPERATURE STRENGTH AND DUCTILITY REALIZED BY COUPLING δ PHASE AND TRIP EFFECT

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**ABSTRACT –** The high-temperature (delta, δ) phase in steels is traditionally considered detrimental to mechanical properties with severe embrittlement. This study challenges that perspective by strategically coupling the δ phase with transformation-induced plasticity (TRIP) to develop a novel duplex stainless steel exhibiting an excellent combination of strength and ductility at cryogenic temperatures. The δ phase exerts suppressive and stimulative impacts on thermal-induced and strain-induced martensite formations, respectively. Through optimization of the δ content, a critical fraction of γ phase is retained at -150 °C, enabling a sustained TRIP effect. This microstructure design results in outstanding mechanical properties, including a tensile strength of ~1 GPa and a plastic strain of ~30% during deformation at -150 °C. The proposed approach provides a generalizable strategy for overcoming the cryogenic-temperature brittleness and is anticipated to be applicable to a wide range of alloy systems.

**Key words**: Duplex stainless steel; Delta phase; Austenitic stability; TRIP effect; Cryogenic-temperature strength and ductility

# REJUVENATION MECHANISM INDUCED BY CYCLIC LOADING IN SIMULATION

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**ABSTRACT-**Rejuvenation in metallic glasses (MGs) is a vital process for improving their mechanical and functional properties, yet its underlying atomic-scale mechanisms remain poorly understood. Unlike thermal quenching, strain cyclic loading offers a straightforward and practical approach to induce rejuvenation in MGs. In this study, we employ molecular dynamics simulations to investigate the rejuvenation mechanism in $Cu_{45}Zr_{45}Al_{10}$ MGs under strain cyclic loading. Our results demonstrate that the number of strain cycles plays a key role in modulating the energy state and dynamic relaxation behavior of the material. Analysis of the dynamical and structural responses during mechanical cycling reveals that rejuvenation enhances dynamic heterogeneity across the system—not only within soft regions but also inside structurally rigid zones. Importantly, rejuvenation exerts a comprehensive influence on all atoms, affecting both their dynamic behavior and local structural order. We also observe that non-activated atoms identified through dynamical mechanical spectroscopy correlate strongly with atoms in local five-fold symmetric environments. However, the structural characteristics of activated atoms require further exploration. This work elucidates the micro-scale dynamic and structural evolution associated with strain-cycle-induced rejuvenation in MGs, providing theoretical insights that can guide the design of strategies for tuning the properties of such metastable materials.

# LOCAL STRAIN MODULATION BY THE LPSO PHASE OF LAMELLAR AND BLOCKY MORPHOLOGY IN MG ALLOYS

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**ABSTRACT-** The long period stacking ordered (LPSO) phase has been the research focus of high-performance Mg alloys for more than two decades, especially those aiming for high strength and ductility. The understandings of the effect of LPSO phase on mechanical properties arose mostly from macroscopic or nano-scale experiments, e.g. synchrotron diffraction and TEM characterization, yet the mesoscale studies have been lacking. This is primarily due to the technical obstacles for resolving the slip activities between the very fine LPSO lamellae inside grains, and indexing the orientations of the blocky LPSO and thereafter describing the phase boundary characteristics. This talk firstly reports the advancements in high resolution digital image correlation analysis and dictionary indexing of EBSD patterns, both crucial for understanding the deformation behaviors at mesoscale. Aided by these techniques, the strain localization behavior in Mg matrix induced by LPSO lamellae, and the strain accommodation at the phase boundary between Mg grain and LPSO blocks were investigated. It was found that closely-spaced intragranular lamellae of high elastic stiffness elevate the local stress level and thereby induce localized basal strain, which could lead to micro-crack formation at low strain level. The intergranular LPSO block shares coherent phase boundary with Mg matrix grain at homogenized state. This enables continuous dislocation slip across phase boundary, without any obstructing effect. Therefore, most of the LPSO phase boundaries provide good strain accommodation, with the LPSO blocks co-deform with the adjacent Mg grain. These results provide important new insights for the effect of LPSO phase on ductility of bulk material.

# DESIGN OF TITANIUM ALLOYS INTEGRATING MECHANISM AND INTELLIGENCE

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**ABSTRACT** –Light and strong titanium alloys are key structural materials in aerospace and other fields. At present, artificial intelligence assisted research and development of titanium alloys is gradually developing, but due to the limited understanding of the microscopic deformation and phase transformation mechanisms, we are still far from the intelligent design of titanium alloys.

In the last 20 years, we have developed a multiscale integrated computational design platform for structural metallic materials. We have systematically investigated a variety of atomic processes in the plastic deformation and phase transformation of metals and alloys, in particular Ti-based alloys. Combined with experimental characterization, we have demonstrated the process point defects clustering and strengthening effect caused by dislocations through dipole reactions and revealed new phase transitions and twin mechanisms under plastic deformation or additive manufacturing. Our work regarding the multiscale performance evaluation of Ti-based alloys was selected as one of the best applications of Materials Genome Engineering in China during 2016-2020. In the recent years, with the above knowledge on mechanisms and with the help of artificial intelligence, we focused on the integrated computational design of the of titanium alloys, combined with computational simulation, experimental characterization and data technology, to reveal the relationship between microscopic defect behavior, microstructure evolution, as well as processing and service performance. We have set up several mechanical property model driven synergically by mechanism and data: 1) the relation between composition and tensile properties for additive manufactured Ti64; 2) creep strain prediction for high-temperature Ti alloys; 3) fatigue life prediction for additive manufactured Ti17; 4) fatigue property evaluation for additive manufactured Ti alloy lattices. These results have largely aided the applications of corresponding materials or components.

**Keywords**: Materials genome, Titanium alloys, Artificial intelligence, Mechanical property

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# DAMAGE EVOLUTION OF MULTI-TYPE VOIDS DURING PLASTIC DEFORMATION OF HIGH-CARBON STEEL USING CRYSTAL PLASTICITY FINITE ELEMENT MODELING

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**ABSTRACT –**During the deformation process of high-carbon alloys, three types of voids are formed through three distinct mechanisms: Matrix-cracking Voids (MCVs), Particle-cracking Voids (PCVs), and Interface-debonding Voids (IDVs). The nucleation of these three types of voids exerts different influences on the subsequent void growth, coalescence, and ductile fracture of high-carbon steel. To identify the three types of voids under mesoscopic inhomogeneous deformation, this study establishes a crystal plasticity finite element model (CPFEM) that accounts for different nucleation mechanisms. Specifically, the model employs a non-local dislocation density crystal plasticity constitutive model combined with a local stored energy density criterion to describe the deformation and void nucleation of the matrix in high-carbon steel; An elastic constitutive model paired with a maximum principal stress criterion to characterize the deformation and cracking of particles; A cohesive zone model coupled with a fracture energy criterion to depict the deformation and void nucleation at the particle-matrix interface. The reliability of the developed CPFEM model is verified using the nucleation positions and quantitative changes of the three types of voids obtained from in-situ tensile tests. The results reveal that PCVs are prone to form in particles located within deformation bands and with high shape irregularity; IDVs tend to nucleate at the interfaces of smaller particles in deformation bands; MCVs are likely to develop in grains with high Schmid factors and high aspect ratios. The void area fractions (VAFs) of all three void types exhibit an initial incubation stage followed by exponential growth. Additionally, the study uncovers the influence laws of particle volume fraction and grain size on the nucleation strain, total VAF, and VAF proportion of the three types of voids.

# X-RAY MICROTOMORGRAPHY INVESTIGATIONS OF SAND PARTICLE BREAKAGE AIDED BY DISCRETE PARTICLE TRACKING

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**ABSTRACT** - Particle breakage is well known to have a significant impact on the mechanical behavior of crushable soils. In this study, the in-situ X-ray computed microtomography (μCT) was used to explore the sand particle breakage behavior within a miniature sample of sand subject to single particle crushing test, oedometer test and triaxial test. The major innovation of this study lies in the development and use of a series of advanced discrete particle tracking techniques including include the point cloud registration (PCR), 3D signature of histograms of orientation (SHOT) and SHOT++ in the recognition and tracking of all crushed particles during the sample deformation process.

# MULTI-SCALE INVESTIGATIONS ON DAMAGE AND ANISOTROPIC TENSILE BEHAVIOR OF TITANIUM MATRIX COMPOSITES WITH A NOVEL TIB-NETWORK ARCHITECTURE AT HIGH TEMPERATURE

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**ABSTRACT –** Titanium matrix composites (TMCs) reinforced by discontinuous network of TiB fibers have a good service performance at temperatures exceeding 600℃. The novel TiB-network architecture reinforced its strength, while leading to anisotropic tensile behavior. The damage mechanisms and tensile anisotropic behavior induced by TiB during TMCs deformation processes remain unclear. In this study, tensile tests on TMCs with two different TiB-networks were carried out at 600℃. The results show that a higher TiB fiber distribution density achieves higher ultimate tensile strength of TMCs. To clarify the underlying mechanism, a crystal plasticity constitutive model coupled with continuum damage mechanics (CDM-CP) was established, and the mesoscale deformation, damage evolution, and macroscopic tensile anisotropy of TMCs were accurately simulated. On this basis, the effects of three spatial distribution types of TiB, triple points (Tri-TiB), grain boundary (GB-TiB) and intragranular (In-TiB) on the mesoscopic deformation behavior of the material were quantitatively investigated. It was found that the damage during tension of TMCs occurs preferentially in the Tri-TiB distribution zone, followed sequentially in the GB-TiB and In-TiB distribution zones. Tri-TiB and GB-TiB synergistically exacerbate the mesoscopic heterogeneous deformation of TMCs at grain boundaries, while In-TiB induces intragranular damage in the material. Additionally, the differences in grain and TiB orientations result in the varying of load-transfer efficiency, leading to the anisotropic tensile behavior of TMCs. These findings provide a novel perspective for improving the high-temperature mechanical properties of TMCs through microstructure design.

# OVERCOMING THE SPECIFIC STIFFNESS/DUCTILITY TRADE-OFF IN ZX50/SIC MAGNESIUM COMPOSITES THROUGH SOLUTE-SEGREGATION INTERFACE STRENGTHENING

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**ABSTRACT-** Structural metallic alloys face a fundamental limitation in specific stiffness (≈26 $MJ \cdot kg^{-1}$), which conventional strategies cannot overcome, while particle-reinforced metal-matrix composites (PRMMCs) often suffer from poor ductility due to weak interfacial bonding. This study presents a novel Mg-5Zn-0.2Ca/SiC composite (ZX50/SiC) manufactured via scalable semi-solid stirring and extrusion, achieving an exceptional combination of high specific stiffness (34 $MJ \cdot kg^{-1}$), strength (>300 MPa), and ductility (>7%). The enhanced performance is attributed to Zn/Ca co-segregation at the particle/matrix interface, which strengthens atomic bonding and delays interface decohesion, coupled with the activation of <c+a> dislocations that promote deformation-induced dynamic recrystallization at crack tips, enabling crack blunting and improved damage tolerance. These mechanisms effectively overcome the stiffness-ductility trade-off, providing a pathway for developing high-performance magnesium composites for industrial applications.

# BREAKING THE STRENGTH-DUCTILITY TRADE-OFF IN 600 ℃ HIGH-TEMPERATURE TITANIUM ALLOYS VIA RAPID HEATING

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**ABSTRACT –** Performance optimization of 600 ℃ high-temperature titanium alloys is crucial for advancing aerospace vehicle development. While titanium alloys with a fully lamellar structure exhibit excellent high-temperature strength, they often suffer from a significant reduction in room-temperature ductility, posing a critical challenge in balancing strength and ductility. In this study, a rapid heating (100℃/s) and aging (RHA) process is employed to fabricate Ti60 alloys featuring submicron-sized lamellar α phase ($\alpha_m$), nanosized lamellar α phase ($\alpha_n$), and multiscale silicides. The RHA-treated alloy achieves exceptional room-temperature elongation of 5.32%, representing a 5-fold improvement compared to the β-solution-treated sample. At 600°C, the alloy exhibits remarkable creep resistance: steady-state creep rate reduces from $4.65\times10^{-6}$ $s^{-1}$ to $1.22\times10^{-6}$ $s^{-1}$, with a 2-fold extension in creep life to 105.8 h under 300 MPa compared with the initial state, approaching the performance of β-solution-treated sample. High heating rate effectively inhibits element diffusion, preventing Si and β-stabilizing elements from accumulating at the prior β phase boundary. Consequently, nanosized silicides precipitation during aging treatment is markedly reduced, avoiding stress concentration at the prior β phase boundary. Submicron-sized silicides serve as load-bearing elements. Nanosized silicides not only pin the lamellar α-phase boundaries to suppress grain boundary sliding but also effectively impede dislocation motion via the Orowan strengthening. Simultaneously, submicron-sized lamellar $\alpha_m$ within the matrix acts as a "skeleton" bearing substantial loads and undergoing plastic deformation. The improved room-temperature ductility mainly originates from strain compatibility enabled by heterogeneous α lamellae. The synergistic interaction between the heterogeneous matrix and multiscale silicides significantly enhances the high-temperature creep resistance of Ti60 alloy. This work demonstrates that controlled heterogeneity via RHA effectively reconciles the strength-ductility trade-off, providing a viable pathway for developing next-generation high-temperature titanium alloys for aerospace applications and expanding the service limits of current alloys.

# ENHANCED PYRAMIDAL SLIP IN MAGNESIUM ALLOYS VIA GADOLINIUM ALLOYING AND ITS EFFECT ON PLASTIC DEFORMATION

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**ABSTRACT –** The influence of solute atoms on the deformation mechanisms of magnesium (Mg) alloys was investigated by comparing Mg-1Al, Mg-1Zn, and Mg-1Gd (at.%) alloys. The three alloys were fabricated by hot extrusion under different conditions. Gd restricts recrystallization and grain growth compared to Al and Zn. At similar grain sizes (~14 μm), Mg-1Gd exhibited lower yield strength yet significantly higher strain hardening and elongation than Mg-1Al and Mg-1Zn. Dislocation density-based elastic-viscoplastic self-consistent (EVPSC) simulations, corroborated by surface slip trace analyses, indicates that pyramidal <a> and <c+a> slip became more active in Mg-1Gd than in Mg-1Al and Mg-1Zn. The critical resolved shear stress (CRSS) of basal, prismatic, pyramidal <a>, pyramidal <c+a> slip, and twinning were estimated in the three alloys. Gd addition significantly reduces the $CRSS_{<c+a>}/CRSS_{basal}$ ratio as well as the $CRSS_{<c+a>}/CRSS_{twin}$ ratio, which is responsible for the high ductility and strain hardening in Gd-containing Mg alloys.

# MICROSTRUCTURE AND MECHANICAL PROPERTY OPTIMIZATION OF ADDITIVELY MANUFACTURED TI-MODIFIED HIGH-STRENGTH AL ALLOYS VIA MULTI-STAGE HEAT TREATMENT

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**ABSTRACT** –Ti-modified Al-Li-Cu alloys fabricated by laser powder bed fusion (LPBF) generally exhibit fine equiaxed grains in the as-built condition, providing excellent ductility (~ 19.4%). However, the extremely high cooling rates suppress the precipitation of strengthening phases, leading to relatively low tensile strength (~ 364 MPa). Conventional T6 heat treatment (560 °C/90 min + 170 °C/36 h) increases strength to ~516 MPa, but ductility is severely reduced (~6.7%) due to grain coarsening during solution treatment and the formation of high-aspect-ratio $T_1$-$Al_2CuLi$ precipitates that accelerate dislocation annihilation and weaken strain-hardening capacity. To address these limitations, a multi-stage solution treatment entirely below 500 °C was developed: 375 °C/5 h + 450 °C/2 h + 475 °C/0.5 h. This process promoted secondary $Al_3Ti$ particles nucleation, and regulated eutectic phases while suppressing grain coarsening. After short-term aging, spherical S′-$Al_2CuMg$ precipitates and secondary $Al_3Ti$ phases formed, enhancing strain-hardening capacity. The final properties reached yield strength of 512 MPa and elongation of 12.5%, nearly double the elongation achieved in the T6 condition. This study demonstrates that multi-stage heat treatment offers an effective pathway to synergistically regulate microstructure and simultaneously improve strength and ductility in additively manufactured high-strength aluminum alloys.

# ROLLING TECHNOLOGIES AND EXTREME MANUFACTURING

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**ABSTRACT –** Rolling is a critical process in the production of steel and other metallic materials. Extreme manufacturing refers to the use of advanced manufacturing technologies and high-end equipment to produce structures, components, and systems with extreme dimensions, ultimate precision, and exceptional performance. With the continuous evolution of rolling technology, high-accuracy process modeling, extreme thickness reduction, and heterogeneous layered composites have become important development directions. Ultra-thin strips are widely used in precision sensors, electronic components, and related applications. They feature extremely small thicknesses (0.01–0.1 mm), ultrahigh width-to-thickness ratios (>30,000), stringent flatness requirements (<0.1 mm/m), and high fatigue resistance (over 300,000 bending cycles), making their manufacturing highly challenging. During the rolling of ultra-thin and composite ultra-thin strips, issues such as strip breakage, strip drawing, and limitation of minimum achievable thickness often arise, along with severe shape defects and large residual stresses. The root causes lie in the pronounced size effects and severe work hardening that occur as the strip thickness approaches the micrometer scale; in addition, the roll system exhibits structural complexity, the roll contact conditions are intricate, and the deformation of the rolls becomes comparable to the applied reduction. To address these challenges, our research focuses on size effects in the plastic deformation of ultra-thin metals, roll-system modeling and shape control, the principles of electrically assisted plasticity rolling, surface-roughness transfer from rolls to ultra-thin strips, and the integration of ultra-thin strip rolling processes and equipment. Corresponding numerical models, processing methods, and rolling equipment have been developed. For bimetallic composite ultra-thin strips, we further investigate interfacial evolution and control, as well as the coordinated deformation mechanisms between dissimilar metals. In addition, research progress on rolling technologies and equipment for thick and wide strip specifications will be briefly introduced.

# APPLICATION OF DEEP NEURAL NETWORK MOLECULAR DYNAMICS TO ELUCIDATE THE ATOMISTIC MECHANISMS OF LASER PROCESSING OF TWO-DIMENSIONAL MATERIALS

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**ABSTRACT –** Two-dimensional materials such as graphene have attracted tremendous interest due to their exceptional electronic, optical, thermal, and mechanical properties. However, enabling their practical applications often requires precise control and modification of their nano- and microstructures, such as the intentional introduction of defects, nanoholes, or oxidation at the basal plane or edges. Although lasers and microwaves have been employed to process graphene and graphene oxide flakes dispersed in water for fabricating functional large-scale structures, the underlying thermal and chemical mechanisms governing these processes remain largely unclear. In this talk, we present recent work employing deep neural network molecular dynamics (DNN-MD) simulations to investigate the atomistic mechanisms of laser irradiation and microwave heating of graphene and graphene oxide in aqueous environments. We reveal unique interfacial heat transfer behaviors between graphene (or graphene oxide) and water under ultrafast energy deposition, along with distinct thermal responses dictated by material composition and oxidation level. Furthermore, our simulations uncover possible reaction pathways, including reduction, dehydration, and nanohole formation in graphene oxide, as well as oxidation in pristine graphene. These insights advance the fundamental understanding of coupled thermal–chemical processes in laser–material interactions and provide a foundation for the rational design and optimization of laser- or microwave-based manufacturing of two-dimensional materials in wet environments.

# COMPOSITIONALLY COMPLEX ALLOYS—TOWARD THE DESIGN OF EXCEPTIONAL MATERIALS

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**ABSTRACT –** This paper reports on a new class of compositionally complex steels (CCSs), developed by applying the principles of high-entropy alloys (HEAs) to conventional structural steels. These CCSs, composed of five major elements with each component's atomic fraction exceeding 5%, leverage a high degree of solid-solution strengthening. This unique design allows us to manipulate the alloy's phase regions to simultaneously form both nanosized shearable-carbides and non-shearable B2 particles. Consequently, our CCSs exhibit superior specific strength and ductility, outperforming existing high-strength HEAs and advanced lightweight steels. We systematically investigated the underlying deformation mechanisms, including the intricate interactions between dislocations and this dual nanoprecipitation, as well as high-stress twinning behavior, providing crucial insights for the future design of high-performance structural materials.

# AN ENHANCED MEAN STRESS EFFECT CORRECTION MODEL FOR FATIGUE LIFE PREDICTION OF NOTCHED COMPONENTS

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**ABSTRACT –** Accurate consideration of mean stress effects in the structural integrity assessment of mechanical equipment and engineering components subjected to cyclic loading is essential to ensure reliability in service. In addition, fatigue damage can be aggravated by significant stress concentration sensitivity induced by notch geometry in engineering structures. To overcome the limitation associated with predicting the fatigue life of notched components with mean stress, developing a fatigue life prediction model for notched structures that can simultaneously consider the combined effect of mean stress and notch effect should be paid special attention. This study proposes an enhanced Walker mean stress correction criterion based on the enhanced stress field intensity, which is extended to the fatigue life prediction of notched specimens considering mean stress plastic relaxation. Firstly, a mean stress adjustment criterion for enhanced stress field intensity is constructed in conjunction with elastoplastic finite element analysis to accurately characterize the influence of notch geometry and plastic relaxation effects within the fatigue failure zone at the notch root on fatigue life of notched specimens. Furthermore, the relationship between notch effects and mean stress sensitivity is discussed by introducing relative stress gradient to calibrate the Walker exponent. Moreover, a modified Walker criterion based on enhanced stress field intensity is proposed to predict the fatigue life of components with arbitrary shapes under arbitrary stress ratios. Finally, this study utilizes the proposed model to predict the fatigue life of five different materials notched specimens with different geometries and stress ratios, and to validate the prediction accuracy compared with the conventional Walker, SWT, and Morrow models. The results analysis indicates that the fatigue life of notched specimens predicted by the proposed model is distributed within the 2-fold scatter band and has better superiority relative to other models. It is confirmed that the proposed model can more comprehensively integrate the influence of the mean stress and notch effect on fatigue life of notched specimens.

# FEMTOSECOND X-RAY DIFFRACTION STUDIES OF PLASTICITY AT EXTREME PRESSURES AND STRAIN RATES

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**ABSTRACT –** The advent of hard x-ray free-electron-lasers (FELs), with peak spectral brightness over a billion times greater than any synchrotron, has enabled the study of material response to extreme deformations at previously inaccessible strain-rates. High-power nanosecond optical lasers, synchronized to the FELs, can, via laser-ablation, subject matter to multi-megabar pressures under uniaxial strain with rise times of a just a few picoseconds, corresponding to strain rates in excess of $10^{10}$ $s^{-1}$. (J. Appl. Phys. **132**, 080902 (2022)). The femtosecond pulses from the FEL allow x-ray diffraction patterns from the dynamically compressed material to be obtained in a single shot on a time-scale shorter than the period of the most energetic phonons in the system. Over the past few years such techniques have been used to start to glean an understanding of plastic flow under such extreme conditions. This paper reviews several of the seminal results in this field. We discuss how, at the very highest strain rates and shortest timescales, where dislocations have insufficient time to relieve the huge shear stresses and engender plasticity, the ultimate elastic compressive strength of a metallic crystal can be reached (Science, **342**, 220 (2013)). Furthermore, by utilizing fiber-textured targets, lattice-rotation and twinning can be observed in real-time (Nature, **550**, 496 (2017)), and the dependence of rotation angles on peak pressure used to inform multi-scale models of plastic deformation at these ultra-high strain-rates (Phys. Rev. Materials, **6**, 043605 (2022), Phys. Rev. Materials, **7**, 113608 (2023)). Such is the brightness of the femtosecond x-ray pulses that the absolute intensity of the x-ray thermal diffuse scattering between the Bragg peaks can be used to infer the temperature rise of the sample owing to the compression and plastic work (J. Appl. Phys., **137**, 155904 (2025)), with this thermometry method being shown to be insensitive to both the initial texture and large plasticity-induced texture changes under load. Despite the advances made in work such as that referred to above, our understanding of plastic flow and strength under these remarkable conditions is still very much in its infancy, yet is required if we are to make progress in generating and probing these states of matter which are of relevance in a number of fields, not least the study of the interiors of planets within our own solar system and beyond. Recent advances at the European XFEL in Hamburg now allow data to be collected at greater than Hz rates, which will greatly facilitate further headway in this burgeoning field of research.

# IN-SITU MANIPULATING MECHANISM OF ELECTROMAGNETIC FIELD ON THE MICROSTRUCTURE AND HARDNESS OF TITANIUM ALLOY DURING LASER MELTING DEPOSITION

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**ABSTRACT –** As a non-contact physical field, the electromagnetic field can influence the internal flow of the melt pool and regulate microstructure properties of alloy through electromagnetic force during laser melting deposition (LMD). This study proposes a three-dimensional numerical model of LMD Ti-6Al-4V coupled with an electromagnetic field, and investigates the influence mechanism of electromagnetic on the fluid dynamics of the melt pool during LMD. The results indicated that a steady electromagnetic field can suppress the internal flow of the melt pool. At an appropriate electromagnetic field, the steady electromagnetic field can refine the β columnar grains in LMD titanium alloy, causing some β columnar grains to exhibit fragmentation and equiaxed tendencies, thereby enhancing the hardness of the deposition layer. This work provides a new method for in-situ manipulate the microstructure and mechanical properties of titanium alloys during LMD.

# MECHANISM-INFORMED NEURAL NETWORK MODELING OF RAFTED NICKEL-BASED SINGLE CRYSTAL ALLOYS

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**ABSTRACT-** Rafted nickel-based single-crystal alloys exhibit directionally dependent mechanical degradation, necessitating the integration of anisotropic microstructural characteristics into macroscopic single-crystal plasticity models. This study presents a new mechanism-informed neural network (MINN-based multi-scale crystal plasticity framework coupled with microstructural fabric tensors to address this challenge. The proposed model incorporates single-crystal slip deformation mechanisms and utilizes 12 sets of measurable physical quantities, including stress, strain, and microstructural parameters, as input and output variables to derive microstructure-sensitive hardening models in an unsupervised manner. Isotropic and deviatoric fabric tensors are decomposed into individual slip systems, directly influencing material plastic flow. The investigations reveal that the isotropic component's magnitude correlates with microstructural channel width, modulating slip system strain rates, while the deviatoric component's direction and magnitude jointly govern flow and hardening behavior on the slip systems. These insights enhance the understanding of the multi-scale mechanical behavior of single-crystal alloys and provide a foundation for constitutive modeling. Meanwhile, the proposed framework offers innovative methods and research paradigms to investigate slip deformation mechanisms in anisotropic crystalline alloys.

# SYNERGISTICAL IMPROVEMENT OF STRENGTH AND PLASTICITY O F CADMIUM TELLURIDE SEMICONDUCTOR MATREILAS THROUGH INTERFACE MODIFICATION ENGINEERING SUCH AS GRADIENT ST RUCTURE AND ALLOYING

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**ABSTRACT –** Strength and plasticity of materials are crucial to functional devices in long-term service. Cadmium Telluride (CdTe) is an excellent absorber material for thin film solar cell due to its high light absorption coefficient. In this work, we adopt gain boundary engineering to attain excellent strength and plasticity in CdTe. With the aid of *in situ* transmission electron microscopy (TEM) observation and molecular dynamics (MD) simulation, we reveal the atomic mechanism of the equiaxed crystals with grain size from 5 nm to 10 nm and columnar crystals with grain size from 20 nm -80 nm. The former have excellent plasticity but stress softening, while the latter have high strength but poor plasticity. In the recent years, reasonable gradient structure design can break the constraint relationship between strength and plasticity, and synergistically improve the strength and plasticity of materials. During the compressive stress, the equiaxed crystals achieve plastic deformation through grain boundary sliding and merging, and the columnar crystals provide strength due to the high density of parallel grain boundaries. Moreover, we modify grain boundaries via Cu doping in CdTe. The hardness of Cu-doped CdTe are significantly increased relative to the pristine CdTe, and the quantitative strengthening models are proposed. This work provides two avenues for designing materials with high strength and plasticity and accomplishing commercial applications.

# PREDICTING DISLOCATION PATTERNS AND DISCOVERING THE LAW OF SIMILITUDE BY MACHINE LEARNING

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**ABSTRACT-** Dislocation patterns reflect the complex self-organization nature of dislocations and have strong influence on the mechanical properties of crystalline materials. Although the law of similitude has been widely accepted to quantify the relation between saturation resolved shear stress and pattern wavelength, it remains a big challenge to link the major inputs (e.g. saturation resolved shear stress, crystal orientation and applied strain amplitude) and major outputs (e.g. wave-type and wave-length) of dislocation patterns. In the present work, we develop two black-box machine learning methods to predict the wave-type and wave-length, as well as two white-box machine learning methods to discover explicit formulas linking major inputs and wave-length of dislocation patterns, based on the data of room temperature fully reversed fatigue of FCC metals. The results show that the black-box machine learning methods can well predict over twenty types of patterns consisting of five constitutive patterns (i.e. wall, vein, ladder, labyrinth and cell structures) and their wavelengths. The traditional law of similitude, as well as an improved version that additionally incorporates crystal orientation, are surprisingly discovered from experimental data under the guidance of expert knowledge and physical constraints in the white-box machine learning methods. This improved formulation represents a significant advancement toward establishing a more comprehensive law of similitude.

# DAMAGE OF TOUGH ELASTOMERS AND GELS: INSIGHTS FROM MECHANOCHEMISTRY

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**ABSTRACT -** Tough elastomers and gels can be fabricated in many different ways, among which the double-network and multiple-network structures have been widely adopted in the past two decades. Upon deformation, a clear hysteresis loop can be observed during the loading-unloading cycles, suggesting a clear damage behavior of these materials. This talk starts with the general damage models in continuum level for those tough elastomers and gels. Motivated by the damage mechanism revealed through incorporation scissile mechanophores into multiple network elastomers, a progressively damage model is further developed which captures all the important features of deformation of multiple network elastomers. Recently, we have further incorporated reversible ring-opening mechanophores into multiple network elastomers. Through comparing the difference in fluorescence intensity during loading and reloading process, we are able to identify the damage level. Eventually both stress and damage visualization in tough elastomers can be achieved using a single mechanophore.

# TAILORING THE THERMAL EXPANSION PERFORMANCE OF NiMnGa FERROMAGNETIC SHAPE MEMORY ALLOY THROUGH ROTARY MAGNETIC FIELD: EXPERIMENT AND THEORETICAL MODEL

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**ABSTRACT –** Tunable thermal expansion is a key property for advanced materials. In this paper, the regulating effect of rotary magnetic field (the rotation angle ranges from 0° to 90°) on the thermal expansion (TE) of NiMnGa ferromagnetic shape memory alloy (FSMA) single crystal is first revealed by experiment. The results show that the TE coefficient along the longitudinal direction of the specimen decreases monotonically with the increasing rotation angle of magnetic field, and gradually saturates after the rotation angle reaches a critical value. A rotary magnetic field with the intensity of 1.086 T can cause a continuous variation of the average TE coefficient from $90.5\times10^{-6}$/K to $-25.8\times10^{-6}$/K in a wide temperature window of 125 K (ranging from 298 K to 173 K), and zero TE is achieved at a specific rotation angle. Furthermore, by applying different compressive stresses and mechanical constraints along the longitudinal direction of the specimen, the evolutions of the TE under various magneto-mechanical regulation conditions are explored. To quantitatively describe these new phenomena, a three-dimensional thermo-magneto-mechanically coupled constitutive model is established based on finite deformation theory within an irreversible thermodynamic framework. The model considers various inelastic deformation and magnetization mechanisms, as well as the intrinsic anisotropic TE tensor of martensite. By comparing the predicted results with experimental data, the fidelity of the proposed model is validated. Moreover, other influencing factors, including the magnetic field intensity and crystallographic orientation, on the tailored TE of NiMnGa FSMA are predicted and discussed. This work will pave the way for the precise regulation of TE performance in NiMnGa FSMA.

# MACRO-MICRO ANISOTROPY INDUCED BY LOADING PATH VARIATION IN HOT WORKING OF TITANIUM ALLOYS: INTERPRETABLE AND PHYSICS-INFORMED MODELING

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**ABSTRACT –** The titanium alloy with initially lamellar structure shows strong loading path dependent anisotropic deformation and microstructure evolution in hot working, which affects the forming process. This work introduces an interpretable and physics-informed constitutive modeling framework for titanium alloys that integrates internal state variable theory with machine learning techniques. The proposed approach specifically addresses the challenge of predicting complex anisotropy induced by loading path variations. By coupling physically-based hardening laws with data-driven parameter optimization, the model achieves both mechanistic fidelity and computational efficiency. Experimental validation demonstrates accurate prediction of path-dependent flow stress evolution and microstructural changes across different strain paths. This modeling method holds significant potential for describing complex deformation behaviors caused by loading path variation, particularly in capturing the interplay between macroscopic flow and microstructure evolution. The framework provides practical guidance for optimizing short-process and low-cost primary hot working routes of titanium alloys, offering a balanced solution between physical interpretability and predictive accuracy for industrial applications. Key advantages include reduced calibration effort compared to conventional models and improved generalization capability beyond purely data-driven approaches.

# THE STUDY OF MICROPILLAR CYCLIC COMPRESSION DEFORMATION BEHAVIOR OF Ti-6.5Al-3.5Mo-1.5Zr-0.3Si ALLOY AFTER ELECTROMAGNETIC SHOCK TREATMENT

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**ABSTRACT –** This work employs micropillar cyclic compression experiments to investigate the effect of electromagnetic shock treatment (EST) on the fatigue performance of Ti-6.5Al-3.5Mo-1.5Zr-0.3Si titanium alloy. The study primarily focuses on the micro-pillar cyclic compression response behavior for EST times of 0 s and 0.12 s. Firstly, the microstructure of the micro-pillars with an EST time of 0.12 s was characterized and analyzed. By comparing with the initial samples, the influence of EST on phase structure and grain boundary distribution was determined. Secondly, the micro-pillars underwent 30 and 50 cycles of cyclic compression to obtain the load-strain curves. Based on the variation of load with the number of cycles, the cyclic hardening/softening behavior of EST micro-pillars was investigated. Further characterization of the grain boundaries and dislocation distribution after cyclic deformation was conducted using TEM. The effects of EST on the micro-pillar cyclic deformation response mechanisms were explored, based on the changes in grain boundaries and dislocations.

# COUPLED CRYSTAL PLASTICITY-PHASE FIELD MODELING OF MULTI-MECHANISM DEFORMATION IN FCC METALS: INSIGHTS INTO TWINNING-MEDIATED PLASTICITY

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**ABSTRACT-** Many face-centered cubic metals, such as austenitic steels and high-entropy alloys, exhibit twinning-induced plasticity, which significantly enhances their strength-ductility synergy. A fundamental understanding of the underlying mechanics of deformation twin is therefore crucial for the rational design of advanced, high-performance structural materials. In this study, we develop a fully coupled multi-physics constitutive framework, implemented within the finite element method, to simultaneously model dislocation slip and deformation twin in FCC metals. A strain-gradient crystal plasticity model is employed to capture the evolution of geometrically necessary dislocations and their contribution to the macroscopic stress-strain response. The framework further integrates a phase-field description of twinning, enabling the concurrent simulation of twin nucleation, growth, and morphological evolution. The unified model is numerically implemented and applied to investigate deformation behavior under single-crystal compression and polycrystalline shear deformation. Coupled model prediction is first validated against experimental micropillar compression data. Subsequently, the growth behavior of twins under complex multiaxial stress states in polycrystal is examined, and the correlation between twin volume fraction and the Schmid factor is quantified. This work provides a comprehensive mechanistic insight into the interplay between multiple deformation modes in FCC metals, offering a robust theoretical basis for the microstructure-informed design of strong and ductile metallic materials.

# IMPROVED IRRADIATION RESISTANCE OF A LOW ACTIVATION REFRACTORY MEDIUM ENTROPY ALLOY, VCrFeW0.2, FOR FUSION APPLICATIONS DEMONSTRATED BY MICRO-TENSILE TESTING

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**ABSTRACT-** An as cast, VCrFeW0.2 refractory medium entropy alloy (RMEA) was designed for fusion reactor divertor applications, focusing on reduced cost, low activation and compositional stability (low transmutation rates). The as-cast alloy was irradiated to a fluence of 5.6 x $10^{17}$ ions/$cm^2$ at room temperature with 5 MeV helium ions whose energy have been uniformly attenuated to 0.4 MeV and 5 MeV via energy degradation device prior to sample irradiation. Pre and post irradiation, its mechanical properties were evaluated micro-tensile testing. Prior to irradiation, the VCrFeW0.2 alloy demonstrated good strength and ductility, with a yield strength of 1464 MPa and strain to UTS ($\varepsilon_{UTS}$) of 4.6%, maintaining comparable strength to pure tungsten (1403 MPa) but with greater strain to UTS (1.3%). Post irradiation, the VCrFeW0.2 alloy exhibited remarkable damage resistance; its strength increased by only ~160 MPa, and it retained strain to UTS with a $\varepsilon_{UTS}$ of 2.9%. It performed better than tungsten tested under identical irradiation conditions where there was ~1800 MPa increase in yield strength and a complete loss of plasticity. The micro-tensile results were supported by nanoindentation tests and Vickers hardness testing was also undertaken to show the yield strength values are representative of macro scale, bulk behaviour. TEM and comparison with existing literature on RMEA/RHEA are presented here to understand the reason for difference in performance between VCrFeW0.2 alloy and Tungsten.

# FRACTURE OF NANO-COATINGS ON POLYCRYSTALLINE METALLIC SUBSTRATES IN PLASTIC DEFORMATION AND ITS MODELING

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**ABSTRACT-** Products with functional coatings are critical for extensive applications in clean power sources, electronics, medical devices, etc. Forming sheet metals with coating directly into those parts is an efficient solution. However, the fracture of coatings on polycrystalline metallic substrates in plastic deformation severely deteriorates the performance. A thorough understanding of the coating fracture mechanism correlated with inhomogeneous substrate plasticity is thus critical for the accurate prediction of their failure and further to guide the process design. To address these challenges, this study conducted comprehensive characterization of niobium coating cracks on stainless-steel substrates and established a multiscale model for predicting coating fracture dominated by substrate plasticity. Specifically, distinct coating cracks were identified and categorized into four patterns based on their spatial distribution: those located on intragranular slip bands, low angle grain boundaries, high angle grain boundaries and twin boundaries of the substrate. Crystallographic calculations and statistical analyses confirmed that coating fracture is induced by grain and sub-grain scale strain localization in the substrate, which was integrated into the multiscale modeling framework. For nanocrystalline coatings, molecular dynamics simulations were utilized to derive the cohesive zone model incorporated within the extended finite element method. Subsequently, coating fracture was simulated on a representative volume element of the substrate containing discrete slip bands. Microscopic observations revealed that substrate slips with Burgers vectors oriented at 30° to 50° relative to the surface initiate coating cracks; this phenomenon was generalized via a fracture parameter to enable efficient implementation in macroscopic simulations. In comparison to traditional homogeneous models, the proposed model achieves accurate identification of the coating crack patterns observed in practical samples.

# ANISOTROPIC SHOCK RESPONSE AND TWIN-BOUNDARY-MEDIATED SPALLATION IN CrCoNi MEDIUM-ENTROPY ALLOY INSTRUCTIONS

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**ABSTRACT-** CrCoNi medium-entropy alloys (MEAs) has been regarded as a highly impact resistant material. This study investigates the influence of crystallographic orientation and pre-engineered twin boundaries on the shock deformation and spallation behavior of CrCoNi medium-entropy alloys (MEAs) under extreme strain rates via molecular dynamics (MD) simulations. By analyzing shock propagation along 11 crystallographic directions (including [001], [110], [111]), results reveal significant anisotropy in spall strength, with the [001]-oriented single crystal exhibiting the highest resistance due to suppressed defect nucleation. Twin boundaries, however, act as preferential sites for amorphous phase nucleation and void initiation, accelerating damage accumulation and reducing spall strength compared to single-crystal counterparts. MD simulations elucidate the defect evolution pathway, highlighting shock-induced amorphization through FCC-to- HCP transitions and subsequent dislocation-entanglement-mediated void coalescence. The interplay between orientation-dependent slip activation and twin-boundary-driven microstructural degradation provides critical insights into the dynamic failure mechanisms of MEAs. These findings advance the understanding of extreme-condition deformation in CrCoNi, guiding the design of impact-resistant materials with tailored microstructures.

# CREEP MODELING FOR NICKEL-BASED SUPERALLOY ALIGNING GRAIN BOUNDARY EFFECT AND DISLOCATION MOVEMENT

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**ABSTRACT –** Creep is a critical concern for nickel-based superalloy components produced via additive manufacturing, particularly due to the complex interplay between grain boundary sliding (GBS) and dislocation-driven mechanisms. In this work, a novel crystal plasticity (CP)-based creep model is developed, where a modified constitutive framework is proposed to account for the presence and density of boundary precipitates, with the swept area of dislocation motion calibrated through Monte Carlo simulations. The model was applied to AM-built IN718 samples under both vertical and horizontal loading conditions. Comparison with experimental data confirms the capability of the model to reproduce transient and steady-state creep behavior. Analyses indicate that a characteristic grain boundary thickness of $\delta = 0.05$ yields high-fidelity reproduction of the creep response. The simulation results reveal a more significant strain concentration within grain interiors relative to grain boundaries, as grain-boundary carbides impede dislocation slip and reduce steady-state creep strain by approximately 50%. For the AM material featuring columnar grains, a more uniform stress and strain distribution and a lower creep rate are shown when the material is loaded parallel to the build direction, compared with perpendicular loading conditions. Furthermore, a virtual-laboratory platform was developed to simulate creep behaviors across diverse grain microstructures. This work identifies the role of precipitate distribution as a tunable microstructural feature to enhance creep resistance, providing a predictive tool for creep performance and potentially reducing the reliance on extensive creep testing.

# HOT CORROSION-CREEP DEFORMATION BEHAVIOR OF NI-BASED SINGLE CRYSTAL SUPERALLOY CONSIDERING THE STRESS DEPENDENCE AND FILM COOLING HOLE

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**ABSTRACT –** This study presents new insights into hot corrosion-creep fracture failure mechanism of Ni-based single crystal superalloy, focusing on creep deformation and microstructural evolution considering the creep stress and film cooling hole. Firstly, creep tests of smooth specimens under high, medium, and low stresses were conducted in air and corrosive environments. Analysis of creep curves and microstructural evolution (corrosion products, γ/γ′ phases, voids, etc.) revealed that hot corrosion accelerates plastic deformation and fracture in the single-crystal alloy in a stress-dependent manner. Second, creep tests of the specimens with film cooling holes were conducted in air and corrosive environments, and microstructural evolution was characterized using Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Electron Backscatter Diffraction (EBSD), nanoindentation, etc. The results showed that the corrosion products around the film cooling holes degraded the microstructure's mechanical properties, altered the stress state and activated different slip systems, resulting in severe damage. Finally, the hot corrosion-creep evolution and failure mechanism of Ni-based single crystal superalloy with film cooling holes were revealed. Hot corrosion accelerates creep rupture by reducing the alloy's resistance to plastic deformation, decreasing the effective load-bearing area, altering the stress state, and changing the creep fracture mode.

# NONLINEAR CAUCHY ELASTICITY

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**ABSTRACT –** Most theories and applications of elasticity rely on an energy function that depends on the strains from which the stresses can be derived. This is the traditional setting of Green elasticity, also known as hyper-elasticity. However, in its original form the theory of elasticity does not assume the existence of a strain energy function. In this case, called Cauchy elasticity, stresses are directly related to the strains. Since the emergence of modern elasticity in the 1940s, research on Cauchy elasticity has been relatively limited. One possible reason is that for Cauchy materials, the net work performed by stress along a closed path in the strain space may be nonzero. Therefore, such materials may require access to both energy sources and sinks. This characteristic has led some mechanicians to question the viability of Cauchy elasticity as a physically plausible theory of elasticity. In this paper, motivated by its relevance to recent applications, such as the modeling of active solids, we revisit Cauchy elasticity in a modern form. First, we show that in the general theory of anisotropic Cauchy elasticity, stress can be expressed in terms of six functions, that we call Edelen-Darboux potentials. For isotropic Cauchy materials, this number reduces to three, while for incompressible isotropic Cauchy elasticity, only two such potentials are required. Second, we show that in Cauchy elasticity, the link between balance laws and symmetries is lost, in general, since Noether's theorem does not apply. In particular, we show that, unlike hyperleasticity, objectivity is not equivalent to the balance of angular momentum. Third, we formulate the balance laws of Cauchy elasticity covariantly and derive a generalized Doyle-Ericksen formula. Fourth, the material symmetry and work theorems of Cauchy elasticity are revisited, based on the stress-work 1-form that emerges as a fundamental quantity in Cauchy elasticity. The stress-work 1-form allows for a classification via Darboux's theorem that leads to a classification of Cauchy elastic solids based on their generalized energy functions. Fifth, we discuss the relevance of Carath\'eodory's theorem on accessibility property of Pfaffian equations. Sixth, we show that Cauchy elasticity has an intrinsic geometric hystresis, which is the net work of stress in cyclic deformations. If the orientation of a cyclic deformation is reversed, the sign of the net work of stress changes, from which we conclude that stress in Cauchy elasticity is neither dissipative nor conservative. Seventh, we establish connections between Cauchy elasticity and the existing constitutive equations for active solids. Eighth, linear anisotropic Cauchy elasticity is examined in detail, and simple displacement-control loadings are proposed for each symmetry class to characterize the corresponding antisymmetric elastic constants. Ninth, we discuss both isotropic and anisotropic Cauchy anelasticity and show that the existing solutions for stress fields of distributed eigenstrains (and particularly defects) in hyperelastic solids can be readily extended to Cauchy elasticity. Tenth, we introduce Cosserat-Cauchy materials and demonstrate that an anisotropic three-dimensional Cosserat-Cauchy elastic solid has at most twenty four generalized energy functions.

**Keywords:** Cauchy elasticity, Green elasticity, Hyper-elasticity, Nonlinear elasticity, Linear elasticity, Odd elasticity

# AN ELECTRO-THERMO-MECHANICALLY COUPLED CRYSTAL PLASTICITY MODEL FOR ELECTROPLASTICITY

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**ABSTRACT –** This study establishes an electro-thermo-mechanically coupled crystal plasticity framework incorporating electroplastic effect to elucidate the fundamental mechanisms of current-assisted deformation in pure copper. In this framework, the thermal and athermal effects of electric current are independently described by the crystal plasticity constitutive model in terms of temperature and current density, respectively. The temperature field and current density distribution are obtained by solving the coupled heat conduction equation and current continuity equation. The model parameters are calibrated using experimental stress-strain responses of polycrystalline copper at different temperatures and current densities. Numerical simulations reveal that the thermal effects of electric current primarily manifest as shear modulus softening and enhanced thermal activation of dislocations, which have a relatively minor impact on flow stress. In contrast, the athermal effect significantly reduces both yield stress and hardening modulus by weakening the short-range and long-range resistances, leading to notable differences in flow stress during the work-hardening stage. Microstructural analysis shows that electric current alleviates stress concentrations caused by grain orientation differences and promotes more uniform distributions of dislocation density and slip deformation during plastic deformation. The proposed framework bridges the mesoscale dislocation slip and evolution with macroscale mechanical responses, providing critical insights for optimizing electrically-assisted forming processes through controlled electroplastic deformation. As an outlook, the current work focuses solely on simulating electroplastic effect in EAT deformation. Future research can extend the present model to other EAF processes, such as quantitatively evaluating the suppression effect of electric current on springback in electrically assisted bending process. Additionally, the framework can be coupled with phase-field fracture models to predict crack propagation behavior in metallic materials under applied electric current.

# ADVANCES IN MATERIALS CHARACTERIZATION

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**ABSTRACT –** This paper reviews new developments for materials characterization for constitutive and failure modeling, focusing on compressive fracture strain with bilinear strain paths, laminated aluminum pouch film properties, gradient properties in Al-Steel spot weld. First, the bilinear strain paths subjected to pre-tensile loading followed by compressive loading is capable of predicting the cut-off region for ductile fracture loci and is verified through experiment and numerical simulation. Second, Lithium-ion battery pouch film is composed of polypropylene, aluminum, PET, and nylon. The material properties of the four layers are characterized by the delamination behavior between the aluminum and polymer layers during tensile testing and the polymer properties through nano-indentation testing. Individual layer properties are optimized to satisfy the combined stress-strain curve The modelled properties were verified through wrinkling and forming behaviors. Finally, aluminum-steel resistance spot welding (Al-steel RSW) is considered. This study develops an inhomogeneous sample to extract the material properties for the fusion zone (FZ), heat-affected zone (HAZ), and intermetallic compound (IMC) layers with a single tensile test. The results from inhomogeneous specimen is compared to the ones from homogeneous samples. Fracture mechanisms of Al-steel RSW are examined using a miniature weld performance test and in-situ micro DIC.

# ORIGIN OF TWINNING MODE HIERARCHY IN NITI – A CRITICAL UNDERSTANDING

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**ABSTRACT –** This work resolves a long-standing question on twinning mode in NiTi that $\{11\bar{1}\}$ Type-I is preferred than $\{011\}$ Type-I. A number of experiments has universally demonstrated the coexistence of $\{11\bar{1}\}$ Type-I twins and $\langle 011\rangle$ Type-II twins—as lattice-invariant deformation—within the same habit plane variant of the B19' martensite in NiTi. This coexistence is unusual since, although both $\{11\bar{1}\}$ Type-I and $\langle 011\rangle$ Type-II twins represent valid solutions derived from the phenomenological theory of martensite crystallography, they are not conjugate to each other. The widespread occurrence of $\{11\bar{1}\}$ Type-I twinning mode has not been clearly explained. This work shows calculations of twin boundary (TB) energies and also generalized planar fault energies (GPFEs) for both twinning modes in Type-I. We found that $\{11\bar{1}\}$ twinning is favored over $\{011\}$ since the TB energy is lower by a factor of three and the barriers of $\{11\bar{1}\}$ are much smaller. The accurate determination of TB energy requires ab-initio calculations because the classical interatomic potentials miss the correct positioning of the Ni and Ti atoms. High-resolution experimental images at the atomic level confirm the positioning of Ni and Ti atoms and agree precisely with our calculations of twin interfaces. Furthermore, we show that, for the first time in the literature, experimental electron diffraction images and simulated images agree only when the correct interface is constructed as in this study. We also hypothesize that the given TB energy correlates with the atomic density at the interface throughout the different twinning modes. Then, with the correct offsets, further shear and shuffles establish GPFEs including twin nucleation and migration barriers. In summary, the current study employs Density Functional Theory (DFT) and recently proposed Molecular Dynamics (MD) potentials to gain further insights into twinning in NiTi, while also serving as a critical evaluation of the proposed MD models.

# MDVP: A MECHANISM-BASED DATA-DRIVEN VISCOPLASTIC CONSTITUTIVE MODEL FOR GLASSY POLYMERS

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**ABSTRACT –** Glassy polymers are widely utilized in engineering applications owing to their superior physicochemical properties. However, their complex viscoplastic behavior under large deformation---encompassing strain rate dependency, hydrostatic pressure sensitivity, post-yield softening, and strain hardening---presents significant challenges for efficient and accurate constitutive modeling. This work introduces a mechanism-based data-driven viscoplastic (MDVP) constitutive model for glassy polymers. The model's theoretical framework is rigorously derived from the principle of virtual work and energy balance considerations. A back stress evolution law, characterizing molecular orientation hardening, is incorporated to describe Bauschinger-type reverse yielding during unloading. Within this thermodynamically consistent framework, a lightweight artificial neural network (ANN) defines the plastic flow rule, requiring only 44 loading paths for training. Notably, the ANN's input layer structure can be adaptively adjusted based on available experimental datasets. The MDVP model has been implemented in commercial finite element software. Numerical validations, including simulations of a single homogeneous cube, a perforated plate, a sphere-impacted plate, and an inclusion-embedded shell, demonstrate the model's capability to accurately capture the nonlinear mechanical responses of glassy polymers and their composites under diverse loading conditions. Furthermore, the feasibility of establishing a fundamental MDVP model using data from only six uniaxial tensile tests is demonstrated. Current limitations of the model are also discussed.

# MICROSTRUCTURAL EVOLUTION AND ENHANCED TENSILE PROPERTIES OF Ni-BASED SUPERALLOYS: A COMPARATIVE STUDY OF COUNTER-GRAVITY CASTING AND GRAVITY CASTING VIA IN-SITU SYNCHROTRON RADIATION

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**ABSTRACT –** Enhancing mechanical properties of Ni-based superalloys via optimized casting methods remains a critical challenge. This study compares mechanical behavior, microstructure evolution, and fracture mechanisms of counter-gravity casting (CGC) and gravity casting (GC) K4169 alloys through ex-situ tensile tests and in-situ synchrotron X-ray diffraction. CGC alloy exhibited a higher dislocation density of 1.066 × 1015/m2, representing an increase of 43.36% over the GCalloy, despite both samples comprising γ, γ', γ', δ phases and carbides. CGC alloy shows better structural uniformity, finer dendritic spacing, and improved crystal integrity by reducing δ phase formation, creating ordered dislocation networks, and simplifying crystal orientation, unlike GC alloy with dislocation tangles and large dendrites. During in-situ tensile testing, CGC alloy demonstrated higher lattice strain than GC alloy, indicating superior capacity to accommodate stress and strain, thereby enhancing its strength and plastic deformation. CGC alloy sustained an applied fracture stress of 1212.82 MPa, significantly higher than GC alloy's 967.25 MPa. Strengthening mechanisms, including dislocation interaction, stacking faults, and carbide precipitation, were more pronounced in CGC alloy. Conversely, GC alloy suffered reduced plasticity due to extensive precipitate formation and elevated internal stress caused by phase transitions. CGC alloy exhibited superior tensile properties and toughness through a tough fracture mechanism, whereas GC alloy predominantly failed via brittle cleavage with minor ductile contributions. CGC alloy's multiple synergistic strengthening mechanism (fine grain, nano-precipitation/MC, low distortion interface and ordered dislocations) was first proposed to be responsible for its exceptional performance. These findings highlight CGC's potential for optimizing Ni-based superalloy properties.

# EXTENSIVE MODIFICATION AND APPLICATION OF VISCOPLASTIC SELF-CONSISTENT MODEL IN VARIOUS FIELDS

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**ABSTRACT -** Due to the excellent model flexibility and high calculation efficiency, the classical viscoplastic self-consistent (VPSC) model has become one of the most popular approaches for the prediction of complex deformation processes of polycrystal metal materials. Based on the VPSC framework, our research team made some modifications on this classical model to enhance its applicability. The main contributions of our work can be summarized as the following three aspects:

**1. Incorporation of dynamic recrystallization (DRX) and dynamic precipitation (DP):** To offer a more complete description on the hot deformation process of aluminum alloys, the DRX and DP behaviors are considered into VPSC model through modifying the Kocks-Mecking dislocation model. Note that a novel modification parameter is defined to describe the hindering effect of DP on DRX process. The unified VPSC-DRX-DP model can accurately predict the hot deformation process of 7055 aluminum alloy, including the flow stress, DRX fraction, DP fraction, DP size, etc.

**2. Through-process modeling of Kampmann-Wagner-numerical (KWN) and VPSC model:** This part of work aims at the prediction of the artificial aging process and the subsequent mechanical responses. The classical KWN model and VPSC model are employed to describe the static precipitation behavior and mechanical properties, respectively. Moreover, the KWN model is modified to consider the effect of precipitate free zone (PFZs) and the external stress in stress-aging process. The precipitation information (precipitation fraction and size, PFZ width, etc.) calculated by KWN model will be used in VPSC calculation, and the yield stress and hardening behavior of aged-alloy can be predicted.

**3. Combination of VPSC and micromechanics damage model:** The VPSC model has been extended to dilatational-VPSC (DVPSC) by Lebensohn and Tomé to consider the void growth. However, as proposed by the VPSC model developers, there are two main challenges hindering the wider application of DVPSC: 1) the lack of the void nucleation and coalescence and 2) the effective experimental verification. Aiming at the above challenges, a modified-DVPSC model considering the void nucleation and coalescence was proposed and experimentally verified. The essential model parameters are identified by the X-ray computed tomography (CT) technique. The modified-DVPSC model accurately captures the abrupt stress reduction caused by the coalescence, and give a satisfactory fracture prediction.

# MICROSTRUCTURE-RESOLVED PLASTICITY HETEROGENEITIES AND DAMAGE INITIATION IN NEAR-*A* TI60 UNDER NON-LINEAR LOADING PATHS

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**ABSTRACT –** Near-$\alpha$ titanium alloys used in aero-engine hardware exhibit equiaxed, bimodal, and lamellar microstructures whose phase morphology and spatial distribution strongly govern strain localization and damage initiation. To quantify these effects under service-relevant non-linear loading sequences, we produced three representative Ti60 microstructures via controlled heat treatment and developed a multiscale crystal plasticity framework that explicitly resolves microstructural heterogeneities while enforcing geometrically necessary dislocation (GND) constraints. Model parameters were calibrated and validated using nanoindentation, micropillar compression, and high-resolution microscopy. The framework links grain-level constitutive behavior to observed microscale deformation and damage, reproducing the nucleation, interaction, and spatial growth of intragranular shear bands with markedly higher fidelity than homogenized CP models. Across loading paths, three hierarchical heterogeneity scales, grain size, morphology, and interface character, govern deformation compatibility and, in turn, damage evolution. Among these, microstructure class (equiaxed/bimodal/lamellar) exerts the dominant control on damage sensitivity and initiation sites, surpassing the effects of grain size or geometric arrangement. Crystallographic orientation contrast across primary $\alpha$ and secondary $\alpha$ phase boundaries induces pronounced stress/strain partitioning and hetero-deformation-induced hardening, delaying void nucleation and shear-band coalescence and thereby enhancing damage tolerance. The results provide a physically grounded basis for microstructure optimization of near-α titanium components and improve the predictive capability of damage models for complex loading histories.

# DEFORMATION BEHAVIOR AND MICROSTRUCTURAL EVOLUTION OF HIGH-STRENGTH AND LOW-PLASTICITY MATERIALS UNDER COMPRESSION PROCESS WITH CONFINING PRESSURE

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**ABSTRACT -** High-strength and low-plasticity materials have attracted increasing attention as candidates for lightweight applications in the automotive, aerospace, and other industries. However, it is particularly difficult to manufacture products from such materials owing to their poor plasticity at room temperature. Lightweight materials such as titanium alloys and titanium-aluminum alloys are being increasingly utilized. Nevertheless, their low ductility makes it challenging to shape high-strength alloys at room temperature. In order to improve the plastic deformation capacity and mechanical properties of deformed parts, this paper proposes a forming process under superimposed hydrostatic pressure. TNM alloy was subjected to compression in a high pressure medium with a pressure of 1.5 GPa, which introduced superimposed hydrostatic pressure during the compression process. The deformation behavior and microstructural evolution of TNM alloys under such loading conditions were investigated through experimental studies. Compared to the conventional compression process under normal pressure, which achieved a hardness of 294.1 HV and a compression ratio of 35%, the high pressure compression process achieved a synergistic improvement in both hardness (477 HV) and plasticity (55% compression ratio). Multiscale characterization (SEM/XRD/EBSD) reveals that under a pressure of 1.5 GPa, the thickness of the α phase lamellae decreased significantly, and the grain orientation became more uniform. Additionally, B2 phase fractured into fine-grains, which promoted the formation of dynamically recrystallized grain of the γ phase. The proportion of low-angle grain boundaries increased by approximately 200% compared to conventional upsetting, mainly distributed within the γ lamellae. Notably, the proportion of the special 60° misorientation angle showed a significant increase, indicating that the twinning deformation mechanism in TNM alloys is more active during high pressure compression process. Subsequently, the volume fractions of the phases revealed a significant increase in the γ phase volume fraction, while the volumes fraction of the B2 and $\alpha_2$ phases decreased. Moreover, the B2 phase volume fraction decreased markedly from 11% to 2.9%. Although high pressure significantly altered the microstructure, grain size, and distribution of each phase, it did not induce the formation of new phases. This comprehensive study offers valuable insights into the influence of high pressure on the deformation behavior and of microstructural evolution TNM alloy, providing a promising pathway for solving the severe engineering challenges caused by the low room-temperature plasticity of TNM alloys.

# SCALE-BRIDGING DISLOCATION PLASTICITY IN MGO AT ROOM TEMPERATURE

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**ABSTRACT –** Recent research challenges the conventional perception of ceramics as inherently brittle materials, with dislocations emerging as a promising avenue for enhancing their mechanical properties [1,2]. To investigate the role of dislocations on the multi-scale mechanical properties of ceramics, we conducted multi-scale studies on (001) MgO single crystals with mechanically seeded dislocation densities ranging from ~$10^{12}$ to ~$10^{15}$ $m^{-2}$. Through nano-/micro-pillar compression tests, we revealed a distinctive dislocation density-dependent yield strength, transitioning from nucleation-dominated to multiplication/motion-controlled mechanisms. Notably, our engineered dislocation seeded samples demonstrated exceptional compressive plastic strain exceeding ~70%, alongside maintaining a high yield strength of approximately 2.35 GPa at a scale of ~400 nm in diameter during transmission electron microscope (TEM) in situ compression tests. Complementary bulk compression experiments, supported by digital image correlation (DIC) analysis, confirmed consistent dislocation-mediated deformation behavior while highlighting a significant size effect—the bulk samples exhibited substantially reduced yield strength (~120 MPa) compared to their nano-/micro scale counterparts. Furthermore, three-dimensional Discrete Dislocation Dynamics (3D-DDD) simulations provided deeper insights into the dislocation avalanche and work hardening during compression. These findings collectively offer new perspectives on tunable dislocation-mediated plasticity in MgO across multiple length scales, paving the way for the design of plastic ceramics.

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# STRAIN-RATE EFFECTS ON THE STRENGTH AND FRACTURE OF ADVANCED HIGH-STRENGTH STEELS

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**ABSTRACT –** The performance of Advanced High-Strength Steels (AHSS) under extreme conditions, such as dynamic crash events, is governed by multiscale plasticity mechanisms activated at high strain rates. This study presents a unified experimental and computational framework to unravel these microstructural origins of macroscopic behavior in three AHSS grades: Quenching & Partitioning (Q&P), Dual-Phase (DP), and Twinning-Induced Plasticity (TWIP) steels. A multiscale crystal plasticity finite element (CPFE) model is developed for Q&P steel, explicitly representing the austenite and martensite phases. The model incorporates key plasticity mechanisms under high-strain-rate loading, including dislocation slip and deformation-induced martensitic transformation, successfully predicting the macroscopic stress-strain response and underlying microstructure evolution. The fracture toughness of DP and TWIP steels under extreme dynamic loading is characterized using the essential work of fracture (EWF) method. Fracture simulations successfully capture the crack propagation and validate the EWF values. By directly connecting the activation of microscale plasticity mechanisms to macroscopic properties under extreme conditions, this work provides a foundational framework for designing next-generation AHSS for crash-critical applications.

# ADDITIVE MANUFACTURING AND MECHANICAL BEHAVIOR OF TINBTAZRMO REFRACTORY HIGH-ENTROPY ALLOY

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**ABSTRACT-** There is challenge in additive manufacturing of refractory high entropy alloys (RHEAs). In this work, TiNbTaZrMo RHEA was successfully prepared by additive manufacturing. The material has a unique cellular structure, exhibiting excellent plasticity of 50% and a yield strength of up to 904 MPa. The cellular structure hinders the transfer of dislocations between adjacent cells and restricts the slip of dislocations within the cell, which significantly improves the strength and uniform deformation properties. The cellular structure is conducive to the redistribution of dislocations during the later deformation process, thereby avoiding strain concentration within the grains. An on-demand regulation mechanism of dislocations during the evolution of the cellular structure at different deformation stages is proposed. In addition, the cellular structure in TiNbTaZrMo RHEA is a distributed grain structure formed by element segregation, but it is retained after aging treatment. After appropriate aging treatment, the cell walls in the cellular structure rotate at a small angle relative to the interior of the cell. This rotation of the cell wall enhances the hindering effect of dislocation movement within the cell. Dislocations have more opportunities to interact, proliferate and accumulate, thereby maintaining a high work hardening rate. This study provides new insights into improving the mechanical properties of additively manufactured RHEA.

# A FREQUENCY-DOMAIN AND ENERGY-BASED DAMAGE MODEL FOR FATIGUE IN SPACECRAFT STRUCTURES INDUCED BY RANDOM VIBRATION

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**ABSTRACT-** Reusable spacecraft represent an emerging trend in space technology applications. However, their repeated launch/re-entry missions induce more severe random vibration fatigue challenges than traditional disposable spacecraft, owing to damage evolution and accumulation. Current understanding of the underlying damage mechanisms remains incomplete, while existing life prediction methodologies—whether time-domain or frequency-domain—relying on Miner's linear cumulative damage theory fail to account for load sequence effects and dynamic response-damage coupling. To enhance prediction accuracy and ensure structural integrity, this study first reveals through experiments that the fundamental difference from quasi-static fatigue originates in non-stationary stress distributions, transient energy transfer, and heterogeneous material responses under random vibration. Based on Continuum Damage Mechanics (CDM), a damage coupled constitutive equation is established considering two effects, local stiffness reduction due to damage evolution, and global dynamic characteristic alterations caused by vibrational energy dissipation, thereby linking element-level damage to frequency-domain response shifts. A novel frequency-domain damage evolution equation is then derived within a thermodynamic framework, where stochastic vibrational energy density serves as the damage driving force. Structural failure is newly defined by the emergence of stiffness matrix singularity. Experimental validation confirms the improvement in life prediction accuracy and the convenience in application over conventional approaches, providing an important theoretical model for designing long-life reusable spacecraft structures.

# A DAMAGE EVOLUTION FRAMEWORK BASED ON SHAPE AND VOLUME CHANGES OF SPHERICAL VOIDS UNDER NON-PROPORTIONAL LOADING CONDITIONS

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**ABSTRACT –** Through considering the influence of stress triaxiality and Lode parameter on the fracture strain of materials, many phenomenological ductile fracture models were developed. These models exhibit strong predictive accuracy for damage and fracture under proportional loading. In practical deformation-to-fracture processes, loading is invariably non-proportional. Even in uniaxial tensile processes, necking prior to fracture disrupts the uniaxial stress state, rendering the loading path nonlinear. This study proposes a novel damage accumulation framework that extends phenomenological ductile fracture models to accommodate non-proportional loading. The framework defines the volume expansion/contraction and shape evolution of voids, correlates them with the material's stress triaxiality and Lode coefficient, and thereby enables applicability to arbitrary ductile fracture models. Experiments and finite element simulations including tensile-shear and notched compression tests on pre-stretched and pre-compressed 6061O aluminum plates were conducted. The change of stress state during testing was numerically analyzed. The predictive accuracy of different damage accumulation models was evaluated. Result shows that the proposed framework can describe void nucleation, growth/healing, shape evolution, and coalescence. By applying the framework with different phenomenological ductile fracture models, the prediction accuracy for material fracture behavior under non-proportional tensile-shear-compressive loading was improved significantly.

# MULTISCALE MODELING OF ELECTRICALLY ASSISTED DEFORMATION IN NI-BASED SUPERALLOY ALLOY THROUGH ELECTRON-ATOM COLLISION MECHANISM

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**ABSTRACT -** Electrically assisted manufacturing (EAM) has emerged as a promising strategy for extending the limits of plastic deformation and realizing tailored microstructures. To unravel the underlying mechanisms of EAM and enable its precise control, it is essential to quantify thermal and athermal effects through modeling. Toward this goal, a meso-scale resistivity quantification theory was developed based on the physical mechanism of electron-atom collisions, and a corresponding crystal plasticity model for EAM was established. This study accurately captures the non-uniform temperature field of a Ni-based superalloy during electrically assisted deformation and analyzes its interaction with the deformation process. The results reveal that two factors are critical to electroplasticity: first, the uneven input of electrical energy into grains with different orientations and defect volumes; second, the further non-uniform increase in resistivity induced by temperature heterogeneity. By comparing texture evolution and slip resistance between thermally assisted and electrically assisted deformation processes, the proposed model clarifies the influence of local Joule heating on micro-scale deformation behavior and quantifies the contributions of thermal and athermal effects at different stages of macro-scale deformation. Distinct from conventional models, this work presents a novel physics-based modeling approach, which breaks the closed loop of empirical modeling and indirect validation.

# PLASTIC DEFORMATION AND DAMAGE MECHANISMS IN PARTICLE-REINFORCED METAL MATRIX COMPOSITES: A CRYSTAL PLASTICITY-PHASE FIELD STUDY

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**ABSTRACT-** Particle-reinforced metal matrix composites (MMCs) exhibit high strength but often suffer from limited ductility due to early damage initiation. In this study, a crystal plasticity-phase field method is employed to investigate the plastic deformation and damage evolution in MMCs with varying particle arrangements and gradient microstructures. The model captures the accumulation of geometrically necessary dislocations (GNDs) near particle-matrix interfaces and grain boundaries, which promotes interfacial crack initiation. Simulations show that placing particles near grain boundaries improves ductility only when particle damage is neglected, whereas incorporating particle fracture reveals that intragranular particle placement more effectively enhances ductility, aligning with experimental observations. In gradient-structured composites, grain-size-dependent plasticity and particle distribution jointly influence strain delocalization, stress concentration, and crack propagation. Fine grains strengthen the material through hardening, while coarse grains accommodate deformation, promoting ductility. Particle-induced stress heterogeneity is size-dependent: smaller particles delay damage by homogenizing stress fields, while larger ones accelerate failure through stress localization. The presence of grain and particle gradients increases crack path tortuosity and enhances fracture resistance. This work provides mechanistic insights into the deformation and failure behaviors of MMCs and highlights microstructural strategies for improving the strength-ductility synergy.

# RESEARCH ON DOUBLE-SIDED INCREMENTAL AND ELECTRO-AGING FLEXIBLE FORMING TECHNOLOGY FOR Al–Li ALLOY

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**ABSTRACT –** To address the issues of poor room-temperature formability of Al–Li alloy aerospace components, long manufacturing cycles of traditional molds, and accuracy degradation caused by heat treatment, this study proposes an innovative composite forming method that integrates double-sided incremental forming and electro-aging treatment. A cooperative forming system was developed based on a dual KUKA robotic platform, and a strain-hardening-corrected trajectory algorithm was implemented to achieve high-precision flexible forming of complex surface components. The thermal response characteristics of 2195 Al–Li alloy under pulsed current were systematically investigated, and a short-time process condition centered on 160 °C/1 h was proposed to reveal the mechanism of rapid precipitation strengthening. Using a zirconia ceramic tool head, mechanical loading and electrothermal aging were carried out simultaneously. EBSD and TEM analyses showed that this process effectively coordinates the multi-field coupling of “electrical–thermal–mechanical” effects, promotes nucleation and transformation of precipitates, and significantly enhances the mechanical properties while maintaining forming accuracy. This research provides a new approach for short-cycle, high-performance, and flexible manufacturing of thin-walled aerospace components.

# THERMO-MECHANICAL DEFORMATION AND EARLY-STAGE DAMAGE IN ROTATING COMPOSITE SPACE STRUCTURES

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**ABSTRACT-**Lightweight composite structures used in solar-oriented spacecraft often rotate slowly to maintain optimal illumination, exposing them to coupled thermal and mechanical loads that can initiate deformation and early-stage damage. This study develops a nonlinear thermo-elastic model for a uniformly rotating composite beam representative of a sun-facing appendage. The formulation accounts for geometric nonlinearity, temperature-dependent properties, and through-thickness thermal gradients that generate bending and stress concentrations. A hybrid-coordinate variational method combined with assumed-mode discretization is used to capture the coupling between rotation-induced loads, thermal stresses, and stiffness degradation. Numerical simulations, validated using COMSOL, show that gravity-gradient loading induces harmonic stress cycles, while nonuniform solar heating produces thermal bending that elevates interlaminar shear and matrix cracking risk. The results highlight the deformation mechanisms and potential damage evolution pathways in rotating composite members operating under extreme thermo-mechanical environments.

# MACRO-MICRO ANISOTROPIC ANALYSIS OF BASED ON CRYSTAL PLASTICITY FINITE ELEMENT METHOD

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**ABSTRACT –** The accuracy forming technology of micro-scale components has reached a bottleneck when relying on conventional thermal processing methods, particularly in strategic fields such as hypersonic vehicles and quantum communication. Electroplasticity has demonstrated its unique advantages to enhance material formability and offer a promising route to overcome these limitations. In this study, a representative volume element (RVE) was constructed based on the crystal plasticity finite element method (CPFEM) to systematically simulate the mechanical response and multi-phase microstructural evolution of metallic materials under varying current densities and loading directions. The focus was put on the orientation-dependent electron scattering, electro-thermal coupling-induced phase transformations, and their effects on dislocation behavior at the polycrystalline scale. The results indicate that the angle between current and loading directions critically affects deformation resistance and dislocation motion. Proper alignment of the current can promote grain rotation along the loading direction, improving deformation coordination. Additionally, the aging effect of the current facilitates the formation and coarsening of γ″ precipitates in nickel-based alloys, achieving multi-phase strengthening in the solid-solution state. With increasing current application time, needle-like precipitates grow, while smaller precipitates undergo atomic diffusion and annihilation, leading to a stable precipitate distribution and saturation of the strengthening effect. In-situ transmission electron microscopy (In-situ TEM) was employed to validate the simulation results. This study reveals the coupled mechanisms of current directionality and electro-thermal effects on microstructural evolution and mechanical performance, providing theoretical guidance for the optimization of electrically assisted manufacturing processes.

# CRYOGENIC DEFORMATION BEHAVIOR AND MICROSTRUCTURAL MECHANISMS IN AA6061T6

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**ABSTRACT –** This study investigates the sub-zero/cryogenic deformation of AA6061–T6 using uniaxial tensile tests from 20 °C to −160 °C under quasi-static conditions. With decreasing temperature, the tensile strength increases monotonically, whereas ductility shows a non-monotonic trend, revealing an optimal sub-zero window (≈ −30 °C) where formability improves before deteriorating at deeper cryogenic temperatures. EBSD-based microstructural analysis indicates that low temperatures markedly suppress dynamic recovery, resulting in a higher overall, yet more uniformly distributed, dislocation density. The more uniform distribution reduces local orientation gradients, reflected by stable or slightly lower KAM values relative to room temperature. Moreover, limited thermal activation restricts cross-slip, promoting planar slip bands and pronounced lattice rotations near grain boundaries. Taken together, these factors support more homogeneous plastic flow and delay strain localization at moderate sub-zero temperatures. At extremely low temperatures, however, severely constrained dislocation mobility leads to pile-ups and stress concentration, reducing ductility. Overall, the results clarify how the balance among dislocation storage, recovery suppression, and grain-boundary-mediated deformation governs the temperature-dependent strength-ductility relationship, providing mechanistic insight into the cryogenic formability of AA6061-T6.

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# MODELLING OF CONTINUOUS DYNAMIC RECRYSTALLIZATION OF ALUMINUM ALLOY WITH CRYSTAL PLASTICITY FINITE ELEMENT CONSIDERING EXPLICIT SUBGRAIN STRUCTURE EVOLUTIONS

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**ABSTRACT-** Continuous dynamic recrystallization (CDRX) is one important phenomenon during thermo-mechanical process of metals, which determines the microstructure and texture evolution. Compared to the well modelled discontinuous dynamic recrystallization (DDRX), CDRX is more complex which evolves a gradual subgrain evolution closely related to the dynamic recovery. In the current work, the CDRX behaviors in a high strength alloy hot deformation are studied experimentally. A crystal plasticity finite element based CDRX model is developed considering the explicit subgrain structure evolutions, where the rotation of subgrain is driven by both deformation and recovery. The CDRX model is implemented with a polycrystalline RVE and validated with the high strength aluminum alloy hot deformation stress and microstructure evolutions. The grain orientation dependence of CDRX development is studied numerically and compared with experimental observations. The effects of slip modes including {111}<110> and {111}<110>& {110}<110> on the subgrain evolution and the corresponding CDRX are also explored numerically. The current CDRX model provides a way to simulate the subgrain related recrystallization behaviors explicated and physically.

# REVEALING THE MECHANISMS OF DISLOCATION-GRAIN BOUNDARY INTERACTIONS IN A COCRNI MEDIUM-ENTROPY ALLOY: A COMBINED SIMULATION AND EXPERIMENTAL STUDY

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**ABSTRACT-** The Hall-Petch relationship has long guided the design of strengthened polycrystalline materials by leveraging grain boundaries (GBs) as obstacles to dislocation motion. However, the mechanistic details of dislocation-GB interactions in multi-principal element alloys (MPEAs) remain poorly understood. This knowledge gap limits the rational design of high-strength nanocrystalline MPEAs, where chemical short-range order (SRO) and GB segregation play critical roles. Here, we combine molecular dynamics simulations and nanoindentation experiments to unravel the influence of GB type and SRO on dislocation-GB interactions in a CoCrNi model alloy. We show that interaction mechanisms are governed by GB structure: undissociated GBs absorb dislocations via free volume, twin boundaries block slip via phase transformation, and dissociated GBs activate GB dislocations under stress. While SRO fundamentally modulate interaction stress by altering deformation mechanisms—reducing dislocation absorption at undissociated GBs, enabling transmission at twin boundaries, and enhancing GB dislocation activity at dissociated GBs. Nanoindentation confirms that these interactions locally govern plasticity and critical stresses. These findings provide atomic-level insights into GB-mediated plasticity in MPEAs, offering a mechanistic basis for GB engineering in advanced alloy design.

# QUANTITATIVE EXPLANATION OF TWIN BOUNDARY INDUCED DUCTILITY IN γ-TiAl BASED ON THE COMPETITIVE MECHANISM OF DISLOCATION NUCLEATION

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**ABSTRACT –** The twin boundaries (TBs) play an important role in improving the strength or ductility of γ-TiAl, yet their underlying mechanism remains incompletely elucidated. In this work, we elaborate the ductile mechanism of nanotwinned γ-TiAl and establish a theoretical model to clarify the competitive relationship between slip systems during TB migration-induced ductility under different TB orientations. The atomic mechanism is attributed to the deformation induced TB migration which is accompanied by breaking and re-forming Ti-Ti and Al-Al bonds in the region of easy slip system $(111)[11\bar{2}]$. The TB migration capacity is closely related to the proportion ($\rho$) of the $(111)[11\bar{2}]$ orientation in the nanotwinned structure, which results in the linear trend between the ultimate strain and the $\rho$ in γ-TiAl. Our model further reveals that TB migration is enabled when the dislocation nucleates and slips along the TBs; this activation occurs because the critical stress along the $(111)[11\bar{2}]$ direction being reached earlier than that along other direction. Consequently, nanotwinned γ-TiAl exhibits ductility only within specific TB orientation ranges (e.g., 0-26°, 72-108°, and 160-180° in true nanotwinned γ-TiAl). To further validate the efficacy of TB migration ductility, *in situ* shear testing was implemented on polysynthetic twinned (PST) TiAl single crystals. Subsequent microstructural characterization revealed a TB migration induced ductile mechanism, which experimentally confirms the universal interface-dominated deformation principle in γ-TiAl alloy systems.

# EFFECTS OF TENSION-COMPRESSION ASYMMETRY IN R-VALUE ON PLASTIC FLOW BEHAVIOR: EXPERIMENTS AND MODELING

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**ABSTRACT –** The plastic strain ratio (also known as the Lankford coefficient or r-value) is commonly used, along with yield stress, to characterize the constitutive behavior of sheet metals. Under tensile and compressive stress states which typically exist in plastic forming, the material usually exhibits distinct yield stresses. This a phenomenon known as tension-compression asymmetry in yielding. However, the corresponding asymmetry in r-values has received comparatively limited attention. In this study, tensile and compressive experiments along different in-plane directions were conducted to characterize the tension-compression asymmetry of material yield stress, and particularly the r-value. Based on the non-associated flow rule, an asymmetric plastic potential function was proposed by introducing a stress-state-dependent term into the conventional plasticity model. Finally, a combined forward-reverse deep drawing test was performed. Finite element simulation based on the proposed constitutive model was conducted to analyze the influence of tension-compression asymmetry in yield stress and r-value on prediction accuracy. Results show obvious tension-compression asymmetry in r-values, with compressive values systematically exceeding their tensile counterparts across all tested orientations. This asymmetry significantly affects the stress-strain distribution during plastic deformation. Incorporating this asymmetry into the constitutive model can effectively improve the simulation accuracy of the forward-reverse deep drawing process.