PRISMS Center Annual Workshop
August 24-25, 2023
Dow Room 1017
University of Michigan
Final Program

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

Thursday August 24

8:20am Registration

8:40am Welcome and PRISMS Center Overview
John Allison

Measuring and Modeling Twinning and Detwinning in Mg Alloys
Session Chair: Liang Qi and Brian Puchala

9:00am Local stress effects on deformation twinning and stress induced phase transformations
Guest Speaker: Rod McCabe (Los Alamos National Laboratory)

9:40am 3D in-situ characterization of twinning inside Mg-4Al grains using dark-field X-ray microscopy
Sangwon Lee, Can Yildirim, Carsten Detlefs, John Allison, Ashley Bucsek

10:10-10:30 Break

10:30am PRISMS-Plasticity Overview and application for Modeling of Twinning & Detwinning in Mg and Mg alloys
Mohammadreza Yaghoobi, Duncan Greeley, John Allison and Veera Sundararaghavan

11:00am Quantifying Grain-Scale Twinning and Detwinning Using High Energy Diffraction Microscopy
Duncan Greeley, Mohammadreza Yaghoobi, Kate Shanks, Darren Pagan, Veera Sundararaghavan and John Allison

11:25am Experimental Characterization of Twinning Behavior in Mg and Mg Alloys during Monotonic and Cyclic Loading
Qianying Shi, Tracy Berman, Anto Jerish and John Allison

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

Twinning: Kinetics and Thermodynamics
Session Chair: Anton Van der Ven and David Montiel

1:20pm **Kinetics of Deformation Twinning in Hexagonal Metals**
Guest Speaker: Jian Wang, University of Nebraska

2:00pm **Stability and Growth Kinetics of Twin Embryos in β Ti-Alloys**
Liang Qi

2:30pm **CASM Overview and its application for modeling alloy effects on twinning in Mg**
Brian Puchala, Sesha Sai Behara* and Anton Van der Ven*
*UCSB

3:00-3:20pm Break

Uncertainty Quantification / Machine Learning / Materials Commons
Session Chair: Anton Van der Ven and David Montiel

3:20pm **Bayesian uncertainty quantification as applied to cluster expansions**
Derrick Ober and Anton Van der Ven, UCSB

3:45pm **Predicting microstructurally sensitive fatigue-crack path in WE43 magnesium using high-fidelity numerical modeling and three-dimensional experimental characterization**
Guest Speaker: Brian Phung*, D.A. Greeley, M. Yaghoobi, J.F. Adams, J.E. Allison, A.D. Spear*, *University of Utah

4:15pm **Automatic Microstructure Segmentation with Computer Vision Techniques**
Kyle Farmer and Liz Holm

4:35pm **Using Materials Commons to Build Collaborative Materials Communities**
Glenn Tarcea, Brian Puchala, Tracy Berman and John Allison

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

Friday August 25
Dow Room 1017

Texture Evolution and Recrystallization of Mg Alloys
Session Chair: Katsuyo Thornton and Ashley Bucsek

9:00am Extreme Abnormal Grain Growth: Connecting Mechanisms to Microstructural Outcomes
Liz Holm

9:40am Effects of Zn and Ca on recrystallization behavior and texture evolution in Mg-Zn-Ca alloys deformed at elevated temperatures
Tracy Berman, Mohamaddreza Yaghoobi, Megan Klein and John Allison

10:10am Overview of the PRISMS-PF framework and its application to simulate static recrystallization in Mg alloys.
David Montiel, Mohammadreza Yaghoobi, Tracy Berman, Michael Pilipchuk, Jacob Lepley, Veera Sundararaghavan, John Allison and Katsuyo Thornton

10:40-11:00 Break

11:00am In-situ characterization of static recrystallization in Mg-Zn-Ca using high-resolution X-ray diffraction
Sangwon Lee, Tracy D. Berman, Can Yildirim, Carsten Detlefs, John E. Allison, Ashley Bucsek

11:20 Computational and experimental investigations of temperature-dependent grain boundary segregation
Vadehi Menon, Sambit Das, Qianying Shi, John Allison, Vikram Gavini, Liang Qi

11:40 A computational thermodynamics framework with intrinsic chemical short-range order
Guest Speaker: Bi-Cheng Zhou, University of Virginia

12:30-1:30 Lunch (Provided - Blue Lounge GGB Building)

Grain Boundary Strengthening
Chair: Liz Holm and Amit Misra

1:40 pm **Mesoscale Investigation of Dislocation-Grain Boundary Interactions in Metals and Alloys**
Guest Speaker: Abigal Hunter, LANL

2:20 pm **Exploring the Influence of Micro-Hall Petch on Mechanical Properties Prediction of Mg-4Al Alloys at Micro and Macro Levels**
Mohsen Taheri Andani, Veera Sundararaghavan and Amit Misra

2:40 pm **Modeling geometrically necessary dislocation accumulation in polycrystals: Crystal plasticity simulations and comparison with experiments**
Michael Pilipchuk, A. Lakshmanan, M. Taheri Andani, Amit Misra and Veera Sundararaghavan

3:00-3:20 Break

3:20 pm **PRISMS Indentation: Multi-scale Elasto-plastic Virtual Indentation Module**
Guest Speaker: Aaron Tallman, Florida International University and Mohammadreza Yaghoobi

3:50pm **A study of grain boundary effect on the strain hardening of Mg-4Al using in situ high resolution (HR) EBSD**
Eunji Song, M. Taheri Andani and Amit Misra

4:10 pm **DFT-FE overview & electronic-structure investigation of <c+a> pyramidal dislocations in Mg and Mg-Y alloy with implications towards ductility enhancement**
Sambit Das and Vikram Gavini

4:40 pm **Wrap-Up**