

**PRISMS Center
Annual Workshop Agenda
August 17-18, 2017
Beyster Room 1670
University of Michigan
Preliminary Program**

NOTE: **Times include discussion times. All speakers should allow at least 10 minutes for Q+A at the end of their talks!**

Thursday August 17

8:00am Registration

8:30am Welcome and PRISMS Center Overview
John Allison

Characterizing and Predicting Precipitate Evolution
Session Chair: Katsuyo Thornton

9:00pm Precipitate Evolution in Mg-Rare Earth Alloys
Guest Speaker: Jian-Feng Nie, Monash University

9:40pm Quantitative characterization of precipitate evolution in Mg-Rare Earth alloys
Ellen Solomon and Emmanuelle Marquis

10:20-10:40 Break

10:40am Application of CASM to the Mg-Rare Earth system
Anirudh Natarajan, Brian Puchala, Anton Van der Ven

11:20am Predicting precipitate evolution in Mg-Nd and Mg-Y using PRISMS-PF
Steve DeWitt, John Allison and Katsuyo Thornton

12:00 Uncertainty Quantification in First Principles Based Phase Diagram Calculations
Brian Puchala, Liang Tian, Anirudh Natarajan, Anton Van der Ven

12:30-1:50 Lunch (Provided - Pierpont Commons East Room)

Predicting Dislocation Effects
Session Chair: Amit Misra

1:50 Precipitate strengthening using dislocation dynamics
Guest Speaker: Sylvie Aubry, Lawrence Livermore National Laboratory

- 2:30** **Dislocation-precipitate interactions in Mg alloys**
Zhihua Huang, John Allison, Amit Misra
- 2:50** **Real-space methods in density functional theory and electronic structure study of energetics of dislocations in Al and Mg**
Sambit Das, Phani Motamarri and Vikram Gavini
- 3:30-3:45pm Break**
Integration, Collaboration and Information Sharing
Chair - Margaret Hedstrom
- 3:45pm** **The Citrination Platform for Data Storage, Discovery, and Materials Development**
Guest Speaker: Kyle Michel, Citrine Informatics
- 4:25pm** **Materials Commons**
Brian Puchala, Glenn Tarcea, Tracy Berman, Terry Weymouth and John Allison
- 5:15-8pm** **Poster session and reception with hors d'oeuvres**
East Room Pierpont Commons

Friday August 18
Beyster Hall Room 1670

Predicting Tensile Behavior

Session Chair: Sam Daly

- 9:00am Measurements and Crystal Plasticity Simulations of
Microstructure-Scale Deformation in Tantalum**
Guest Speaker: Corbett Batteille, Sandia National Laboratory
- 9:40am Quantifying local deformation in Mg alloys**
Zhe Chen and Sam Daly
- 10:20am Using PRISMS-CPFEA to model microstructural influences on
tensile Deformation in HCP Metals**
Sriram Ganesan and Veera Sundararaghavan

11:00-11:20 Break

Predicting Deformation and Fatigue Behavior

Chair - Wayne Jones

- 11:20 Microstructure effects on fatigue crack growth in Mg alloys**
Jake Adams, John Allison, Wayne Jones
- 12:00 Using PRISMS-Plasticity for simulating fatigue behavior**
Shardul Panwar and Veera Sundararaghavan

12:40-2:00 Lunch (Provided - in Pierpont Commons East Room)

Predicting Microstructure Evolution

Session Chair: Steve DeWitt

- 2:00pm Phase Field Methods: From Materials Design to Phase Field
Crystals**
Guest Speaker: Peter Voorhees, Northwestern University
- 2:40 Modeling Nucleation Using PRISMS-PF**
David Montiel, Steve DeWitt and Katsuyo Thornton
- 3:10 Computational methods to represent phase transformations with
coherent or incoherent interfaces**
Greg Teichert and Krishna Garikipati
- 3:40-4:00 Break***

- 4:00** **Phase Field Crystal Method**
Jason Luce and Katsuyo Thornton
- 4:30** **Incorporating strongly anisotropic interfacial energy into PRISMS-PF**
Beck Andrews, Steve DeWitt and Katsuyo Thornton
- 5:00** **Concluding Comments**