

**PRISMS Center Annual Workshop  
August 22-23, 2024**

**University of Michigan  
Preliminary Program**

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

**Thursday August 22**

**8:20am**      **Registration & Coffee**  
**8:40am**      **Welcome and PRISMS Center Overview**  
John Allison

**Measuring and Modeling Twinning and Detwinning in Mg Alloys**

*Session Chair: Liang Qi and Veera Sundararaghavan*

**9:00am**      **The effect of grain size on deformation twinning in textured magnesium and its alloys**  
*Guest Speaker: Jian-Feng Nie, Monash University*

**9:40am**      **Resolving the 3D evolution of deformation twins inside a grain under tension with in-situ DFXM**  
*Sangwon Lee and Ashley Bucsek*

***10:10-10:30 Break***

**10:30am**      **PRISMS-Plasticity: Overview and its application to understand activity of extension twins in Mg-Y alloys**  
*Chaitali Patil, John Allison and Veera Sundararaghavan*

**10:55am**      **The observation of twinning formation in Mg-Y alloys**  
*Qianying Shi, Tracy Berman and John Allison*

**11:20**      **Surrogate models for PRISMS-Plasticity**  
*Kyle Farmer and Liz Holm*

***12:00-1:00 Lunch (Provided - Blue Lounge GGB Building)***

**Measuring and Modeling Twinning and Detwinning in Mg Alloys (Continued)**

*Session Chair: Liang Qi and Veera Sundararaghavan*

**1:20pm**      **Elucidating the Role of Internal Stresses on Twin Network Formation and Morphology in HCP Metals**  
*Guest Speaker: Darshan Bamney, LANL*

**2:00pm**      **PRISMS Multi-Physics: Development of an integrated CASM/Phase-Field/CPFE framework and its application to simulate twin morphology evolution in Mg alloys.**

David Montiel, Chaitali Patil, Brian Puchala, Anton Van der Ven, Katsuyo Thornton, Veera Sundararaghavan

***Deformation Mechanisms and Grain Boundary Strengthening***

*Chair: Amit Misra and Chaitali Patil*

**2:20 pm**      **Computational and Experimental Study of Geometrically Necessary Dislocation Densities in PRISMS-Plasticity**

Michael Pilipchuk, Veera Sundararaghavan, et al

**2:40pm**      **Quantification of grain boundary effects on the geometrically necessary dislocation density evolution and strain hardening of polycrystalline Mg-4Al using *in situ* tensile testing in scanning electron microscope and HR-EBSD**

Eunji Song and Amit Misra

***3:10-3:30pm Break***

**3:30 pm**      **DFT-FE overview & electronic-structure informed <c+a> cross-slip barrier predictions in binary Mg alloys.**

Sambit Das and Vikram Gavini et al

**4:00 pm**      **Atomistic simulations of competitive nucleation of deformation twinning and pyramidal dislocations from grain boundaries of Mg and Mg alloys**

Viadehi Menon and Liang Qi

**4:20**      **Use of PRISMS-Fatigue to simulate microstructural effects on fatigue in additive manufactured metals**

Mohammadreza Yaghoobi

**5:00-7pm**      **Poster session and reception with hors d'oeuvres**  
**Beyster Lobby (Tischmann Hall)**

**Friday August 23**

**Grain Boundary Segregation, Texture Evolution and Recrystallization of Mg Alloys**

*Session Chair: Katsuyo Thornton and Ashley Bucsek*

**9:00am      A complete first draft of the spectral model for grain boundary segregation**

Guest Speaker: Chris Schuh, Northwestern University

**9:40am      Computational studies of grain boundary segregation and migration in Mg alloys at finite temperatures**

Vadehi Menon, Sambit Das, Qianying Shi, John Allison, Vikram Gavini,  
Liang Qi

**10:00am      Modeling the nucleation process during recrystallization in HCP alloys**

Liz Holm

**10:30-10:50 Break**

**10:50am      Constructing a FAIR dataset describing static recrystallization kinetics in Mg-Zn-Ca alloy**

Tracy Berman, Qianying Shi and John Allison

**11:15 am      Integrated modeling of static recrystallization in Mg-Zn-Ca alloy using the PRISMS framework**

Supriyo Chakraborty, David Montiel, Katsuyo Thornton

**12:00-1:00    Lunch (Provided - Blue Lounge GGB Building)**

***Advanced Simulation and Characterization Methods and Data Infrastructure***

*Session Chair: Anton Van der Ven and Liz Holm*

**1:00            Micromechanical Modeling of Phase Transformation Materials**

Guest Speaker: Ananya Renuka Balakrishna, UCSB

**1:40pm      CASM Overview**

Brian Puchala, Sesha Sai Behara\* and Anton Van der Ven\* \*UCSB

**2:00pm      Overview of the PRISMS-PF framework improvements in performance, ease of use and recent applications.**

David Montiel, Katsuyo Thornton et al

**2:30-2:50pm Break**

- 2:50pm**      **Metadata and cyberinfrastructure for structural materials research at CHESS**  
Guest Speaker: Kate Shanks, Cornell High Energy Synchrotron Source (CHESS)
- 3:30pm**      **Laboratory-scale high-energy diffraction microscopy: A validation study**  
Seunghee Oh and Ashley Bucsek
- 3:50pm**      **The Materials Commons Approach to FAIR data**  
Glenn Tarcea, Brian Puchala, Tracy Berman and John Allison
- 4:15 pm**      **Wrap-Up**