PRISMS Center Annual Workshop
August 9-12, 2022
Tentative Virtual Program (all times Eastern Time Zone)

Tuesday August 9

9:55/10:00am **Welcome and PRISMS Center Overview**
John Allison

Grain Strengthening in Mg and Mg Alloys
Session Chair: Veera Sundararaghavan

10:20am **PRISMS Grain Strengthening Use Case Overview**
Veera Sundararaghavan

10:30am **Atomistic Simulation of Dislocation-Grain Boundary Interactions in Mg**
Yong-Jie Hu, Vaidehi Menon and Liang Qi,

11:00am **Estimation of Micro-Hall-Petch Coefficients in Mg-4Al as a Function of Grain Boundary Parameters**
Moshen Tahari, Aaditya Lakshmanan, Veera Sundararaghavan, John Allison, Amit Misra

11:30am **Modeling Grain Size Strengthening Using PRISMS-Plasticity**
Gurmeet Singh, Aaditya Lakshmanan, Mohammedreza Yaghoobi and Veera Sundararaghavan

12:00 pm ***Break (30 min)***

12:30 am **TEM study of Dislocation Interactions with Grain Boundaries in Mg Alloys**
Jeremy Yoo, Moshen Tahari and Amit Misra

12:50 pm **Atomistic Simulation of Solute Segregation at Grain Boundaries in Mg Alloys at Finite Temperatures**
Vaidehi Menon and Liang Qi

1:10pm **Experimental Characterization of Grain Boundary Segregation in Mg Alloys**
Qianying Shi and John Allison

1:30 pm **DFE-FE 1.0 Overview and Application to Mg Alloys**
Sambit Das and Vikram Gavini

2:00 pm ***Open Discussion***

Wednesday August 10

9:55-10am Convene/Welcome

Predicting and Measuring Twinning and Detwinning in Mg Alloys
Session Chair: Amit Misra

10:00am **Twin Network Formation and Morphology in HCP Metals**
Guest Speaker: Laurent Capolungo (Los Alamos National Laboratory)

10:40am **An Integrated PRISMS Modeling Framework for Modeling of Twinning & Detwinning in Mg and Mg alloys**
David Montiel, Mohammadreza Yaghoobi, Brian Puchala, Anton Van der Ven, Katsuyo Thornton, Veera Sundararaghavan and John Allison

11:10pm **Using HEDM and PRISMS-Plasticity to Quantify and Model Twinning and Detwinning in Mg Alloys**
Duncan Greeley, Mohammadreza Yaghoobi, Darren Pagan and John Allison

11:40pm **Quantifying Twin Behavior by In-Situ SEM Measurements During Monotonic and Cyclic Loading in Mg and Mg alloys**
Tracy Berman, Zhe Chen and John Allison

12:00pm ***Break (30 min)***

12:30pm **Theoretical Predictions for CRSS of Twinning in HCP Metals**
Guest Speaker: Huseyin Sehitoglu (University of Illinois)

1:10pm **CASM 1.0 Overview & Application to Twinning in Mg Alloys**
Brian Puchala and Anton Van der Ven

1:30pm **PRISMS-Plasticity Overview & Application to Simulation of Twinning and Detwinning in Mg Alloys**
Mohammadreza Yaghoobi, Veera Sundararaghavan and John Allison

2:00pm ***Open Discussion***

Thursday August 11

9:55-10am Convene/Welcome

Modeling and Measuring Microstructural Evolution
Session Chair: Katsuyo Thornton

10:00am **Simulation of Precipitation in Al-Li alloy**
Guest Speaker: Javier Llorca (IMDEA)

10:40am **PRISMS Texture Evolution Use Case Overview**
John Allison

10:45am **Texture Evolution in Mg-Zn-Ca Alloys: Simulation and Measurements**
Tracy Berman, Mohamaddreza Yaghoobi and John Allison

11:10am **A multiscale, multimodal approach to characterizing static recrystallization in Mg-3Zn-0.1Ca with in-situ nf-HEDM, ff-HEDM, and DFXM**
Sangwon Lee, Reza Roumina, Kate Shanks, Can Yildirim, Tracy Berman, John Allison and Ashley Bucsek

11:40am **PRISMS-PF Overview and Application to Recrystallization Simulation**
David Montiel and Katsuyo Thornton

12:00pm Break (30 minutes)

Advances in High Energy Diffraction Microscopy (HEDM)
Session Chair: John Allison

12:30pm **Characterization of Grain Distortions using HEDM**
Guest Speaker: Kelly Nygren, Cornell High Energy Synchroton Source (CHESS)

1:10pm **The Development of a Laboratory-scale HEDM Instrument**
Ashley Bucsek

1:40pm Open Discussion

Friday August 12

9:55/10:00am Convene/Welcome

Capturing and Using Materials Information
Session Chair: Brian Puchala

10:00 am **The National Scientific Data Fabric**
Guest speaker: Valerio Pascucci, University of Utah

10:40pm **Materials Commons 2.0 Overview**
Glenn Tarcea, Brian Puchala, Tracy Berman and John Allison

11:10pm **Added value and increased organization: Capturing experimental data provenance in Materials Commons 2.0**
Tracy Berman

11:30 pm Break (30 min)

Measuring and Modeling Microstructural Effects on Fatigue in Mg Alloys
Session Chair: Mohamaddreza Yaghoobi

12:00pm **PRISMS-Fatigue: New Developments**
Guest Speaker (tentative): Kris Stopka (Purdue University), Mohammadreza Yaghoobi, Veera Sundararaghavan, John Allison and David McDowell (Georgia Tech)

1:30pm **Graph Theory Approach for Modeling Fatigue Crack Paths**
Siddhartha Srivastava and Veera Sundararaghavan

2:00pm **HEDM Characterization of Fatigue Crack Paths in WE 43 Mg**
Duncan Greeley, Jake Adams, Peter Kenesei, Wayne Jones, Ashley Spear and John Allison

2:30pm **Concluding Remarks**
John Allison