# 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 O+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: Liana Oi and Brian Puchala

9:00am Local stress effects on deformation twinning and stress induced phase transformations

<u>Guest Speaker:</u> <u>Rod McCabe</u> (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 allows

Mohammadreza Yaghoobi, Duncan Greeley, John Allison and Veera Sundararaghavan

11:00am Quantifying Grain-Scale Twinning and Detwinning Using High Energy Diffraction Microscopy

<u>Duncan Greeley</u>, 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  $\beta$  Ti-

**Alloys** <u>Liang Qi</u>

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

<u>Guest Speaker:</u> <u>Brian Phung\*</u>, 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** 

<u>Glenn Tarcea,</u> 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

<u>Tracy Berman,</u> 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.

<u>David Montiel</u>, 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

  <u>Guest Speaker: Bi-Cheng Zhou</u>, University of Virginia
- 12:30-1:30 Lunch (Provided Blue Lounge GGB Building)

Grain Boundary Strengthening

Chair: Liz Holm and Amit Misra

## **Mesoscale Investigation of Dislocation-Grain** 1:40 pm **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 Elastoplastic Virtual Indentation Module Guest Speaker: Aaron Tallman, Florida International University and Mohammadreza Yaghoobi 3:50pmA 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

Wrap-Up

4:40 pm