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 Solute Clustering and Precipitate Evolution in Mg 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 Battaille, 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 **Modeling the influence of microstructural features on microstructurally short cracks in a Mg alloy**
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 **A unified computational framework for phase transformations with coherent and incoherent interfaces**
Greg Teichert and Krishna Garikipati

3:40-4:00 Break

4:00 **Phase Filed Crystal Modeling for HCP Metals**
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**