PRISMS Center Annual Workshop
August 22-23, 2024
Room 1017 Dow Building - University of Michigan North Campus
DRAFT 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**

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, 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 **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

5:00-7pm Poster session and reception with hors d'oeuvres
Borg Warner Lobby (GG Brown Ground Floor)

Friday August 23
Room 1017 Dow Building

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, 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 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, 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**