PRISMS Center Annual Workshop
August 8-9, 2019
Beyster Room 1670
University of Michigan
Final Program

NOTE: Times include discussion times. All speakers should allow time for Q+A at the end of their talks!

Thursday August 8

8:00am **Registration**

8:30am **Welcome and PRISMS Center Overview**
John Allison

Plasticity and Dislocation-Precipitate Interactions *Session Chair: Liang Qi*

9:00am **The Case for a Physical Theory of Plasticity: Prospects and Impact on Metals Research**
Guest Speaker: Anter El-Azab, Purdue University

9:40am **Dislocation-precipitate interactions in Mg alloys**
Zhihua Huang, John Allison, Amit Misra

10:00am **Modeling dislocation-precipitate interactions**
Chaoming Yang and Liang Qi

10:20-10:40 Break

Grain Boundary Strengthening in Mg *Session Chair: Amit Misra*

10:40am **Modeling the effect of grain size in crystal plasticity**
Veera Sundararaghavan and Aaditya Lakshmanan

11:00am **Quantifying Slip Band-Grain Boundary Interactions**
Mohsen Taheri, Aditya Lakshmanan, John Allison, Veera Sundararaghavan and Amit Misra

11:20am **Search for minimum-energy grain boundary structures using phase field crystal models and atomistic simulations**
Jason Luce, Chaoming Yang, Mingfei Zhang, Yong-Jie Hu, Katsuyo Thornton and Liang Qi

12:00pm **DFT-FE: A massively parallel real-space code for large-scale DFT calculations; & electronic structure studies of defects in Mg**
Phani Motamarri, Sambit Das and Vikram Gavini

12:30-1:30 Lunch (Provided - Pierpont Commons East Room)

Measuring and Predicting Fatigue Behavior *Session Chair: Veera Sundararaghavan*

1:45pm **Examining Sub-grain-level Plasticity and Fatigue Crack Growth Using High Energy Diffraction Microscopy**
Guest Speaker: William Musinski, Air Force Research Laboratory, WPAFB, OH

2:25pm **Two and Three Dimensional Characterization of Fatigue Short-Crack Growth in Magnesium Alloys**
Duncan Greeley and John Allison

2:45pm **Cyclic Deformation and Low Cycle Fatigue in Mg and Mg alloys**
Aeriel Leonard-Murphy and John Allison

3:15 **PRISMS-Plasticity Modeling of Monotonic and Cyclic Deformation in Mg and Mg alloys**
Mohammadreza Yaghoobi, Veera Sundararaghavan and John Allison

3:45-4:00pm Break

Alloying Effects *Session Chair: Sam Daly*

4:00pm **Rare-earth effect on Microstructure Evolution and Deformation Behavior of Mg Alloys**
Guest Speaker: Carl Boehlert, Michigan State University

4:40pm **Investigation of Deformation Twinning in Mg Alloy during in-situ Compression**
Zhe Chen and Sam Daly, UCSB

5:30-8pm Poster session and reception with hors d'oeuvres
Beyster Lobby

Friday August 9
Beyster Hall Room 1670

Predicting Corrosion Behavior of Mg Alloys *Session Chair: Katsuyo Thornton*

9:00am **A Variational Principle for Mass Transport**
Guest Speaker: Dallas Trinkle, University of Illinois

9:40am **Modeling and Experimental Studies of Corrosion in Mg Alloys**
David Montiel, Stephen DeWitt, Ransom Stamps, Emmanuelle Marquis, and Katsuyo Thornton

10:20-10:50 Break

Capturing and Using Materials Information *Chair: Brian Puchala*

10:50am **Using Materials Commons for Collaborative Materials Research**
Glenn Tarcea, Brian Puchala, Tracy Berman, Steve DeWitt and John Allison

11:20am **Extreme Data Management Analysis and Visualization for Materials Science and Exascale Computing**
Guest Speaker: Valerio Pascucci, University of Utah

12:00-1:00 Lunch (Provided - in Pierpont Commons East Room)

Designing Complex Alloys *Chair: Liang Qi*

1:15 pm **Using CASM to Determine the First Principles Determination of the Al-rich part of Al-Cu Phase Diagram**
Guest Speaker: Sha Liu, Ioannis Papadimitriou, Javier Llorca, IMDEA Advanced Materials Institute, Madrid Spain

1:45 **The *prisms.multiscale* Suite of Tools and its Use to Optimize the Strength of Complex Mg Alloys**
Stephen DeWitt, Brian Puchala, Qianying Shi, Anirudh Natarajan, Chaoming Yang, Zhihua Huang, Katsuyo Thornton, Amit Misra, Liang Qi, Anton Van der Ven, and John Allison

2:15 **Integrating Calphad and Experiments to Provide Direction for Complex Mg Alloy and Heat Treatment Optimization**
Qianying Shi and John Allison

2:40 **First-principles Thermodynamics of Multicomponent Alloys**
Anirudh Natarajan and Anton Van der Ven

3:10 **Using CASM and Materials Commons for Collaborative Complex Alloy Modelling**
Brian Puchala, John Thomas, John Goiri, Glenn Tarcea, John Allison and Anton Van der Ven

3:40 **Concluding Remarks**