PRISMS Center Annual Workshop
August 22-23, 2024
Room 1017 Dow Building - University of Michigan North Campus
FINAL 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/Fruit + Danish**

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, Tracy Berman, Michael Pilipchuk, Can Yaldirim, Carsten Detlefs, Veera Sundararaghavan, John Allison 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, Qianying Shi, John Allison and Veera Sundararaghavan

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

11:20 **Preparing the groundwork for 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, John Allison, Katsuyo Thornton, Veera Sundararaghavan

Deformation Mechanisms and Grain Boundary Strengthening
Chair: Amit Misra and Chaitali Patil

2:20 pm **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

2:40pm **Computational and Experimental Study of Geometrically Necessary Dislocation Densities in PRISMS-Plasticity**
Michael Pilipchuk, Tracy Berman, John Allison, Veera Sundararaghavan

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

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

5:00-6:30pm Poster session and reception with hors d'oeuvres
Borg Warner Lobby (GG Brown Ground Floor)

Friday August 23
Room 1017 Dow Building

8:30am **Coffee/Fruit + Danish**

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 alloys**
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, Michael Pilipchuk, David Montiel, Veera Sundararaghavan, 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 2.0 - Overview and recent applications.**
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, Supriyo Chakraborty, Jason Landini, Zachary Croft, Beck Andrews, Alexander Menash and Katsuyo Thornton

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, Yuefeng Jin, Sangwon Lee, Wenxi Li, Ken Geauvreau, Matthew Williams, Robert Drake and Ashley Bucsek

3:50pm **The Materials Commons approach to FAIR data**
Glenn Tarcea, Brian Puchala, Tracy Berman, David Montiel and John Allison

4:15 pm **Wrap-Up**