

# Program for PF24, May 19-23, 2024

## Hangzhou, China

Dragon Hotel (杭州黄龙饭店)

May 19 <sup>th</sup>	May 20 <sup>th</sup>	May 21 <sup>st</sup>		May 22 <sup>nd</sup>		May 23 <sup>rd</sup>		Room
Registration Desk Open 10:00-20:00  Welcome Reception (18:00-20:00)	Plenary Talks (9:00-17:00) Crystal Ballroom  Poster Session	8:30-12:10	13:30-18:00	8:30-12:10	14:00-18:00	8:30-12:10	14:00	Room
		Topic 1	Topic 1	Topic 1	Social Activities	Topic 1	Departure	Pearl Room 1
		Topic 2a	Topic 2a	Topic 2a		Topic 2a		Pearl Room 2
		Topic 2b	Topic 2b	Topic 2b		Topic 2b		Bauhinia Room 1
		Topic 4	Topic 3	Topic 4		Topic 4		Bauhinia Room 2
		Topic 5	Topic 5	Topic 3		Topic 5		Spring Room

Topic 1-Solidification and additive manufacturing (Page 3)

Topic 2a- Solid state processes in functional materials (Page 5)

Topic 2b- Solid state processes in structural materials (Page 7)

Topic 3-Electrochemical reactions, corrosion, and oxidation (Page 10)

Topic 4-Brittle and ductile fracture (Page 12)

Topic 5-New method development, integration with ML, et al. (Page 14)

Poster Session (Page 16)

Banquet is scheduled on the May 21<sup>st</sup> (18:30-20:30) in Crystal Ballroom.

# Plenary Talks

Crystal Ballroom, May 20th, Monday (9:00-17:00)

Time	Title	Speaker	Chair
9:00-9:30	Opening Ceremony Opening Speech by Prof. Yunzhi Wang Welcome Speech by Local Hosting Organization		Jie Wang
9:30-10:20	Materials and Processes as Understood by Phase-Field Simulations: Solidification, Solid State Transformation, and High-Temperature Creep	Ingo Steinbach (Ruhr-University Bochum)	Yong Du
<b>Coffee Break</b>			
10:50-11:40	Recent Progress in the Application of Phase-Field Models to Multi-Phase and Multi-Component Alloy Microstructure Evolution	Nele Moelans (KU Leuven)	Yuhong Zhao
<b>Lunch</b>			
14:00-14:50	Development and Application of Phase-Field Models for Microstructure Evolution under Complex Processing Conditions	Katsuyo Thornton (University of Michigan)	Damien Tournet
14:50-15:40	Opening New Horizons in the Prediction of Environmentally-Assisted Material Degradation: Phase Field Models for Hydrogen Embrittlement and Corrosion	Emilio Martinez-Paneda (University of Oxford)	Baixiang Xu
<b>Coffee Break</b>			
16:10-17:00	Materials/Mechanics-GPT and the Integration of Artificial Intelligence with Phase-Field Simulations	Tong-Yi Zhang (Hong Kong University of Science and Technology - Guangzhou)	Long-Qing Chen

## Parallel Oral Sessions

### Topic 1. Solidification & Additive Manufacturing

Time	Speaker	Affiliation	Title
<b>Pearl Room 1, May 21, Topic 1-I, Chair: Damien Tournet</b>			
8:30-9:00	Tomohiro Takaki	Kyoto Institute of Technology	Phase-Field Modeling and Simulation of Fragmentation and Deformation During Solidification
9:00-9:30	Mathis Plapp	Ecole Polytechnique	Phase-Field Modeling of Dendritic Growth in Crystals with Strongly Anisotropic Surface Free Energy
9:30-9:50	Raphael Schiedung	The Interdisciplinary Centre for Advanced Materials Simulation	Mobility Corrections in Phase-Field Models for Material Solidification
9:50-10:10	Tamás Pusztai	Wigner Research Centre for Physics	Exploring Equilibrium and Steady-State Solutions with Elliptic PDE Solvers
<b>Coffee Break</b>			
<b>Pearl Room 1, May 21, Topic 1-II, Chair: Mathis Plapp</b>			
10:30-11:00	Yuhong Zhao	University of Science and Technology Beijing	Phase-Field Modelling of Dendrites and Precipitates to Guiding Alloy Design and Process Optimization
11:00-11:30	Xiaofeng Yang	University of South Carolina	Efficient Numerical Algorithms for the Phase-Field Dendritic Model
11:30-12:00	Mohsen Asle Zaeem	Colorado School of Mines	Integrating Machine Learning with Atomistic-Informed Phase-Field Simulations for Prediction of Microstructures During Rapid Solidification
<b>Pearl Room 1, May 21, Topic 1-III, Chair: Qingcheng Yang</b>			
13:30-14:00	Jincheng Wang	Northwestern Polytechnical University	Cracking Mechanism of GH3536 Superalloy During Directed Energy Deposition Additive Manufacturing
14:00-14:30	Min Yi	Nanjing University of Aeronautics and Astronautics	Phase-Field Modeling from Additive Manufacturing Microstructure Evolution to Aerospace Structures
14:30-14:50	Guillaume Boussinot	Access E.V.	Pattern Formation in Additively Manufactured Binary Al-Ni And Ternary Al-Ni-Ce Eutectic Alloys
14:50-15:10	Leiji Li	Shanghai Jiao Tong University	Quantitative Phase Field Modeling of Morphological Evolution in The Rapid Directional Solidification Under Additive Manufacturing Conditions

15:10-15:30	Upadesh Subedi	Silesian University of Technology	Temperature Dependence of Free Energies in A Phase Field Model for Selective Laser Melting of Tin Powder on Copper Substrate
<b>Coffee Break</b>			
<b>Pearl Room 1, May 21, Topic 1-IV, Chair: Abhik Choudhury</b>			
15:50-16:20	Murali Uddagiri	Ruhr University Bochum	Microstructure Evolution of Multi-Component Single Crystal Ni-Based Super Alloys Under Additive Manufacturing Process Conditions
16:20-16:40	Yangyiwei Yang	TU Darmstadt	Tailoring Material Properties Via Powder Bed Fusion: Multiphysics-Multiscale Phase-Field Simulations of Process-Property Relationships
16:40-17:00	Fathollah Varnik	Ruhr-University Bochum	A Phase-Field-Based Model for The Simulation of Reactive Gas Flows in Particle Beds
17:00-17:20	Téo Boutin	Commissariat À L'Énergie Atomique	Phase Field Model of Dissolution: Application to Porous Media Formation
17:20-17:40	Xiaoqian Huang	Universite Claude Bernard Lyon 1	Thermodynamically Consistent Phase Field Modeling for Freeze Crystallization in A Binary System

<b>Pearl Room 1, May 22, Topic 1-V, Chair: Tomohiro Takaki</b>			
8:30-9:00	Damien Tournet	IMDEA Materials	Phase-Field Insights into Microstructure Selection During Solidification of Hcp Mg Alloys
9:00-9:30	Munekazu Ohno	Hokkaido University	Quantitative Phase-Field Modeling of Non-Equilibrium Interface Dynamics During Rapid Solidification
9:30-9:50	Guillaume Boussinot	Access E.V.	Review on The Non-Diagonal Phase Field Model and Its Applications
9:50-10:10	Li Yue	Northwestern Ploytechnical University	A Continuum Phase-Field Model with Interfacial Concentration Ordering Parameters
<b>Coffee Break</b>			
<b>Pearl Room 1, May 22, Topic 1-VI, Chair: Yuhong Zhao</b>			
10:30-11:00	Abhik Choudhury	Indian Institute of Science	Diffuse-Interface Formulations for Coupling Process and Microstructure Simulations Within the Smooth-Boundary Framework
11:00-11:20	Mingwang Zhong	Northeastern University - USA	Grain Texture Selection During Rapid Alloy Solidification
11:20-11:40	Yuhan Cai	Karlsruhe Institute of Technology	Formation of Misoriented Lamellar Microstructures in Mo-Si-Ti Alloy: A Phase-Field Study
11:40-12:00	V. B. Rajkuma	Central South University	Phase-Field Simulation of Eutectic Solidification Microstructures in Al-Zn And Cu-Mg Systems Integrating CALPHAD

Pearl Room 1, May 23, Topic 1-VII, Chair: Jincheng Wang			
8:30-9:00	Qingcheng Yang	Shanghai University	A Thermodynamically Consistent Phase-Field-Micromechanics Model of Solid-State Sintering with Coupled Diffusion and Deformation
9:00-9:20	Weipeng Chen	North University of China	Temperature And Solute Diffusion In A-Mg Dendrite Growth of Mg-5wt.%Zn Alloy: A Phase-Field Study
9:20-9:40	Sa Ma	Central South University	Parallel-GPU-Accelerated Large-Scale Quantitative Phase-Field Simulation of Dendrite Growth for Al-Si-Mg Casting Alloys
9:40-10:00	Chuanqi Zhu	Tohoku University	Diffuse Interface Model for Alloy Solidification Under Non-Equilibrium Cooling Conditions
<b>Coffee Break</b>			
Pearl Room 1, May 23, Topic 1-VIII, Chair: Murali Uddagiri			
10:20-10:40	Lei Wang	Northwestern Polytechnical University	Applications of Phase-Field Method in The Study of Solidification Defects Formation
10:40-11:00	Kai Wang	TU-Darmstadt	Electro-Chemo Coupled Phase Field Modeling of Grain Growth in SrTiO <sub>3</sub> Polycrystalline Material
11:00-11:20	Wenbo Liu	Xi'an Jiaotong University	Sintering of Ceramic Nuclear Fuels: Phase-Field Simulation
11:20-11:40	Sandeep Sugathan	Kookmin University	Phase Field Study of Solid-State Sintering Process in Binary Alloys
11:40-12:00	Ayush Suhane	The University of British Columbia	Atomistically Informed Phase Field Modeling for Austenite Grain Growth

## Topic 2a. Solid State Processes in Functional Materials

Pearl Room 2, May 21, Topic 2a-I, Chair: Jiamian Hu			
8:30-9:00	Long-Qing Chen	The Pennsylvania State University	Thermodynamic Basis for Phase-Field Method of Ferroelectrics
9:00-9:30	Houbing Huang	Beijing Institute of Technology	Electric-Field-Induced Crystallization of Hf <sub>0.5</sub> Zr <sub>0.5</sub> O <sub>2</sub> Thin Film Based on Phase-Field Modeling
9:30-9:50	Yu-Jia Wang	Institute of Metal Research, Chinese Academy of Sciences	Prediction and Observation of Polar Topological Domain Structures in Ferroelectric Thin Films
9:50-10:10	Jianhua Ren	Sun Yat-Sen University	Stabilization and Control of Weakly Correlated Polar Skyrmions In Ferroelectric Thin Films
<b>Coffee Break</b>			
Pearl Room 2, May 21, Topic 2a-II, Chair: Zijian Hong			

10:30-11:00	Jie Wang	Zhejiang University	Phase Field Modeling of Topological Domain in Ferroelectric and Ferromagnetic Materials
11:00-11:30	Zhong-Hui Shen	Wuhan University of Technology	Phase-Field Programming Polarity Heterogeneity of Energy Storage Dielectrics by Bidirectional Intelligent Design
11:30-11:50	Ke Xu	Beijing Institute of Technology	Insight into Domain Structure and Energy Storage Properties of Antiferroelectric Via Phase-Field Methods

**Pearl Room 2, May 21, Topic 2a-III, Chair: Houbing Huang**

13:30-14:00	Yann Le Bouar	Université Paris-Saclay	Modeling of The Electrical Resistivity of Microstructures
14:00-14:30	Zijian Hong	Zhejiang University	Phase-Field Simulations of Polar Skyrmions
14:30-14:50	Ren-Ci Peng	Xidian University	The Role of Space Layer in Domain Dynamics of $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$ Thin Films Via Phase-Field Simulations
14:50-15:10	Shiyu Tang	Beijing Institute of Technology	Multi-Field Manipulation of Topological Domains on BFO Nano islands By Phase-Field Simulations
15:10-15:30	Xu Hou	The Hong Kong Polytechnic University	Effect of Grain Size on The Electrocaloric Properties of Polycrystalline Ferroelectrics

**Coffee Break**

**Pearl Room 2, May 21, Topic 2a-IV, Chair: Yann Le Bouar**

15:50-16:20	Tao Xu	Kyoto University	Mechanical Rippling for Rich Ferroelectric Topologies in $\text{SrTiO}_3$ Nanofilms
16:20-16:40	Zhanpeng Zhang	Xiangtan University	Thermodynamic Analysis of Stress-Mediated Electrocaloric In Ferroelectrics
16:40-17:00	Yinping Zeng	Changsha University of Science and Technology	Gibbs Energy and Phase-Field Modeling of Phase Transformation Under an External Magnetic Field
17:00-17:20	Xuhui Lou	Sichuan University	Electromechanical Grain Boundary Model with Formation Mechanism in Polycrystalline Ferroelectrics

**Pearl Room 2, May 22, Topic 2a-V, Chair: Zhong-Hui Shen**

8:30-9:00	Yu Su	Beijing Institute of Technology	Phase-Field Study of The Strongly Enhanced Capacitive Energy Density in Ferroelectric Films with Superfine Columnar Nanograins
9:00-9:30	Xiaoqin Ke	Xi'an Jiaotong University	Phase-Field Modelling on The Phase Transition Mechanisms and Associated Properties of Ferroelectric Materials
9:30-9:50	Ling Fan	Karlsruhe Institute of Technology (KIT)	A Phase-Field Model For Ferroelectric Materials—Based On The Multiphase-Field Approach

**Coffee Break**

<b>Pearl Room 2, May 22, Topic 2a-VI, Chair: Yu Su</b>			
10:30-11:00	Fei Li	Xi'an Jiaotong University	The Origin of Ultrahigh Piezoelectricity in Relaxor-Ferroelectric Solid Solution Crystals
11:00-11:30	Xiaoyan Lu	Harbin Institute of Technology	Phase Coexistence and Critical Behaviors in Ferroelectric Materials
11:30-11:50	Shuai Yuan	Guilin University of Electronic Technology	Hexagonal Close-Packed Skyrmion Lattices in Ferroelectric Ultrathin PbTiO <sub>3</sub> Films

<b>Pearl Room 2, May 23, Topic 2a-VII, Chair: Tiannan Yang</b>			
8:30-9:00	Jiamian Hu	University of Wisconsin-Madison	Design of Narrowband Magnonic Terahertz Emitter by Dynamical Phase-Field Simulation
9:00-9:20	Shouzhe Dong	Beijing Institute of Technology	Voltage-Controlled Magnetic Double-Skyrmion States in Magnetoelectric Elliptical Nanostructures by Phase-Field Model
9:20-9:40	Yu Wang	Central South University	Coherent Magnitude-Fluctuated Spin Waves Emitted by Magnetic Skyrmions
9:40-10:00	Jiajun Sun	Zhejiang University	Strain Mediated Transition Between Skyrmion And Antiskyrmion In Ferromagnetic Thin Films

**Coffee Break**

<b>Pearl Room 2, May 23, Topic 2a-VIII, Chair: Jie Wang</b>			
10:20-10:50	Tiannan Yang	Shanghai Jiao Tong University	Excited-State Evolution Dynamics of Ferroelectric Domains: A Phase-Field Study
10:50-11:10	Yixuan Jiang	Lanzhou University	Phase-Field Modelling on Mechanically Induced Phase-Transition in PMN-0.3PT Single Crystal
11:10-11:30	Sizheng Zheng	Zhejiang University	The Origin of The Chiral Phase Transition in Ferroelectric/Dielectric Superlattices
11:30-11:50	Changqing Guo	Beijing Institute of Technology	Evolution of Domain Structures in Flexible Ferroelectric Thin Film Systems by Phase-Field Simulations

## Topic 2b. Solid State Processes in Structural Materials

<b>Bauhinia Room 1, May 21, Topic 2b-I, Chair: Qingping Sun</b>			
8:30-9:00	Guozheng Kang	Southwest Jiaotong University	Phase Field Simulation on The Functional Properties of Shape Memory Alloys
9:00-9:30	Jiaming Zhu	Shandong University	Microstructure Evolution and High-Performance Design of Materials Via Phase Field Simulations
9:30-9:50	Hesham Salama	Interdisciplinary Centre For Advanced Materials Simulation (ICAMS)	Phase-Field Simulation Framework for Modeling Martensite and Bainite Formation in Steel

9:50-10:10	Hongwei Zhang	Northeastern University	Morphological Evolution of Ferrite-Austenite Interface and Cementite Grains in Divorced Eutectoid Transformation of Fe-1.05wt%C Alloy
<b>Coffee Break</b>			
<b>Bauhinia Room 1, May 21, Topic 2b- II , Chair: Guozheng Kang</b>			
10:30-11:00	Qingping Sun	The Hong Kong University of Science and Technology	Development of Ultrahigh Fatigue Life Shape Memory Alloys for Solid-State Refrigeration Technology: Challenges and Opportunities
11:00-11:30	Hong-Hui Wu	University of Science and Technology Beijing	Phase Field Simulation Study on Microstructure Evolution of Low Carbon Steel
11:30-11:50	Ben Niu	Dalian University of Technology	Disorder-Order Transformation and Phase-Filed Simulation of Coherent B2/L21 Phase in Irradiated BCC Fe-Cr-Al Alloys
11:50-12:10	Qianglong Liang	Xi'an Jiaotong University	Fatigue-Resistant Elastocaloric Effect in Hypoeutectic TiNi58 Alloy with Heterogeneous Microstructure

<b>Bauhinia Room 1, May 21, Topic 2b-III, Chair: Rongpei Shi</b>			
13:30-14:00	Yao Shen	Shanghai Jiao Tong University	Dual-Mesh Crystal Plasticity Finite Element (CPFE) – Phase Field (PF) Coupled Model For Dislocation And Twin Plasticity
14:00-14:30	Xu Zhang	Southwet Jiaotong University	Deformation Mechanism of Dual Heterogeneous Materials: A Combined Crystal Plasticity FEM and Phase Field Modeling
14:30-14:50	Xiaohua Niu	Xiamen University of Technology	A Phase Field Model for The Motion of The Prismatic Dislocation Loops by Both Climb and Self-Climb
14:50-15:10	Hong Liu	Shanghai Jiao Tong University	Multiscale Simulation Study on Precipitation Behavior in Light Alloys
<b>Coffee Break</b>			
<b>Bauhinia Room 1, May 21, Topic 2b-IV, Chair: Yao Shen</b>			
15:50-16:20	Rongpei Shi	Harbin Institute of Technology (Shenzhen)	Origin of Morphological Variation of Grain Boundary Precipitates in Metallic Alloys
16:20-16:50	Tianlong Zhang	The Hong Kong University of Science and Technology	Design of Compositionally Modulated Strong Yet Ductile Ti Alloys
16:50-17:10	Mengyuan Hao	Northwest Institute of Nonferrous Metals	Heterogeneous Precipitate Microstructure Design In B-Ti Alloys By Regulating The Cooling Rate



17:10-17:30	Xiaoke Wu	Central South University	A Novel Nucleation Model for Multi-Component Alloys During Solid-State Phase Transition and Its Incorporation into Phase-Field Model with Finite Interface Dissipation
17:30-17:50	Jakub Mikula	Institute of High-Performance Computing, Agency for Science, Technology and Research	Phase Field Model of Heat Treatment and Strengthening In Maraging Steel

**Bauhinia Room 1, May 22, Topic 2b-V, Chair: Saswata Bhattacharya**

8:30-9:00	Yipeng Gao	Jilin University	Grain Boundary Engineering Using Self-Organized High-Index Twins: A Phase Field Study
9:00-9:30	Benoit Appolaire	Université De Lorraine	Phase-Field Cosserat Crystal Plasticity Towards Modelling Nucleation in Recrystallization
9:30-9:50	Haipeng Li	Jilin University	Phase Field Modeling and Stress Field Analyses of Twin-Twin, Twin-Grain Boundary Reactions Mediated by Disclinations In Mg Alloys
9:50-10:10	Yongsi Wei	Jilin University	Analytical Solution and Phase Field Simulations of Stress Fields Associated with Twin-Twin Reactions in Mg Alloys

**Coffee Break**

**Bauhinia Room 1, May 22, Topic 2b-VI, Chair: Benoit Appolaire**

10:30-11:00	Saswata Bhattacharya	Indian Institute of Technology, Hyderabad	Morphology Selection in Bimetallic Nanoparticles: A Phase-Field Study
11:00-11:30	Dongke Sun	Southeast University	Lattice Boltzmann-Phase Field Modeling of The Coherent Hexagonal-To-Orthorhombic Transition in The Elastic Strain Field
11:30-11:50	Caihao Qiu	City University of Hong Kong	Grain Growth Controlled by Disconnection-Mediated Interface Migration
11:50-12:10	Liu Huo	Ruhr-Universität Bochum	A Multi-Phase Field Simulation of The Grain Growth in Smco Polycrystal Assisted by Magnetic Fields

**Bauhinia Room 1, May 23, Topic 2b-VII, Chair: Dong Wang**

8:30-9:00	Yongsheng Li	Nanjing University of Science and Technology	Three Dimensional Phase-Field Simulation of Kinetics Evolution of Lamellar $\Gamma$ -TiAl Alloys
9:00-9:20	Jinlin Li	Dalian University of Technology	Phase-Field Simulation of Coherent $\Gamma/\Gamma'$ Microstructures In Co-Based Superalloys

9:20-9:40	Min Yang	Northwestern Polytechnical University	Effect of $\Gamma'$ Volume Fraction On Creep of Ni-Based Single-Crystal Superalloys: A View from Evolutions of Internal Stress and Strain Fields
9:40-10:00	Ahmadreza Riyahi Khorasgani	Ruhr University of Bochum	Phase Field Modeling of Kirkendall Voids in A Compositionally Graded Superalloy
<b>Coffee Break</b>			
<b>Bauhinia Room 1, May 23, Topic 2b-VIII, Chair: Yongsheng Li</b>			
10:20-10:50	Dong Wang	Xi'an Jiaotong University	Phase Field Simulations Assisted Multiscale Microstructure and Property Design of Alloys
10:50-11:10	Yuanchao Yang	Xi'an Jiaotong University	Phase Field Investigation of The Influence of Transformation Induced Plasticity in Lath Martensite
11:10-11:30	Xiaolin Tian	North University of China	Spinodal Decomposition Mediated Misorientation Dependence of Grain Boundary Segregation: A Phase-Field-Crystal Study
11:30-11:50	Zheyuan Liu	Central South University	Atomic Scale Insights into The Self-Assembly of Alternating Aln/Tin Lamellar Nanostructure Via Spinodal Decomposition in Altin Coating
11:50-12:10	Ali Khajezade	University of British Columbia	Phase Field Modeling of Anisotropic Grain Growth

### Topic 3. Electrochemical reactions, corrosion, and oxidation

<b>Bauhinia Room 2, May 21, Topic 3- I , Chair: Lei Chen</b>			
13:30-14:00	Yong Du	Central South University	Multiphase Transformation and Mechanical Analysis of Sn-Based Nanoparticle During Lithiation Via CALPHAD-Guided Phase-Field Approach
14:00-14:30	Kejie Zhao	Purdue University	Corrosive Fracture and Its Interplay with Electrochemistry in Battery Electrodes
14:30-14:50	Umair Hussain	Indian Institute of Technology Madras	Voltammetric Study of Phase Separating Materials in Li-Ion Battery Using Phase-Field Modelling
<b>Coffee Break</b>			
<b>Bauhinia Room 2, May 21, Topic 3- II, Chair: Yong Du</b>			
15:30-16:00	Lei Chen	University of Michigan-Dearborn	Optimization of External Pressure in Pouch Cell Manufacturing Through Large-Scale Phase-Field Simulations
16:00-16:20	Rui Zhang	Beijing Huairou Laboratory	Electrode Microstructure Design for Electrochemical Energy Storage Devices

16:20-16:40	Li Ting Gao	Shanghai University	Elucidating the Role of Rational Separator Microstructures in Guiding Dendrite Growth and Reviving Dead Li
16:40-17:00	Chuanjie Cui	University of Oxford	Phase Field Modelling of Stress Corrosion Cracking

**Spring Room, May 22, Topic 3- III, Chair: Geng Zhang**

8:30-9:00	Ying Zhao	Tongji University	Phase-Field Formulation for Predicting Void Evolution at The Li--Electrolyte Interface in All-Solid-State Batteries
9:00-9:20	Sachin Poudel	Silesian University of Technology	A Computational Model for Examining the Role of Externally Applied Stress on Dendrite Growth Pattern in Solid State Lithium-Ion Batteries
9:20-9:40	Yuyang Lu	Westlake University	Phase Field Simulation for Crack Propagation in Polycrystalline Particles in Lithium Ion Batteries
9:40-10:00	Yang Bai	Max-Planck-Institut FÜR Eisenforschung GmbH	Chemomechanical Phase-Field Modeling of Phase Transformation During Iron Oxide Reduction with Hydrogen

**Coffee Break**

**Spring Room, May 22, Topic 3- IV, Chair: Ying Zhao**

10:20-10:50	Geng Zhang	Fujian Science & Technology Innovation Laboratory for Energy Devices of China	Improved Electrochemical Phase-Field Model and Its Application to Ionic Deposition and Intercalation
10:50-11:10	Pan Wang	Central South University	A Quasi-Smooth Manifold Element (QSME) Method for Fast and Accurate Numerical Simulation of Stress Corrosion
11:10-11:30	Yajie Li	Shanghai University	Microstructure Optimization of Dendrite Inhibiting Battery Separators Via Phase-Field Modeling

## Topic 4. Brittle and Ductile Fracture

**Bahinia Room 2, May 21, Topic 4- I , Chair: Yong Ni**

8:30-9:00	Jiaying Wu	South China University of Technology	A Generalized Phase-Field Cohesive Zone Model for Fracture
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9:00-9:30	Bai-Xiang Xu	TU Darmstadt	Cohesive Phase-Field Chemo-Mechanical Modeling of Inter- and Trans- Granular Fracture of Polycrystalline Materials: Application in Lithium Ion Battery Cathode Materials
9:30-9:50	Shucheta Shegufta	Friedrich-Alexander-Universität Erlangen-NÜRNberg	Fracture of Porous Media with Thermally Driven Healing of Damage: From Peridynamics To Phase Field Formulations
9:50-10:10	Bin Li	Guangdong Technion-Israel Institute of Technology	Crack Path Selection in Brittle Anisotropic Materials

**Coffee Break**

**Bauhinia Room 2, May 21, Topic 4- II, Chair: Bai-Xiang Xu**

10:30-11:00	Yong Ni	University of Science and Technology of China	Phase Field Modeling of Some Crack Path Problems
11:00-11:20	Yong Zhang	Tongji University	On the Coupling of Fracture and Dielectric Breakdown in Piezoelectric Materials
11:20-11:40	Lin Chen	Northeastern University	Mixed-Mode Crack Opening Computation in The Phase Field Method
11:40-12:00	Qionghuan Zeng	Northwestern Polytechnical University	Phase-Field Investigation on The Effect of Grain Size on The Propagation Behavior of Intergranular Corrosion Cracks in Austenitic Stainless Steels

**Bauhinia Room 2, May 22, Topic 4- III, Chair: Zhanli Liu**

8:30-9:00	Yongxing Shen	Shanghai Jiao Tong University	A Scheme for Crack Nucleation in The Phase Field Approach to Brittle Fracture
9:00-9:20	Yuanfeng Yu	Northwestern Polytechnical University	A Length Independent Regularized Phase Field Model for Brittle and Quasi-Brittle Fracture
9:20-9:40	Tao Zhang	South China University of Technology	Phase-Field Modeling of Storage Particle Delamination and Electrolyte Cracking in Cathodes of Solid-State Batteries
9:40-10:00	Pei-Liang Bian	Hohai University	A Variationally-Consistent Phase-Field Cohesive Zone Model for Mixed-Mode Fracture Based on Energy Decomposition Scheme

**Coffee Break**

**Bauhinia Room 2, May 22, Topic 4- IV, Chair: Jianying Wu**

10:20-10:50	Pengyang Zhao	Shanghai Jiao Tong University	Integrated Modeling of Microstructural and Micromechanical Evolution Subjected to Thermal-Mechanical Loadings
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10:50-11:10	Xiaofei Hu	Dalian University of Technology	Mesoscopic Phase Field Modelling of Progressive Damage in Hydroxyl-Terminated Polybutadiene (HTPB) Propellant of Solid Rocket Motor
11:10-11:30	Wenxiang Shi	Southwest Jiaotong University	A Diffusional-Mechanically Coupled Phase Field Model of Shape Memory Alloys in Hydrogen-Rich Environment
11:30-11:50	Shuo Yang	Shanghai Jiao Tong University	An Acceleration Scheme for The Phase Field Fatigue Fracture Simulation
11:50-12:10	Ye Feng	Northwestern Polytechnical University	Phase-field method of cohesive fracture: mixed-mode cohesive law and frictional contact

**Bauhinia Room 2, May 23, Topic 4- V, Chair: Pengyang Zhao**

8:30-9:00	Zhanli Liu	Tsinghua University	Reveal the Mixed Tensile-Shear Ductile Fracture of Impulsively Loaded Metal Plates by Developing A Phase-Field Fracture Model
9:00-9:20	Yudong Ren	Tongji University	Physically Consistent Nonlocal Macro-Meso-Scale Damage Model for Brittle Fracture
9:20-9:40	Wanxin Chen	The Technical University of Darmstadt	Cohesive Phase-Field Fracture Simulation of Wetting Impact on Chemo-Mechanical Bulk and Interfacial Damage: Application in Li-Ion Battery Cathode Materials
9:40-10:00	Yuanyuan Wang	Dalian University of Technology	Phase-Field Modeling of Crack Propagation Assisted by Irradiation Environment in Tungsten

**Coffee Break**

**Bauhinia Room 2, May 23, Topic 4- VI, Chair: Yongxing Shen**

10:20-10:50	Hongjun Yu	Harbin Institute of Technology	A Thermodynamic Consistent Phase Field Model for The Fracture of Micropolar Medium Considering the Tension-Torsion Coupling Effect
10:50-11:10	Lukas Schöller	Karlsruhe Institute of Technology (KIT)	Phase-Field Modeling of Crack Propagation Considering Multi-Crack Order Parameters and Mechanical Jump Conditions
11:10-11:30	Zaiyong Wang	Taiyuan University of Technology	Numerical Study of Multiple Hydraulic Fractures Propagation in Poroelastic Media Based on Energy Decomposition Phase Field Method
11:30-11:50	Chang Liu	Southwest Jiaotong University	A Phase-Field Model for The Fracture Behavior of Ferroelectric Materials with Flexoelectric Effect
11:50-12:10	Fucheng Tian	Hokkaido University	Dynamic instability of rapid fracture in soft materials

## Topic 5. New Method Development

Spring Room, May 21, Topic 5-I, Chair: Daniel Schneide			
8:30-9:00	Alphonse FINEL	Université Paris-Saclay	A New FFT-Based Mechanical Solver for Abrupt Interfaces
9:00-9:30	Ken Elder	Oakland University	Moire Patterns, Dislocations and Defects in Graphene and Hexagonal Boron (Hbn) Layers
9:30-9:50	Bohyun Yoon	Kyung Hee University	Anisotropic Grain Boundary Properties in Grain Growth Modelling: A Phase-Field Approach Using Spherical Gaussian Function
9:50-10:10	Ming Tang	Rice University	Accelerating Microstructure Evolution Simulations with Convolutional and Graph Neural Networks with Adaptive Spatiotemporal Resolution
<b>Coffee Break</b>			
Spring Room, May 21, Topic 5-II, Chair: Ken Elder			
10:30-11:00	Lijun Zhang	Central South University	Phase-Field Modeling of Microstructure Evolution: Ready for Materials Design?
11:00-11:20	Dong-Uk Kim	Kookmin University	An Efficient Phase Field Approach to Growth of Stoichiometric Compounds of Aluminum Alloys
11:20-11:40	Qing Wang	Dalian University of Technology	Design and Evolution of Coherent Microstructure In BCC/B2 High-Entropy Alloys Via the Cluster-Formula Approach and Phase-Field Method
11:40-12:00	Peng Wu	Harbin Institute of Technology	Multi-Scale Simulation of Voids Migration at Cu-Sn Interface Under Electromigration Effect
Spring Room, May 21 Topic 5-III, Chair: Lijun Zhang			
13:30-14:00	Daniel Schneide	Karlsruhe Institute of Technology	Chemo-Elastic Benchmarks in The Context of (Multi)Phase-Field Modeling
14:00-14:30	Pil-Ryung Cha	Kookmin University	Development Endeavors of Microstructure Prediction Models at The ICAPE (Integrated Computer-Aided Process Engineering) Center for Structural Materials
14:30-14:50	Nanxi Chen	Tongji University	Solving Phase Field AC-CH Equations Using A Novel PF-Pinns Framework

14:50-15:10	Anil Kunwar	Silesian University of Technology	Unveiling New Horizons in Materials Interface Understanding Through the Synergy of Phase Field Simulations and Machine Learning Techniques
<b>Coffee Break</b>			
<b>Spring Room, May 21, Topic 5-IV, Chair: Alphonse FINEL</b>			
15:30-16:00	Marco Salvalaglio	TU-Dresden	Coarse-Grained Phase Field Crystal Modeling of Elasticity and Defects
16:00-16:30	Jianshan Wang	Tianjin University	Modelling Polymorphic Transformations and Debonding of Bacterial Filagellar Filaments
16:30-16:50	Di Qiu	Shanghai University	Predicting Grain Boundary Dislocation Structures Using Microscopic Phase-Field Model and Neural Networks
16:50-17:10	Lan Shang	Zhejiang Lab	Physics-Informed Neural Networks for The Phase-Field Simulation of Ferroelectric Microstructure Evolution

<b>Spring Room, May 23, Topic 5-V, Chair: Akinori Yamanaka</b>			
8:30-9:00	Namin Xiao	Beijing Institute of Aeronautical Materials	Design of Titanium Alloy for Aero-Engines Using an ICME Framework
9:00-9:30	Zhi-Feng Huang	Wayne State University	Modeling Two-Dimensional Layered Materials Via Phase Field Crystal Method
9:30-9:50	Nan Wang	Guangdong Technion - Israel Institute of Technology	Connecting Continuum And Quantum Mechanical ELETROMIGRATION Theories at Mesoscale Using Phase Field Crystal Method
9:50-10:10	Takumi Morino	Yokohama National University	Phase-Field Model for CALPHAD Coupling : Closed-Form Expression for The Interface Composition Satisfying Local Equilibrium

**Coffee Break**

<b>Spring Room, May 23, Topic 5-VI, Chair: Namin Xiao</b>			
10:30-11:00	Akinori Yamanaka	Tokyo University of Agriculture and Technology	Bayesian Data Assimilation-Integrated Phase-Field Modeling of Fracture
11:00-11:20	Sen Liu	Shanghai Jiao Tong University	Asymptotic Homogenization Framework for Fracture of Heterogeneous Materials Based on The Phase Field Approach
11:20-11:40	Vincent Feyen	KU Leuven	Scale-Bridging Quantitative High Driving Force Phase-Field Model Applied To The B To A Phase Transformation In Pure Titanium

## Poster Session

No.	Presenter	Affiliation	Title
<b>P1. Solidification &amp; Additive Manufacturing</b>			
P1-1	Raphael Schiedung	ICAMS - The Interdisciplinary Centre For Advanced Materials Simulation	Openphase Studio: The Microstructure Simulation Suite
P1-2	Wenhang Ning	University of Science and Technology Beijing	Evolution of Iron-Rich Phase During Solidification of Al-Si-Fe Alloys
P1-3	Shunsuke Kanki	Kyoto Institute of Technology	Estimation of Solid-Liquid Interfacial Properties in Pure Metal Solidification by Integrating Phase-Field with Molecular Dynamics Simulations Using Data Assimilation
P1-4	Namito Yamanaka	Kyoto Institute of Technology	Multi-Phase-Field Lattice Boltzmann Modeling and Systematic Simulations for Semi-Solid Deformation
P1-5	Konosuke Ikeda	Kyoto Institute of Technology	Multi-Phase-Field Lattice Boltzmann Modeling of Microstructure Evolutions Affected by Melt Pool Flow During Powder Bed Fusion
P1-6	Yuki Takahashi	Kyoto Institute of Technology	Efficient Large-Scale Simulations of Multi-Phase-Field Method for Various Scanning Strategies in Metal Additive Manufacturing
P1-7	Ayano Yamamura	Kyoto Institute of Technology	Data Assimilation For Precise Evaluation of Columnar Dendrite Growth Via Phase-Field Method-X-Ray Tomography Integration
P1-8	Murali Uddagiri	Ruhr University Bochum	Phase Field Simulation of Eutectic Solidification of a Multi-Phase Multicomponent Al-Based Alloy
P1-9	Wout Mertens	KU Leuven	Unraveling Cooling Rate Impact on Ti Phase Transition: Integrated Simulations and Experiments
P1-10	Tamás Pusztai	Wigner Research Centre For Physics	Phase-Field Modeling of Unconventional Morphologies Formed in Biomineralizing Systems
P1-11	Hao Wang	Clausthal University of Technology	Statistical Mechanics Informed Phase Field Modelling of Li <sub>2</sub> SiO <sub>3</sub> Solidification from The Li <sub>2</sub> O-SiO <sub>2</sub> Melt
P1-12	Heran Wang	Xi'an Jiaotong University	Phase-Field Simulation of The Effect of Stress Field on Pseudospinodal Decomposition
P1-13	Shinji Sakane	Kyoto Institute of Technology	Systematic Evaluation of Settling Equiaxed Dendrite During Solidification by The Phase-Field Lattice Boltzmann Simulations
P1-14	Yuanzuo Wang	Beijing University of Technology	Phase Field Approach to Stress Corrosion Crack of Elastoplastic Solid
P1-15	Siqin Liu	Beihang University	Phase Field Modeling of Transcrystalline Growth During Additive Manufacturing of Semi-Crystalline Thermoplastic Polymer Composites
P1-16	Ying Gao	Xi'an University of Technology	Atomistic Investigation of Coarsening Kinetics of Supported Nanoparticles Using the Phase Field Crystal Model



P1-17	Yashan Zhang	Northwestern Polytechnical University	Mechanism of grain boundary angle on solidification cracking in directed energy deposition Hastelloy X superalloys
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<b>P2. Solid State Processes in Structure and Functional Materials</b>			
P2-1	Xlin-Wei Wu	Tianjin University	An Electro-Thermo-Mechanical Coupling Phase-Field Model of Defect'S Evolution Induced By Electromigration In Interconnects
P2-2	Wenkui Yang	North University of China	Dislocation Loop and Irradiation-Induced Synergistic-Competitive Mechanism in Cu-Rich Precipitates: A Phase-Field Study
P2-3	Hassaan Ali	Hongik University	Phase Field Modeling of Strain Induced Phase Transformations in Mote2
P2-4	Xiong Shuai	Jiangxi University of Science and Technology	Simulation of Microstructure Evolution and Response of Mechanical Properties and Corrosion Resistance of Aluminum Alloy in Early Aging
P2-5	Liqiang He	Xi'an Jiaotong University	Large Electrostrain With Nearly-Vanished Hysteresis in Eco-Friendly Perovskites by Building Coexistent Ferroelectric Glasses
P2-6	Aoi Nakazawa	Kyoto Institute of Technology	Continuous Simulation from Powder Compaction to Sintering Using High-Performance Multi-Phase-Field Computing
P2-7	Juan Zhang	Southwest Jiaotong University	A Phase-Field-Finite-Element Simulation on Ratchetting of Medium Manganese TRIP Steel
P2-8	Shenglong Wang	Nanjing University of Science and Technology	Morphology and Phase Boundary Evolutions of Co-Based Superalloy with Lattice Mismatch Strain
P2-9	Zhiheng Luo	Guangdong Technion-Israel Institute of Technology	Effects of Space Charge on Freestanding Ferroelectric Thin Films
P2-10	Tianjiao Dong	Xi'an Jiaotong Universit	Phase Field Simulations for The Crossover from Sharp Martensitic Transformation into Smooth Strain Glass Transition by Fine Precipitates
P2-11	Yunting Su	Xi'an Jiaotong University	Computer Simulations for Shuffle-Regulated Strain Glass Transition in Compositionally Modulated Ti-Nb Alloys
P2-12	Jianwei Li	Xi'an Jiaotong University	Effects of External Stress On Microstructure Evolution In $\Gamma$ -Tial Alloys By Phase Field Method
P2-13	Tianmeng Zhang	Guangdong Technion – Israel Institute of Technology (GTIIT)	Exploring the Role of Dislocations in Solid-State Dewetting Through Phase Field Crystal Method
P2-14	Jiyuan Ding	Jilin University	A Disclination-Based Theory of Twin-Twin Reactions: Complete Analyses of Symmetry-Correlated Deformation Pathways, Twinning Disclination Generation and Resulting Stress Concentration

P2-15	Silong Quan	East China University of Technology	Study on Interfacial Dislocation Network Transition and Formation Mechanism in Van Der Waals Heterojunctions
P2-16	Yuefeng Sheng	Shanghai University/China	Phase Field Method Study on The Microscopic Mechanism of Twinning and Dislocations In Mn-Cu Damping Alloys
P2-17	Chunfeng Du	Jilin University	A Lie-Algebra-Based Description of Disclination Densities and The Quantification of Partial Disclinations In Deformed Polycrystalline Metals
P2-18	Meixiong Zhu	Institute of Metal, Research Chinese Academy of Sciences	Enhancing Energy Storage Performance in Bifeo <sub>3</sub> Films Via Oxygen Vacancies and Strain Engineering
P2-19	Zhenzhi Liu	Shanghai University	An Integrated Simulation Scheme to Predict Microstructural Evolution and Creep Behavior for A Nine-Component Ni-Based Superalloy
P2-20	Kohta Kasai	Kyoto University	Quasiparticle-Like Structures and Behaviors of Magnetic Skyrmion Lattice Defects from Phase-Field Simulations
P2-21	Huimei Li	Institute of Metal, Research Chinese Academy of Sciences	Electric-Field-Induced Topological Transition in Pbtio <sub>3</sub> /Sr <sub>2</sub> io <sub>3</sub> Superlattice
P2-22	Xi Liu	Central South University	Phase Field Simulation of Grain Ripening During Liquid Phase Sintering of Nbc Matrix Cermets
P2-23	Yiqi Guan	Central South University	Phase-Field Simulation of Core-Rim Structure During Early Sintering in Tic-WC-Ni Cermet
P2-24	Hong Mao	Hunan Institute of Science and Technology	Strain-Induced Grain Boundary Migration and Grain Rotation in Polycrystalline Metals: Atomic-And Meso-Scale Phase Field Simulations
P2-25	Jiachen Hu	Southwest Jiaotong University	Plastic Deformation of Magnesium Single Crystal: A Crystal Plasticity Coupled Twinning Phase Field Simulation
P2-26	Rongpei Shi	Harbin Institute of Technology (Shenzhen)	The Influence of Particle Size and Its Distribution on Microstructure Evolution and Densification Kinetics During Sintering - A Phase-Field Simulation Study
P2-27	Dan Sun	Nuclear Power Institute of China	Phase-Field Simulation of Recrystallization Coupling Bubble Evolution During Irradiation in UO <sub>2</sub>
P2-28	Bo Xu	Sichuan University	Toward Tunable Functional Properties of Niti Shape Memory Alloys by Grain Size Engineering: A Phase Field Study
P2-29	Ming Zhao	Sichuan University	Total Internal Reflection of Shear Waves In Elastic/Dielectric Elastomer Bi-Materials

### P3. Electrochemical Reactions, Corrosion and Oxidation

P3-1	Jiachen Wang	North University of China	Phase-Field Simulation of Interface Growth of Magnesium Metal Anodes During Electrodeposition
P3-2	Haodong Zhang	Karlsruhe Institute for Technology	Thermodynamics of Dielectric Materials

#### P4. Brittle and Ductile Fracture

P4-1	Zhipeng Yao	Friedrich-Alexander-Universität Erlangen-NÜrnberg	A Phase Field Model for Interface Sliding and Interface Failure Parameterized by DFT Data
P4-2	Wenquan Zhou	Northwest A&F University	Investigations into The Deformation Behavior of Graphene Loops by Using Phase Field Crystal Model
P4-3	Xin Li	Nanjing University of Aeronautics and Astronautics	A Phase-Field Fracture Model for Fatigue Behavior in Fiber-Reinforced Composites Considering Anisotropic Fatigue Effects

#### P5. New Method Development and Integration with ML.

P5-1	Zhaobo Liu	Beijing Institute of Technology	Electric-Field-Induced Crystallization of Hf <sub>0.5</sub> Zr <sub>0.5</sub> O <sub>2</sub> Thin Film Based on Phase-Field Modeling
P5-2	Hwanwook Lee	Hongik University	Phase-Field Simulation of Thin Film Deposition and Crystallization
P5-3	Woojin Jung	Kyunghee University	Advanced Phase-Field Modeling of Constituent Redistribution In U-Zr Fuel Considering Fission Gas
P5-4	Yechan Kim	Hongik University	Multiphysics Modeling of Thermal Disturbance in Three-Dimensional Phase-Change Memory
P5-5	Yao Yang	Zhejiang Lab	Deep Multi-Task Learning with Multi-Scale Features for Metal-Organic Framework Properties Prediction
P5-6	Hongwen Zhang	Zhejiang Lab	Predicting Crystal Material Property by Combining Composition and Structure
P5-7	Hongmin Zhang	Karlsruhe Institute of Technology	Effect of Wall Free Energy Formulation on The Wetting Phenomenon: Conservative Allen-Cahn Model
P5-8	Xin SU	Guangdong Technion-Israel Institute of Technology	Modeling Grain Boundary Motion Driven by Electric Current
P5-9	Ingo Steinbach	Ruhr-University Bochum	Quantum Phase Field
P5-10	Liu Xi	Dalian University of Technology	A Quantitative Phase-Field Model of Gas Bubble Evolution in Phase Boundary of Uranium-Based Fuels
P5-11	Jiajun Zhao	Dalian University of Technology	Three-Dimensional Phase-Field Modelling of Fission Gas Resolution Effect on Nano-Sized Bubble Formation in UO <sub>2</sub>
P5-12	Xuejian Wang	Friedrich-Alexander University of Erlangen-NÜrnberg	An Extended Phase-Field-Drift-Diffusion Model for Oxygen Vacancy Migration in Single-Crystal Barium Titanate

P5-13	Meiling He	Central South University	Determination of Elastic-Plastic Parameters of Binder Phase in Cemented Carbide Using Nanoindentation And Finite Element Simulation
P5-14	Xiaoxiao Chen	Wuhan University of Technology	Programming Polarity Heterogeneity of Energy Storage Dielectrics by Bidirectional Intelligent Design