



The 4th International Symposium on Phase-Field Modelling in Materials Science.

July 22th - 25th 2019, Bochum (Germany)

## Program



## Monday 22. July 2019

9:00-10:00	Welcome		
10:00-10:10	Introduction (Prof. Steinbach)		
10:10-11:00	<b>Plenary I:</b> Prof. Long-Qing Chen, Pennsylvania State University, USA <b>Discovery and Design of Mesoscale Structures for Novel and Optimum Properties Guided by Phase-field Simulations</b> Chair: <i>Ingo Steinbach</i>		
11:00-11:10	Break		
11:10-12:30	<b>Session I:</b> <b>Solid state phase transformation</b> Chair: <b>Yunzhi Wang</b>  Chemo-mechanical multiphase-field modeling on the mesoscopic length scale: Applications to microstructural processes during heat treatment of steels <b>Daniel Schneider</b> , Karlsruhe Institute of Technology (KIT) and Karlsruhe University of Applied Sciences, Germany  Multiscale simulation of precipitation in Al-Cu alloys <b>Hong Liu</b> , KU Leuven, Belgium	<b>Session II:</b> <b>Solidification</b> Chair: <b>Damien Tournet</b>  Solid-liquid interfacial properties estimated from phase-field and molecular dynamics simulations <b>Munekazu Ohno</b> , Hokkaido University, Japan  Thermodynamic description and thermophysical properties of Mg-Gd alloys and quantitative phase-field simulation of their solidification process <b>Lijun Zhang</b> , Central South University, China  Phase-field investigation on the dynamic contact angle in a peritectic transition <b>Yuhan Cai</b> , Karlsruhe University of Applied Sciences, Germany  Phase-field modelling of nucleation in a binary glass forming system <b>Anders Ericsson</b> , Lund University, Sweden	<b>Session III:</b> <b>Emerging materials and industrial applications</b> Chair: <b>Yong Ni</b>  A phase-change memory device simulation using electrothermal and phase-change models <b>Kwon Yongwoo</b> , Hongik University, Republic of Korea  Multi-phase-field modelling of microstructure formation during the crystallization of a ternary alloy for phase-change memory applications <b>Raphaël Bayle</b> , PMC-Ecole Polytechnique/CEA Leti/STMicroelectronics, France  Phase field simulation on the mechanical controllability of toroidal ordering in ferroelectrics <b>Weijin Chen</b> , Sun Yat-sen University, China  Phase field modeling of topological phase transition in ferromagnetic materials <b>Jie Wang</b> , Zhejiang University, China
12:30-14:00	Lunch		
14:00-15:50	<b>Session IV:</b> <b>Solid state phase transformation</b> Chair: <b>Daniel Schneider</b>  <b>Highlight 30Min</b> Peter Voorhees <b>Coarsening of Bicontinuous Structures: A Comparison between Experiment and Simulation</b>  A Phase-Field Model for Segregation-Assisted Grain Boundary Phase Separation and Its Application to FeMn System <b>Reza Darvishi Kamachali</b> , Max-Planck-Institut für Eisenforschung (MPIE), Germany  Phase Field Simulation of Alpha/Beta Phase Transformation in Titanium Alloy Welds <b>Rajeev Ahluwalia</b> , Institute of High Performance Computing, Singapore  Phase-field/CALPHAD methods for multi-phase and multi-component microstructures <b>Chuanlai Liu</b> , Max-Planck-Institut für Eisenforschung, Germany  Domain dynamics in strain engineered bismuth ferrite thin films: a phase-field study <b>Soumya Bandyopadhyay</b> , Indian Institute of Technology Hyderabad, India	<b>Session V:</b> <b>Solidification</b> Chair: <b>Lijun Zhang</b>  Janin Eiken <b>A multi-phase-field approach for solidification considering phase, temperature and composition dependent local molar volumes</b>  Rod to lamellar transition during anisotropic two-phase eutectic growth <b>Sumeet Khanna</b> , Indian Institute of Science, Bangalore, India  Effects of branching on primary dendrite arm spacing in directional solidification of Al-Cu alloy <b>Jaehoon Lee</b> , Hokkaido University, Japan  Phase-field simulation on morphological diversity of solidification structure with different preferred growth directions <b>Kim Geunwoo</b> , Hokkaido University, Japan  Effect of Crystalline Anisotropy on Spacing Homogenization in Lamellar Eutectics <b>Maxime Ignacio</b> , LPMC, Ecole Polytechnique, France	<b>Session VI:</b> <b>Emerging materials and industrial applications</b> Chair: <b>Alain Karma</b> Shenyang Hu <b>Mesoscale Model of Volumetric Swelling in Monolithic UMo Nuclear Fuels by Coupling Phase Field Approach and Rate Theory</b>  Pattern formation during dewetting of a solid-state thin film – A phase field study <b>Miral Verma</b> , Indian Institute of Technology, Kanpur, India  Phase-Field Modeling of void growth kinetics in irradiated metallic fuels <b>Yong Lu</b> , Xiamen University, China  Formation Mechanism of script lamellar structure in Directionally-Solidified MoSi <sub>2</sub> /Mo <sub>5</sub> Si <sub>3</sub> Eutectic by Phase Field Simulation <b>Chuanqi Zhu</b> , Institute for Materials Research, Tohoku University, Japan  Application of the phase-field model for finite interface dissipation for general material problems <b>Matthias Stratmann</b> , OpenPhase Solutions GmbH, Germany
15:50-16:20	Break		
16:20-18:00	<b>Session VII:</b> <b>Solid state phase transformation</b> Chair: <b>Peter Voorhees</b>  Finite Strain Phase-Field Microelasticity Theory for Modeling Microstructural Evolution <b>Yunzhi Wang</b> , The Ohio State University, United States  Phase field modeling of 2D and 3D equilibrium shapes of the precipitate under influence of coherency stresses <b>Bhalchandra Bhadak</b> , Indian Institute of Science, Bangalore, India  Large scale phase-field simulations of solid state sintering <b>Johannes Hötzer</b> , Hochschule Karlsruhe, Deutschland  Phase-field simulation of lath martensite microstructure in low-carbon steel	<b>Session VIII:</b> <b>Solidification</b> Chair: <b>Janin Eiken</b>  Phase-field as a benchmark for other models of solidification and microstructure evolution <b>Damien Tournet</b> , IMDEA Materials Institute, Spain  Phase-field Solidification Texture Model for Powder Bed Fusion Additive-Manufacturing Process <b>Kamalnath Kadirvel</b> , Ohio State University, United States of America  PF-LBM modeling of equiaxed dendritic growth and motion in undercooled melt with forced fluid flow <b>Sen Luo</b> , Northeastern University, China  Modelling defects formation in late-stage solidification using a novel phase-field-crystal	<b>Session IX:</b> <b>Emerging materials and industrial applications</b> Chair: <b>Reza Darvishi Kamachali</b> Phase-field modelling of non-isothermal grain coalescence in additive manufacturing <b>Bai-Xiang Xu</b> , TU Darmstadt, Germany  Full-field simulations with OpenPhase: scientific and technical developments <b>Johannes Görler</b> , OpenPhase Solutions GmbH, Germany  Grain-Size and Frequency Dependent Behaviors of BaTiO <sub>3</sub> Nanoceramics: A Phase-Field Study <b>YU SU</b> , Beijing Institute of Technology, China  Phase-Field Modeling of Gas Bubble Morphology in Solids

**Oleg Shchyglo**, *ICAMS, Ruhr University  
Bochum, Germany*

method  
**Nan Wang**, *Guangdong Technion - Israel  
Institute of Technology, China*

**Amy Kaczmarowski**, *Sandia National  
Laboratories, United States of America*

Investigation of the Evolution Kinetics of Porous  
Metals During Dealloying by Phase-field Method  
**SanQiang SHI**, *The Hong Kong Polytechnic  
University, China*

Simulation of a rising bubble in a quiescent  
liquid: Coupled Phase-field Navier-Stokes model  
**Farshid Jamshidi**, *Karlsruhe University of  
Applied Sciences, Germany*

Phase-field simulation of solidification and  
homogenization in quinary high Mn steels  
**Won Tae Kim**, *Cheongju University, Korea*

18:00-21:00 Barbeque

## Tuesday 23. July 2019

9:00-9:50	Plenary II: Prof. Dr. Alain Karma, University of Boston, USA <b>Phase-field Modeling of Fracture</b> Chair: <i>Mathis Plapp</i>		
9:50-10:10	Break		
10:10-12:00	Session X: <b>Solid state phase transformation</b> Chair: <b>Yann Le Bouar</b>	Session XI: <b>Recrystallization and grain growth</b> Chair: <b>Mathis Plapp</b>	Session XII: <b>Mathematical and numerical aspects</b> Chair: <b>Oleg Shchyglo</b>
Highlight 30Min	<b>Dong Wang</b> <b>Phase field simulations assisted novel strain glass design</b> Variant selection during $\alpha$ precipitation in Ti-6Al-4V alloy under stress and around dislocation <b>Jinhu Zhang</b> , <i>Institute of Metal Research, China</i>	<b>Samuel Forest</b> <b>A Cosserat crystal plasticity and phase field approach to grain boundary migration</b> Modeling of abnormal grain growth during carburization in Nb-alloyed steel <b>Kinoshita Takahisa</b> , <i>Hokkaido University, Japan</i>	<b>Machiko Ode</b> <b>An application of machine learning to estimate interface conditions in KKS phase-field model</b> High-Speed High-Throughput Thermodynamic and Phase Equilibrium Calculation and Its Application in Phase Field Simulation <b>Shuanglin Chen</b> , <i>CompuTherm, LLC, USA</i>
	Effect of strong chemo-mechanical coupling on phase-transformation kinetics and microstructure stability <b>Ingo Steinbach</b> , <i>Ruhr-University Bochum, Germany</i>	Phase-field modeling of abnormal anisotropic grain growth in polycrystalline ceramic fibers <b>Julia Kundin</b> , <i>Ruhr Universitaet Bochum, Germany</i>	Coupling phase-field and CALPHAD models for multicomponent systems using thermodynamic tensor models. <b>Yuri Coutinho</b> , <i>KU Leuven, Belgium</i>
	A phase-field study of elastic stress effects on phase separation in ternary alloys <b>Saswata Bhattacharya</b> , <i>Indian Institute of Technology Hyderabad, India</i>	A phase-field investigation on the processing-dependent microstructure during selective laser sintering <b>Yangyiwei Yang</b> , <i>TU Darmstadt, Germany</i>	A regularized phase field model for anisotropic motion-by-curvature <b>Thomas Philippe</b> , <i>Physique de la Matière Condensée, Ecole Polytechnique, CNRS, France</i>
	Phase field modeling of deformation twinning in beta-metastable titanium alloys <b>Benoit Appolaire</b> , <i>Université de Lorraine, France</i>	Quantitative phase field modeling of discontinuous dynamic recrystallization for magnesium alloy during thermomechanical processing <b>Yulan Li</b> , <i>Pacific Northwest National Laboratory, United States</i>	Multi-phase-field modelling of void migration caused by electromigration in bamboo interconnect line <b>Akimitsu Ishii</b> , <i>Tokyo University of Agriculture and Technology, Japan</i>
12:00-14:00	Lunch		
14:00-14:50	Plenary III: Prof. Dr. Tomohiro Takaki, KIT, Kyoto, Japan <b>High-performance phase-field computing of solidification and grain growth</b> Chair: <i>Ingo Steinbach</i>		
14:50-15:10	Break		
15:10-17:00	Session XIII: <b>Solid state phase transformation</b> Chair: <b>Dong Wang</b>	Session XIV: <b>Recrystallization and grain growth</b> Chair: <b>Samuel Forest</b>	Session XV: <b>Mathematical and numerical aspects</b> Chair: <b>Machiko Ode</b>
Highlight 30Min	<b>Valery Levitas</b> <b>Phase transformations, dislocations and their interaction: Nano and microscale phase field approaches</b> A framework for modeling the interaction of phase boundaries with dislocations <b>Michael Budnitzki</b> , <i>Institute for Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Germany</i>	<b>Matthias Militzer</b> <b>Simulating the role of solutes and mobility distributions on grain growth and recrystallization using phase field modelling</b> A phase field model for Cu <sub>6</sub> Sn <sub>5</sub> compound evolution in binary Cu-Sn system under thermomigration effects. <b>Anil Kunwar</b> , <i>KU Leuven, Belgium</i>	<b>Fathollah Varnik</b> <b>Modelling metallic foam: A combined phase field Lattice Boltzmann approach</b> Simulation of Capillary-Driven Kinetics with Multi-PhaseField and Lattice-Boltzmann <b>Raphael Schiedung</b> , <i>Ruhr Universität Bochum, Deutschland</i>
	A Phase-field study on $\tau \rightarrow m$ martensitic phase transformation in zirconia ceramics <b>Mohan Kumar Rajendran</b> , <i>TU Bergakademie Freiberg, Institute of Mechanics and Fluid Dynamics, Germany</i>	Prediction of recrystallization texture in extruded aluminium alloys using phase field modeling <b>Ali Khajezade</b> , <i>The University of British Columbia, Canada</i>	Breakup of liquid jets: Thermodynamic perspectives <b>Fei Wang</b> , <i>Karlsruhe Institute of Technology, Germany</i>
	Modelling the stress-induced multi-variant martensitic transformation in nanoindentation <b>Mohsen Rezaee-Hajidehi</b> , <i>Institute of Fundamental Technological Research (IPPT), Polish Academy of Sciences, Poland</i>	Phase-field Simulations and Time-Resolved X-ray Experiments: a method for determining large datasets of grain boundary properties <b>Jin Zhang</b> , <i>Northwestern University, USA</i>	Higher Order Evolutionary Structural Optimization with Phase Field Modeling <b>Ingo Münch</b> , <i>KIT, Germany</i>
	Mesoscale Modeling of Metal-Hydrogen Interactions <b>Tae Wook Heo</b> , <i>Lawrence Livermore National Laboratory, USA</i>	Simulation of equilibrium morphology of WC in WC-Co hard metals by phase-field method <b>Li Han</b> , <i>Central South University, China</i>	Homogenization and averaging models for phase-field modeling <b>Mohammad Sarhil</b> , <i>Institute of Mechanics / Universität Duisburg-Essen, Germany</i>
17:00-17:30	Break		
17:30-21:00	Poster Session		

## Wednesday 24. July 2019

9:00-9:50	Plenary IV: Prof. Yong Ni, CAY Key Laboratory, University Hefei, China <b>Emergent pattern formation induced by stress-driven multiple instabilities</b> Chair: <i>Yunzhi Wang</i>		
9:50-10:10	Break		
10:10-12:00	Session XVI: <b>Solid state phase transformation</b> Chair: <b>Valery Levitas</b>	Session XVII: <b>Recrystallization and grain growth</b> Chair: <b>Matthias Militzer</b>	Session XVIII: <b>Mathematical and numerical aspects</b> Chair: <b>Fathollah Varnik</b>
Highlight 30Min	Rongpei Shi <b>Revisiting heterogeneous nucleation at grain boundaries: The role of faceted nucleus and grain boundary interaction</b>	Mathis Plapp <b>Topological defects in two-dimensional orientation-field models for grain growth</b>	Sukeharu Nomoto <b>Multi-phase field model with finite interface dissipation coupling with thermodynamics data estimated by machine learning</b>
	Co-precipitation kinetics of $\gamma'$ and $\gamma''$ phases in Ni-based superalloy using multi-phase field model <b>Kamal Nath Kadirvel</b> , <i>Ohio State University, United States</i>	Modelling of Magnetic Driving Force in Grain Boundary Migration: Using Multi-Phase Field Method <b>Liu Huo</b> , <i>ICAMS, Ruhr-Universität Bochum, Germany</i>	On Phase-field modeling with two phases <b>Michael Fleck</b> , <i>University Bayreuth, Germany</i>
	Microstructure defects and stability in Ni base superalloys <b>Yann Le Bouar</b> , <i>LEM, CNRS/ONERA, France</i>	Investigation of sintering between coarse and multiple fine particles using Phase field simulations <b>Niharika Dalbehera</b> , <i>National Institute of Technology Rourkela, India</i>	Parallel Simulation of Solidification and Fluid Flow with OpenPhase <b>Marvin Tegeler</b> , <i>ICAMS, Germany</i>
	Phase-field study of microstructure control using external Magnetic and Elastic fields <b>Rupesh Chafle</b> , <i>Indian Institute of Technology Kanpur, India</i>	Phase Field Modelling of Diffusion Induced Grain Boundary Migration in Binary alloys <b>Deepjyoti Mukherjee</b> , <i>KTH Royal Institute of Technology, Stockholm, Sweden</i>	Multi-GPUs parallelization for AMR-phase-field simulation of dendrite growth <b>Shinji Sakane</b> , <i>Kyoto Institute of Technology, Japan</i>
	Effect of elasticity and plasticity on the Widmanstätten growth in metallic alloys <b>Hocine Lebbad</b> , <i>LEM (CNRS/ONERA) &amp; UBC, France &amp; Canada</i>	Phase Field Modelling of Microstructural Evolution in Porous Ni/Yttria Stabilized Zirconia Electrodes <b>Ming Chen</b> , <i>Department of Energy Conversion and Storage, Technical University of Denmark, Denmark</i>	The Sharp Phase Field Method and its application to grain growth and microstructure evolution in Ni-based superalloys <b>Alphonse Finel</b> , <i>Laboratoire d'Etudes des Microstructures, France</i>
12:00-22:00	Excursion/Dinner		

## Thursday 25. July 2019

9:00-9:50	Plenary V: Prof. Dr. Axel Voigt TU Dresden, Germany <b>Defects at grain boundaries: a coarse-grained description by the amplitude expansion of the phase-field crystal model</b> Chair: <i>Marco Salvalaglio</i>	
9:50-10:10	Break	
10:10-12:00	Session XIX: <b>Phase-field crystal</b> Chair: <b>Axel Voigt</b>	Session XX: <b>Plastic deformation and fracture</b> Chair: <b>Alphonse Finel</b>
Highlight 30Min	Marco Salvalaglio <b>Closing the gap between atomic-scale lattice deformations and continuum elasticity within the phase field crystal framework</b>	Antoine Ruffini <b>Phase-field model coupling dislocations and pores in FCC materials</b>
	Phase Field Crystal Simulation of Crack Extension and Brittle-Ductile Transition Behavior on Nano-Scale <b>Gao Ying-jun, Guangxi University, China</b>	Modelling of crack propagating through heterogeneous material using a phase field approach <b>Hervé HENRY, PMC, École Polytechnique, CNRS, France</b>
	Phase field simulation of 6XXX Al-Mg-Si alloys during the whole ageing process and its experimental verification <b>Yong Du, Central South University, China</b>	Bifurcation Theory of Plasticity, Damage and Failure <b>Alexander R. Umantsev, Department of Chemistry and Physics, Fayetteville State University, USA</b>
	Phase Field Crystal Study of Triple Junction Migration <b>Zhirong Luo, Yulin University, China</b>	Contact phase-field modeling for materials with spatial irregularities <b>Alexandre GUEVEL, Duke University, USA</b>
		Multiscale Model for Interlayer Defects in Bilayer Materials <b>Yang Xiang, Hong Kong University of Science and Technology, China</b>
12:00-13:30	Lunch	
13:30-14:30		Session XXII: <b>Plastic deformation and fracture</b> Chair: <b>Alexander R. Umantsev</b> Phase field and atomistic modeling of solute-defect interaction in alloys <b>Jaber Rezaei Mianroodi, Material Mechanics, RWTH Aachen University, Germany</b> Phase field modeling interplay between dislocation glide and interface shear <b>Linghui He, University of Science and Technology of China, China</b> Numerical investigations on a phase-field description of cohesive zones -- Convergence and applicability to irregular meshes <b>Stephan Roth, TU Bergakademie Freiberg, Deutschland</b>
14:30	Conference end	