

# **4<sup>th</sup> International Conference on Material Modeling**

**Berkeley, California, USA**

**May 27-29, 2015**

**Local Organizing Committee:**

**Sanjay Govindjee, Co-Chair  
Panos Papadopoulos, Co-Chair  
Albrecht Bertram**

## Scientific Organizing Committee

- Douglas J. Bammann, *Mississippi State University, USA*
- Federic Barlat, *Pohang University of Science and Technology, South Korea*
- Albrecht Bertram, *University of Magdeburg, Germany*
- Francesco dell'Isola, *Universita di Roma La Sapienza, Italy*
- Pawel Dluzewski, *Institute of Fundamental Technological Research, PAN, Poland*
- Fionn Dunne, *Imperial College London, UK*
- Yuri Estrin, *Monash University, Australia*
- Samuel Forest, *Mines ParisTech, France*
- Marc Geers, *Eindhoven University of Technology, The Netherlands*
- Sanjay Govindjee, *University of California, Berkeley, USA*
- Istvan Groma, *Eoetvoes University, Budapest*
- Dave McDowell, *Georgia Institute of Technology, USA*
- Karol Miller, *University of Western Australia, Australia*
- Nobutada Ohno, *Nagoya University, Japan*
- Roberto Paroni, *University di Sassari, Italy*
- Srinivasan M. Sivakumar, *Indian Institute of Technology, Madras, India*
- Arun Srinivasa, *Texas A&M University, USA*
- Bob Svendsen, *RWTH Aachen University, Germany*
- George Voyiadjis, *Louisiana State University, USA*
- Quan-Shui Zheng, *Tsinghua University, PRC*



**U.S. Association for Computational Mechanics**

# Schedule

## Wednesday, May 27

### Garbarini Lounge

8:30 – 10:30 Registration and Check-in

### Session 1: 10:30 – 12:00

#### Blum Hall 100 – Micro- and Nano-Scale Modeling of hcp Alloys

Chair: F. Dunne

- 10:30 – 10:48 C. Tome, *Introducing Probabilistic Distributions at the Mesoscale for the Modeling of Hexagonal Materials*
- 10:48 – 11:06 Y. Yoshihara, Y. Tadano, Y. Ito, *Constitutive Modeling of Commercial Pure Titanium Using Crystal Plasticity Homogenization Method*
- 11:06 – 11:24 M. Cuddihy, F. Dunne, *An Investigation into Length-Scale Effects in hcp Alloys*
- 11:24 – 11:42 H. Abdolvand, A. Wilkinson, *Investigation of Localized Deformation in Twins and the Surrounding Neighbourhoods*
- 11:42 – 12:00 J. Kacher, M. de Jong, M. Asta, A. Minor, *Twinning Interactions in Re and Re – 10% W*

#### Hearst 290 – Nonlinear Elasticity and Viscoelasticity

Chair: A. Gupta

- 10:30 – 10:48 R. Brasil, J.M. Balthazar, *Elastic Constitutive Laws and Stability Analysis*
- 10:48 – 11:06 D. Jalocha, A. Constantinescu, R. Neviere, *Prestrain Dependent Constitutive Model for Highly Filled Elastomers*
- 11:06 – 11:24 D. Okumura, A. Sasaki, N. Ohno, *Swelling-induced Buckling Patterns in Gel Films with a Square Array of Holes Subjected to Pretensions*
- 11:24 – 11:42 T. Healey, *Stability Boundaries for Highly Stretched Elastic Sheets*

#### Bechtel 240 – Plasticity and Viscoplasticity

Chair: J. Mosler

- 10:30 – 10:48 J. Kratochvíl, M. Kolar, M. Benes, P. Paus, *Modeling of Cross-Slip as the Most Important Single Process Underlying Plastic Properties of Materials*
- 10:48 – 11:06 F. Farukh, L. Bing, L. Zhao, A. Roy, V. Silberschmidt, *Micromechanical Deformation of Single-Crystal Nickel-based Superalloy: Direct Dislocation Dynamics and Crystal Plasticity*
- 11:06 – 11:24 G. Lancioni, G. Zitti, *Deformation Patterning in Crystal Plasticity Induced by Non-Convex Plastic Energies*
- 11:24 – 11:42 M. Priddy, N. Paulson, S. Kalidindi, D. McDowell, *Strategies for Rapid Parametric Assessment of Microstructure-Sensitive Fatigue for HCP Systems*
- 11:42 – 12:00 F. Azzouz, A. Gaubert, P. Kanoute, C. Mariconi, *Cyclic Inelastic Constitutive Equations of the Hot Turboengine Components*

## **Sibley Auditorium – Multiscale Modeling**

Chair: S. Klinkel

- 10:30 – 10:48 S. Klinge, P. Steinmann, *Determination of Material Parameters Corresponding to Viscoelastic Curing Polymers*
- 10:48 – 11:06 D. Jeulin, B. Figliuzzi, M. Faessel, F. Willot, M. Koishi, N. Kowatari, *Modelling the Microstructure and the Viscoelastic Behaviour of Carbon Black Filled Rubber Materials from 3D Simulations*
- 11:06 – 11:24 D. Sodhani, S. Reese, *Finite Element Based Full Field Micromechanical Modeling of Stress Softening in Filler Reinforced Elastomers*
- 11:24 – 11:42 S. Wang, *Multi-Scale Modeling of Proteins and Cells – A Protocol for Complex Systems*

## **Dai 250 – Experimental Identification and Material Characterization**

Chair: L. Nahlik

- 10:30 – 10:48 P. Rangaswamy, C. Cady, M. Lewis, *Thermo-Mechanical Characterization of Silicone Foams*
- 10:48 – 11:06 F. Bedoui, T-L. Nguyen, P. Gelineau, *Combined Small Angle X-Ray Scattering and Dynamic Mechanical Analysis Investigation of the Confined Amorphous Layer Properties in Semi-Crystalline Polymers*
- 11:06 – 11:24 C. Pacheco, M. Vesenjok, R. Jha, S. Reddy, G. Dulikravich, H.R.B. Orlande, *Inverse Parameter Identification Using Bayesian Statistics and Response Surfaces*
- 11:24 – 11:42 B. Lan, M.J.S. Lowe, F. Dunne, *Non-Destructive Bulk HCP Texture from Ultrasound: A Solution to the Inverse Problem*
- 11:42 – 12:00 S. Belhas, A. Bendaas, C. Belamri, *Matrix Fibers Interfaces Role in Relaxation Phenomena in an Al-Cu Alloy Strengthened with SiC Fibers*
- 12:00 – 1:30 Lunch Break

## **Session 2: 1:30 – 3:00**

### **Blum Hall 100 - Micro- and Nano-Scale Modeling of hcp Alloys**

Chair: J. Brooks

- 1:30 – 1:48 E. Busso, *On the use of Ti-based Alloys in Aeroengine Applications*
- 1:48 – 2:06 T. White, J. Patten, D. Eakins, *Progress Towards the Study of Grain-level Adiabatic Shear Localisation in Titanium Alloys at High Strain-rates*
- 2:06 – 2:24 Z. Zhang, F. Dunne, *Formation of Adiabatic Shear Bands in Textured HCP Metals*
- 2:24 – 2:42 W. Proud, *The Shock Response of HCP Metals*

### **Hearst 290 – Nonlinear Elasticity and Viscoelasticity**

Chair: A. Gupta

- 1:30 – 1:48 A. Freed, A. Srinivasa, *Logarithmic Strain and its Material Derivative for a QR Decomposition of the Deformation Gradient*
- 1:48 – 2:06 F. Zhao, *Continuum Constitutive Modeling for Isotropic Hyperelastic Materials*
- 2:06 – 2:24 H. Altenbach, V. Eremeyev, *On Effective Properties of Solids and Structures at the Nanoscale*

- 2:24 – 2:42 E. Rouhaud, C. Gay, B. Panicaud, *Conditions to Establish Hyper-elasticity from Hypo-elastic Models. Applications to the Identification of Models of Complex Fluids*
- 2:42 – 3:00 J. Goddard, *Hyperdissipativity vs. Hyperelasticity*

### **Bechtel 240 – Plasticity and Viscoplasticity**

Chair: *Y. Dafalias*

- 1:30 – 1:48 W. Sumelka, M. Nowak, *Fractional Calculus for Plasticity – Non-Associative and Induced Plastic Anisotropy*
- 1:48 – 2:06 H. Feigenbaum, Y. Dafalias, *Directional Distortional Hardening at Large Plastic Deformations*
- 2:06 – 2:24 L-W Liu, H-K Hong, *Modelling of Aluminum Alloy AL6061 Using an Elastoplastic Model with Distortion Hardening*
- 2:24 – 2:42 S. Parma, Z. Hrubý, R. Marek, J. Plešek, H. Feigenbaum, Y. Dafalias, *Identification of Parameters of a Directional Distortional Hardening Model*
- 2:42 – 3:00 Z. Hrubý, J. Plešek, S. Parma, R. Marek, I. Stepanek, Z. Prevorovsky, L. Korec, H. Feigenbaum, Y. Dafalias, *Influence of the Yield Offset Definition on Calibration and Numerical Implementation of Directional Distortional Hardening Model*

### **Sibley Auditorium – Multiscale Modeling**

Chair: *D. Jeulin*

- 1:30 – 1:48 S. Xu, Y. Chen, D. McDowell, *A Concurrent Atomistic-Continuum Study of Dislocation Pile-Ups at Grain Boundaries*
- 1:48 – 2:06 J. Fan, R. Stewart, T. Xu, *Accuracy Verification and Model Size Effects on Crack-Tip Behavior with Atomistic-Based Multiscale Simulations*
- 2:06 – 2:24 Q. Tong, S. Li, *A Multiscale Molecular Dynamics for Representing Continuum Mechanical Loads*
- 2:24 – 2:42 M. Ulz, P. Wurm, *On the Use of Stochastic Approximation for Coupling the FEM and MD in Quasi-Static Isothermal Problems*
- 2:42 – 3:00 C. Chen, S. Aubry, T. Ooppelstrup, C. Dudley, T. Arsenlis, E. Darve, *Fast Multipole Method for Dislocation Dynamics Simulation*

### **Dai 250 - Experimental Identification and Material Characterization**

Chair: *M. Jabereen*

- 1:30 – 1:48 G. Díaz, S. Behr, G. Schneider, J. Mosler, *Fracture Properties of Bio-inspired Ceramic-polymer-composites – Modelling and Experimental Investigation*
- 1:48 – 2:06 V. Shim, N.T. Cao, Y.B. Guo, G.F. Gao, *Meso-scale Computational Modeling of High-Strength Concrete*
- 2:06 – 2:24 T. Jankowiak, A. Rusinek, A. Farid, *Material Behavior Description Under Dynamic Loading Based on Taylor's Test*
- 2:24 – 2:42 X. Truant, *Experimental and Numerical Study of Structural Panel Welded by Friction Stir Welding (FSW)*
- 2:42 – 3:00 J. Weickenmeier, E. Mazza, E. Kuhl, *Mechanical Modeling of Tissue Interaction in Facial Tissues*
- 3:00 – 3:30 Coffee Break

### Session 3: 3:30 – 5:00

#### Blum Hall 100 - Micro- and Nano-Scale Modeling of hcp Alloys

Chair: Esteben Busso

- 3:30 – 3:48 M. Martin, *Delayed Hydride Cracking in Zirconium Alloys – Microstructural Modelling and the Challenge of Developing an Engineering Assessment*
- 3:48 – 4:06 R. Traylor, J. Kacher, A. Minor, *Observation of Size-dependent HCP to FCC Phase Transformation of Ti*
- 4:06 – 4:24 J. Brooks, H. Basoalto, *Constitutive Modelling Approaches for Titanium Alloys with Application to Process Simulation*
- 4:24 – 4:42 M. Lowe, F. Dunne, P. Huthwaite, B. Lan, A. van Pamel, *Modelling of Ultrasound Wave Propagation in Heterogeneous Materials*

#### Hearst 290 – Nonlinear Elasticity and Viscoelasticity

Chair: Bob Svendsen

- 3:30 – 3:48 R. Segev, D. Kim, *Notes on the Mechanics of an Octopus's Arm*
- 3:48 – 4:06 R. Paroni, *From 3D Nonlinear Elasticity to 1D Elastic Models for Thin-walled Beams*
- 4:06 – 4:24 B. Panicaud, E. Rouhaud, M. Wang, F. Sidoroff, R. Kerner, *Eulerian Approach with the Lie Derivative for a Thermodynamic Construction of Constitutive Models*
- 4:24 – 4:42 J. Harrison, *New Methods in the Calculus of Variations*

#### Bechtel 240 – Plasticity and Viscoplasticity

Chair: J. Kratochvil

- 3:30 – 3:48 M. Jabareen, *A General Finite Plasticity Model with a Smooth Elastic-Plastic Transition*
- 3:48 – 4:06 L. Delannay, H. Tummala, G. Lemoine, M. Fivel, T. Pardoen, *Influence of Grain Shape on Dislocation Slip Activity Inside Free-Standing Thin Films*
- 4:06 – 4:24 Y. Ma, H. Zhu, *The Mechanical Behaviour of 3-D Stochastic Fibrous Materials*
- 4:24 – 4:42 J. Dirrenberger, V. Favier, O. Castelnau, *Representative Volume Element Size for Viscoplastic Properties in Face-centered Cubic Metals*
- 4:42 – 5:00 K. Kourousis, D. Agius, C. Wang, A. Subic, *Constitutive Modeling of Additive Manufactured Ti-6Al-4V Cyclic Elastoplastic Behaviour*

#### Sibley Auditorium – Multiscale Modeling

Chair: K. Hackl

- 3:30 – 3:48 X. Markenscoff, *Hadamard Instability Analysis of "Negative Creep" in Coupled Chemo-Thermo-Mechanical Systems*
- 3:48 – 4:06 A. Marchenko, S. Forest, M. Mazière, J-L Strudel, *Polycrystalline Modeling of Dynamic and Static Strain Aging Phenomena in Commercially Pure Alpha Titanium* (Presented by E. Nizery)
- 4:06 – 4:24 T. Schueler, R. Jaenicke, H. Steeb, *Effective Nonlinear Modeling of Asphalt Concrete on the Basis of  $\mu$ -CT Scans*
- 4:24 – 4:42 J. Maveur, *A Study of Higher-Order Boundary Conditions at Elastic-Plastic Interfaces in Micropolar Single Crystals*

4:42 – 5:00 E. Couka, F. Willot, P. Callet, D. Jeulin, *Modeling and Optical Properties of a Hematite Coating: Ellipsometry Data vs. Fourier-based Computations*

### **Dai 250 - Experimental Identification and Material Characterization**

Chair: S. Reese

3:30 – 3:48 G. Gerstein, A. Bruchanov, N. Volchok, F. Nürnberger, *The Effect of Texture in Modeling Deformation Processes of Body-centered-cubic Steel Sheets*

3:48 – 4:06 A. Milenin, R. Kuziak, M. Lech-Grega, W. Szczepan, M. Pietrzyk, *Numerical Modeling and Experimental Identification of Residual Stresses in Hot-Rolled Sheets*

4:06 – 4:24 C. Belamri, S. Belamri, *The Relaxation Origin in an Al – (20% at Ag.) Single Crystal Alloy from Ambient to 530K*

4:24 – 4:42 P. Sielicki, T. Lodygowski, *Numerical and Experimental Modelling of Masonry Under Explosive Loading*

## **Thursday, May 28**

### **Session 4: 8:30 – 10:00**

#### **Blum Hall 100 - Micro- and Nano-Scale Modeling of hcp Alloys**

Chair: Carlos Tome

8:30 – 8:48 R. Banerjee, H. Fraser, *Application of Experimental and Computational Approaches to Explore the Richness of Microstructures in Beta-Stabilized Titanium*

8:48 – 9:06 A. Minor, *In-situ TEM Deformation of Lightweight Alloys and Local Strain Measurements with Diffraction Imaging*

9:06 – 9:24 T-S. Jun, Z. Zhen, F. Dunne, B. Britton, *A Study of Local Deformation Mechanism in Two-Phase Ti Alloys Using Micromechanical Testing and CPFEM Modelling*

9:24 – 9:42 M. Sangid, A. Venkataraman, K. Chatterjee, A. Beaudoin, J. Rotella, J-S. Park, P. Kenesei, *Grain Level Residual Stress Measurements in Ti-7Al as a Result of Multi-Axial Loading*

9:42 – 10:00 V. Tong, J. Jiang, A. Wilkinson, B. Britton, *Quantifying Accuracy of Deformation Measurements Near Grain Boundaries Using High Resolution Electron Backscatter Diffraction*

#### **Hearst 290 – Nonlinear Elasticity and Viscoelasticity**

Chair: Jim Casey

8:30 – 8:48 Y. Kim, I. Yoshitake, *Hyperelasticity Modeling for Track-work in Advanced Rapid Transit*

8:48 – 9:06 A. Gupta, A. Roychowdhury, *Inhomogeneous Elastic Shell*

9:06 – 9:24 J. Walton, *Residual Stress with Application to Wave Propagation*

9:24 – 9:42 M. Lewis, *The Use of Multiplicative Decomposition of Relative Volume in Modeling Nonlinear Elastic Foams*

## **Bechtel 240 – Dislocation Dynamics**

Chair: *S. Ghosh*

- 8:30 – 8:48 I. Groma, P. Ispanovity, Z. Vandrus, *Possible Directions to Extend the Validity of the Current 2D Continuum Theory of Dislocations*
- 8:48 – 9:06 B. Svendsen, *Statistical-mechanics-based Continuum Models for Discrete Dislocation Networks*
- 9:06 – 9:24 M. Zaiser, K. Spiliotis, E. Aifantis, *Some Remarks on the W-A Model*
- 9:24 – 9:42 M. Monavari, M. Zaiser, S. Sandfeld, *Microstructural Comparison of Continuum Models for Dislocation Plasticity*

## **Sibley Auditorium – Multiscale Modeling**

Chair: *V. Silberschmidt*

- 8:30 – 8:48 V. Kouznetsova, A. Sridhar, A. Krushynska, M. Geers, *Transient Computational Homogenization for Locally Resonant Metamaterials*
- 8:48 – 9:06 A. Javili, G. Chatzigeorgiou, A. McBride, C. Linder, P. Steinmann, *Computational Homogenization at Finite Strains Accounting for Size Effects via Surface Energy*
- 9:06 – 9:24 S. Klinkel, B. Kohlhaas, *An FE<sup>2</sup> Model for Shape Memory Alloy Fiber-Compounds*
- 9:24 – 9:42 H-B. Ly, V. Monchiet, D. Grande, *Permeability in Multiporous Materials: A Multiscale Modeling Approach*
- 9:42 – 10:00 W. Wagner, F. Gruttmann, *On a Homogenization Method for Heterogeneous Shells and Sandwich Plates*

## **Dai 250 – Strain Gradient and Nonclassical Approaches**

Chair: *K. Garikipati*

- 8:30 – 8:48 J. Liu, M. S. Kah, *Strain Gradient Elastic-Plasticity Theory for Micro-Scaled Deformations*
- 8:48 – 9:06 S.M. Mousavi, *Dislocation-Based Fracture Mechanics in Gradient Elasticity*
- 9:06 – 9:24 A. Bertram, R. Glüge, *On Finite Gradient Materials with Internal Constraints*
- 9:24 – 9:42 A. McBride, D. Gottschalk, D. Reddy, A. Javili, *Computational and Theoretical Aspects of a Grain-Boundary Model*
- 9:42 – 10:00 H. Pouriayevali, E. Bruder, B-X. Xu, *Grain-Grain Boundary Interaction in a Gradient Crystal Plasticity Description: Formulation and Numerical Implementation*
- 10:00 – 10:30 Coffee Break

## **Session 5: 10:30 – 12:18**

### **Blum Hall 100 - Micro- and Nano-Scale Modeling of hcp Alloys / Atomistic to Continuum Transitions**

Chair: *David Rugg*

- 10:30 – 10:48 M. Ghazisaeidi, *Material Behavior from First Principles: Atomic-Scale Investigation of Deformation Mechanisms in Mg Alloys*
- 10:48 – 11:06 Z. Zheng, D. Balint, F. Dunne, *Discrete Dislocation and Crystal Plasticity Analyses of Load Shedding in Polycrystalline Titanium Alloys*
- 11:06 – 11:24 D. Xu, H. Wang, R. Yang, A. Huang, D. Rugg, *MD Simulation of the Deformation and Fracture Mechanism of hcp Titanium Under Fatigue*



- 11:24 – 11:42 S. Ghosh, J. Cheng, *Physics-Based Crystal Plasticity FE Models for Predicting Deformation and Twinning in Polycrystalline Magnesium Alloys*
- 11:42 – 12:00 B. Szajewski, W. Curtin, *Analysis of Spurious Image Forces in Atomistic Simulations of Dislocations*

### **Hearst 290 – Nonlinear Elasticity and Viscoelasticity**

*Chair: Jim Casey*

- 10:30 – 10:48 B. Nadler, M. Rubin, *An Eulerian Constitutive Formulation of Anisotropic Viscoelastic Solids and Fluids*
- 10:48 – 11:06 O. Mattei, A. Carini, *Variational Formulations for the Linear Viscoelastic Problem in the Time Domain*
- 11:06 – 11:24 V.K. Devendiran, K. Kannan, P. Ravindran, *A Study of Two Dimensional Torsional Deformation and “Sheet-Pulling” for Non-Linear Rate-Type Viscoelastic Materials*
- 11:24 – 11:42 C. Naumann, J. Ihlemann, *On the Thermodynamics of Viscoelastic Models of Convolution Type at Large Deformations*

### **Bechtel 240 – Dislocation Dynamics**

*Chair: I. Groma*

- 10:30 – 10:48 K.C. Le, *Dislocation Mechanism of Microstructural Changes in Ductile Single Crystals*
- 10:48 – 11:06 M. Koster, K.C. Le, B. Nguyen, *Shear Band Formation in Ductile Single Crystals under Compression*
- 11:06 – 11:24 Y. Xiang, Y. Zhu, *A Continuum Model for Dislocation Dynamics in Three Dimensions and Applications to Micro-Pillars*
- 11:24 – 11:42 C. Silbermann, C. Khanh, M. Baitsch, J. Ihlemann, *Analysis of Plane Strain Deformation of Aluminum Single Crystals using Continuum Dislocation Theory*

### **Sibley Auditorium – Multiscale Modeling**

*Chair: V. Kouznetsova*

- 10:30 – 10:48 F. Maresca, V. Kouznetsova, M. Geers, *Multiscale Modeling of Hierarchical Microstructures: A Framework for Laminated Morphologies Applied to Martensitic Steels*
- 10:48 – 11:06 C. Mareau, S. Berbenni, *Self-Consistent Modelling of Heterogeneous Materials with an Elastic-Viscoplastic Behavior: Application to Polycrystals*
- 11:06 – 11:24 E. Hervé-Luanco, *Analytical Extension of the (n+1)-phase Model to Non Linear Behavior*
- 11:24 – 11:42 F. Bedoui, P. Gelineau, L. Cauvin, *Viscoelasticity of Nano-platelets Reinforced Polymer: Micromechanical Modeling and Microstructural Investigation*
- 11:42 – 12:00 J. Novak, *Efficient Modelling of Random Heterogeneous Materials*

## **Dai 250 – Strain Gradient and Nonclassical Approaches**

Chair: A. Bertram

- 10:30 – 10:48 K. Garikipati, Z. Wang, S. Rudraraju, *A 3D Field Formulation and IGA Solutions to Point and Line Defects using Toupin's Theory of Gradient Elasticity at Finite Strain*
- 10:48 – 11:06 A. Basak, A. Gupta, *Plastic Flow with Incoherent Interfaces and a Junction in a Tricrystal*
- 11:06 – 11:24 J. Plešek, R. Marek, Z. Hruby, S. Parma, H. Feigenbaum, Y. Dafalias, *Implementation of Directional Distortional Hardening Models for Metal Plasticity*
- 11:24 – 11:42 R. Marek, J. Plešek, Z. Hruby, S. Parma, H. Feigenbaum, Y. Dafalias, *Study of Benefits and Limitations Linked to Implementation of Directional Distortional Hardening Models*
- 11:42 – 12:00 F. Alisafaei, N. Garg, C-S. Han, *Modeling of Length Scale Dependent Deformation in Polymers – Experiments, Theory and Simulations*
- 12:00 – 12:18 A. Roy, Q. Liu, M. Demairal, V. Silberschmidt, *A Comprehensive Investigation of Indentation Size Effects in F.C.C. and B.C.C. Single Crystals*
- 12:00 – 1:30 Lunch Break

## **Session 6: 1:30 – 3:00**

### **Blum Hall 100 – Polymeric Materials**

Chair: A. Freed

- 1:30 – 1:48 P. Rakesh, M.K. Gupta, *Recent Developments in Natural Fiber Reinforced Composites*
- 1:48 – 2:06 G. Laschet, M. Spekowius, P. Hul, R. Spina, C. Hopmann, *Two-Level Homogenization of 3D Polypropylene Microstructures of an Injection Moulded Component*
- 2:06 – 2:24 L. Brassart, Q. Liu, Z. Suo, *Viscous Mixing*
- 2:24 – 2:42 G. Montella, P. Neff, S. Govindjee, *Modelling Tire Derived Material for Moderately Large Deformations*
- 2:42 – 3:00 A. Krischok, C. Linder, *A Stabilized Finite Element Formulation for Poroelasticity Models Undergoing Large Deformations*

### **Hearst 290 – Nonlinear Elasticity and Viscoelasticity / Biomaterials**

Chair: M. Sangid

- 1:30 – 1:48 J. Casey, *A Kinematical View of Parallel Transport Along a Curve on a Surface*
- 1:48 – 2:06 H. Zou, Z. Liu, J. Wu, J. Liu, Y. Zhang, *Simulation of a Needle Inserted into Liver*
- 2:06 – 2:24 V. Silberschmidt, M. Wang, X. Gao, A. Abdel-Wahab, S. Li, E. Zimmermann, C. Riedel, B. Busse, *Crack Growth in Cortical Bone Tissue: X-FEM Modelling*
- 2:24 – 2:42 M. Eskandari, A. Javili, C. Linder, E. Kuhl, *Exploring Instabilities in Bi-Layered Structure with Focus on Chronic Lung Disease*
- 2:42 – 3:00 M.J. Razavi, X. Wang, *Computational Understanding of Cortical Folding and Brain Developmental Disorders*

## **Bechtel 240 – Dislocation Dynamics**

*Chair: V. Gavini*

- 1:30 – 1:48      X. Markenscoff, *The Elastodynamics of Defects*
- 1:48 – 2:06      S. Sandfeld, M. Zaiser, *Dislocation Structure Formation in a Continuum Model of Dislocation Dynamics*
- 2:06 – 2:24      N. Bertin, L. Capolungo, M. Upadhyay, C. Pradalier, *An FFT-based Formulation for Efficient Mechanical Fields Computation in Periodic Discrete Dislocation Dynamics*
- 2:24 – 2:42      A. Hosseinzadeh Delander, *Dislocation Dynamics Simulation of Plastic Deformation in Phosphorus-alloyed Oxygen-free Copper (Cu-OFP) Single Crystal*

## **Sibley Auditorium – Multiscale Modeling**

*Chair: Friedrich Gruttmann*

- 1:30 – 1:48      J. Soric, T. Lesicar, Z. Tonkovic, *Multiscale Computational Approach Using Strain Gradient Formulation at Microlevel*
- 1:48 – 2:06      Z. Liu, W.K. Liu, *A Statistical Descriptor Based Volume-integral Micromechanics Model of Heterogeneous Material with Arbitrary Inclusion Shape*
- 2:06 – 2:24      M. Doskar, J. Kruis, J. Novak, *Wang Tiles in Numerical Homogenization Models*
- 2:24 – 2:42      M. Leuschner, F. Fritzen, *Reduced Order Computational Homogenization for Materials with Nonlinear Interfaces*

## **Dai 250 – Nanomechanics**

*Chair: A. Minor*

- 1:30 – 1:48      J. Zimmerman, L. Hale, *Atomic-Scale Modeling of Helium-3 Bubble Growth in Aging Palladium Tritides*
- 1:48 – 2:06      X. Wang, L. Zhang, *Mechanics of Graphyne-enabled Cholesterol Removal from Protein Cluster*
- 2:06 – 2:24      Y. Kinoshita, A. Matsubara, N. Ohno, *First-Principles Study of Torsional Resistance of Faceted Boron Nitride Nanotubes*
- 2:24 – 2:42      L. Wang, J. Lee, *Work Conjugacy Between Stress and Strain in Molecular Dynamics*
- 3:00 – 3:30      Coffee Break

## **Session 7: 3:30 – 5:00**

### **Blum Hall 100 – Creep, Damage, Fracture, and Fatigue**

*Chair: J. Moeller*

- 3:30 – 3:48      S. Reese, S. Wulfinghoff, M. Fassin, *Anisotropic Damage Coupled with Plasticity – Model Development, Finite Element Implementation and Applications*
- 3:48 – 4:06      G. Xu, M. Demkowicz, *Brittle Intergranular Fracture Frustrated by Intermittent Dislocation Emission in Nickel*
- 4:06 – 4:24      L. Malcher, E. Mamiya, *Numerical Study for the Improved CDM Model Regarding Cyclic Loading Conditions*

- 4:24 – 4:42 D. Krause, *A Novel Hysteresis Energy Based Fatigue Failure Criterion for an Epoxy Based Polymer Using a Viscoplastic Material Model*
- 4:42 – 5:00 E. Sozumert, V. Silberschmidt, E. Demirci, M. Acar, B. Pourdeyhimi, *Damage in Random Fibrous Networks*

### **Hearst 290 – Granular Materials and Particle Systems**

Chair: *K. Sagiyama*

- 3:30 – 3:48 Y. Dafalias, X. Li, P. Fu, *Is Critical State Theory for Granular Materials Complete?*
- 3:48 – 4:06 S. Luding, K. Saitoh, V. Magnanimo, *Master Equation for the Probability Distribution Functions of Overlaps Between Particles in Two Dimensional Granular Packings*
- 4:06 – 4:24 M. Kulosa, M. Neumann, M. Boeff, G. Gaiselmann, V. Schmidt, A. Hartmaier, *Characterization of Porous Ceramics Derived from a Combination of Stochastic and Mechanical Modelling*
- 4:24 – 4:42 K. Hackl, M.S. Kahn, *Modeling of Microstructures in a Cosserat Continuum Using Relaxed Energies*

### **Bechtel 240 – Dislocation Dynamics**

Chair: *C. Silbermann*

- 3:30 – 3:48 V. Gavini, M. Iyer, B. Radhakrishnan, *Electronic Structure Study of an Edge Dislocation in Aluminum*
- 3:48 – 4:06 R. Sills, W. Cai, *Characterizing Solute Drag on Perfect and Extended Dislocations*
- 4:06 – 4:24 A. Romanov, E. Aifantis, *Reaction-Kinetics Models for Structural Defects and Implication to Certain Nanotechnology Problems*
- 4:24 – 4:42 D. Molodov, *Grain Boundary Dynamics: Model Experiments on Bicrystals*
- 4:42 – 5:00 N. Safara Nosar, G. Engberg, M. Sandström, *Predicting the Microstructural Evolution of a 13% Chromium Steel During Hot Working with a Physically Based Model*

### **Sibley Auditorium – Multiscale Modeling / Statistical Mechanics**

Chair: *D.L. McDowell*

- 3:30 – 3:48 B. Golden, D-F Li, S. Lean, N. O'Dowd, *Microstructural Deformation of a Power Plant Steel: Modelling the Granular Response of a Martensitic Steel*
- 3:48 – 4:06 C. Ling, J. Besson, S. Forest, E. Bosso, F. Latourte, B. Tanguy, *Multi-scale Simulation of Uniaxial Tension of Pre-cracked Single Crystal and Polycrystalline Irradiated FCC Steels Specimens*
- 4:06 – 4:24 P. Kustra, A. Milenin, M. Pietrzyk, D. Svyetlichnyy, *Physical and Numerical Modeling of Hyperfine Wire Drawing of MgCa08 Alloy in Heated Dies Accounting for Recrystallization in Mic*
- 4:24 – 4:42 T. Gu, E. Herve-Luanco, H. Proudhon, O. Castelnau, S. Forest, *Multiscale Modeling of the Elastic Behavior of Architected and Nanostructured Cu-Nb Composite Wires*

**6:30 pm Conference Dinner – Berkeley Faculty Club**

## Friday, May 29

### Session 8: 8:30 – 10:00

#### Blum Hall 100 – Creep, Damage, Fracture, and Fatigue

Chair: L. Delannay

- 8:30 – 8:48 T-H. Pham, J-J. Marigo, J. Laverne, *Effect of Non-Uniform Stress Field on Bi-dimensional Cohesive Crack Initiation and Propagation*
- 8:48 – 9:06 L. Nahlik, K. Stegnerova, Z. Majer, P. Hutar, *Numerical Estimation of Stepwise Crack Propagation in Ceramic Laminates with Strong Interfaces*
- 9:06 – 9:24 J. Möller, E. Bitzek, *On the Influence of Crack Front Curvature on the Fracture Behavior of Nano-Scale Cracks*
- 9:24 – 9:42 J. Zghal, C. Mareau, F. Morel, *Development of a Polycrystalline Approach for the Modelling of High Cycle Fatigue Damage: Application to a HSLA Steel*
- 9:42 – 10:00 E. Nizery, S. Forest, H. Proudhon, J-Y. Buffiere, J. Chevy, *Modelling Fatigue Crack Initiation at Fractured Particles in Aluminum Alloys*

#### Hearst 290 – Composites

Chair: V. Silberschmidt

- 8:30 – 8:48 T. Matzies, H. Rapp, *Analytical Damage Modelling of 2-D Braided Textile Composites*
- 8:48 – 9:06 B. Drach, I. Tsukrov, A. Drach, H. Bayraktar, J. Goering, *Finite Element Modeling of Damage Initiation and Propagation in Three-Dimensional Woven Composites*
- 9:06 – 9:24 N. Garg, F. Alisafaei, G. Chandrashekar, *A Numerical Study on Length Scale Dependent Deformation in Micro-fiber Composites*
- 9:24 – 9:42 M. Ribeiro, R. Fujiyama, *Mechanical Behaviour of Composite Material Polyester Matrix Reinforced for Industrial Waste Wood*
- 9:42 – 10:00 M. Serpilli, *Mathematical Models for Thin Piezoelectric Interphases: An Asymptotic Approach*

#### Bechtel 240 – Phase-Transforming Materials

Chair: S. Morris

- 8:30 – 8:48 F. D. Fischer, M. Petersmann, S. Mayer, T. Waitz, *Martensite at High Temperatures – Is it Possible?*
- 8:48 – 9:06 L. Casalena, F. Yang, D. Coughlin, X. Chen, M. Bowers, Y. Gao, H. Paranjape, P. Anderson, Y. Wang, R. Noebe, M. J. Mills, *Transformation and Deformation Mechanisms in High Temperature Shape Memory Alloys with Nanoprecipitates*
- 9:06 – 9:24 M. Bhargava, S. Chakraborty, A. Tewari, S. Mishra, *Microstructure Based Material Model for Transformation Induced Plasticity (TRIP) Steels*
- 9:24 – 9:42 M. Budnitzki, M. Kuna, *Stress Induced Phase Transitions During Scratching of Silicon*
- 9:42 – 10:00 F. Adziman, R. Reed, *Microstructure Evolution Modelling of the Rotary Welding of Nickel Based Superalloys*

## **Sibley Auditorium – Multiscale Modeling / Multiferroic Materials**

Chair: Jonathan Zimmerman

- 8:30 – 8:48 J-W. Simon, B. Bednarczyk, B. Stier, S. Reese, *Multiscale Modeling of the Damage Behavior of Textile Composites*
- 8:48 – 9:06 A. Karakoc, J. Paltakari, E. Hiltunen, *A Stochastic Micromechanical Model for Fiber Network Deformation*
- 9:06 – 9:24 M. Hickman, P.K. Basu, *Stochastic Multiscale Optimization of Short-Fiber Reinforced Composites*
- 9:24 – 9:42 S. Santapuri, *Micro-Magneto-Electro-Mechanical Framework for Multiferroic Materials*
- 9:42 – 10:00 G. Dulikravich, R. Jha, N. Chakrabort, M. Fan, J. Schwartz, C. Koch, *Algorithms for Multi-Objective Design Optimization of Hard Magnetic Alloys Using Experimental Data*
- 10:00 – 10:30 Coffee Break

## **Session 9: 10:30 – 12:00**

### **Blum Hall 100 – Creep, Damage, Fracture, and Fatigue**

Chair: TBA

- 10:30 – 10:48 X. Zhang, C. Linder, *Phase Field Modeling of Fracture in Si Electrodes at Large Deformation*
- 10:48 – 11:06 O. Soto, J. Baum, R. Lohner, *A Mixed Strain/Displacement Finite Element Formulation for Fracture Computation in Blast and Impact Coupled Fluid-Solid Problems*

### **Hearst 290 – Composites**

Chair: TBA

- 10:30 – 10:48 O. Bayrak, V. Silberschmidt, E. Demirci, *Finite-element Modelling of Graphene-Reinforced Nanocomposites: Introduction of Quantitative Microstructural Data*
- 10:48 – 11:06 T. Siriwardanage, Y Kim, *Thermal-conduction Modeling of a Composite Material Embedded in a Concrete Substrate*
- 11:06 – 11:24 X. Wang, A. Jivkov, *3D Meso-Structure Modelling of Concrete for Failure Analysis in Tension and Compression*

### **Bechtel 240 – Phase-Transforming Materials**

Chair: F.D. Fischer

- 10:30 – 10:48 H. Feigenbaum, D. LaMaster, C. Ciocanel, *A Thermodynamics-Based 3D Model for the Magneto-Mechanical Behavior of Magnetic Shape Memory Alloys*
- 10:48 – 11:06 J. Mosler, A. Bartels, *On the Influence of Homogenization Assumptions in Phase Field Theories*
- 11:06 – 11:24 K. Sagiyama, K. Garikipati, S. Rudraraju, *An Unconditionally Stable Time-Integration Scheme for Problems of the Mechano-chemical Spinodal Decomposition*
- 11:24 – 11:42 S. Morris, *On Polymorphic Phase Changes Occurring via an Incoherent Intermediate State*

## **Sibley Auditorium – Electronic Materials**

*Chair: S. Klinge*

- 10:30 – 10:48 M. Klassen, B-X Xu, R. Müller, *Static and Dynamic Analysis of Heterogeneous Dielectric Elastomers*
- 10:48 – 11:06 A. Romanov, A. Smirnov, J. Speck, *Modeling Mechanical Stresses and Dislocations in III-nitride Semipolar Layered Electronic Structures*
- 11:06 – 11:24 P. Dluzewski, M. Mazdziarz, P. Tazowski, *Constitutive and FE Modeling of Residual Stresses and Kirkendall Effect in Semiconductor Structures*
- 11:24 – 11:42 M. Labusch, J. Schröder, M-A. Keip, D. Lupascu, *On the Influence of Ferroelectric Polarization States on the Magneto-electric Coupling in Two-phase Composites*

Information on wireless access is provided at the registration desk in Gabarini Lounge.