



# IMFD RESEARCH SEMINAR PRESENTATION DR. MAYU MURAMATSU, KEIO UNIVERSITY

Hosted by Prof. Bernhard Eidel. · Chair of Micro Mechanics & Multiscale Materials Modeling

## A MULTISCALE METHOD COUPLING MD AND FEM FOR INVESTIGATION ON ATOMISTIC-SCALE DEFORMATION MECHANISMS **UNDER CONTINUUM-SCALE DEFORMATION**







Keio University **Department of Mechanical Engineering** 

Muramatsu@mech.keio.ac.jp https://muramatsu.mech.keio.ac.jp/

#### **Tuesday, May 20, 2025** 14:30 - 16:00

Lecture hall : WEI-1051 Julius-Weisbach-Bau Lampadiussstr. 4, Freiberg

#### **BIOGRAPHY**

- 2011 Ph.D

Keio University, Department of Mechanical Engineering

- 2012-2013 Researcher

National Institute of Advanced Industrial Science and Technology

- 2014-2017 Assistant Professor

Tohoku University

- 2018-Present Senior Assistant Professor (2022-Associate Professor)

Keio University, PI

### **ABSTRACT**

The objective of this study is to develop a multiscale bridging method for investigating nanocrystalline metals based on macroscale deformation. To achieve this objective, we propose a hierarchical multiscale computational method that enables scale bridging to atomic-scale models within a finite element model. In this method, atomic-scale nanocrystal models are associated with finite element integration points and assumed to deform based on macroscale deformation. Nanocrystalline aluminum was selected for the validation of the multiscale method. Finite element method and molecular dynamics methods were used for continuous-scale and atomic-scale simulations, respectively. The concept of the Cauchy-Bourne rule was utilized to transfer deformation information from the continuous scale to the atomic scale. The results of the analysis investigated changes in microstructure due to differences in loading conditions. Additionally, a method to reduce simulation costs was also investigated.

For more information about the Institute of Mechanics and Fluid Dynamics

TU Bergakademie Freiberg | Institute of Mechanics and Fluid Dynamics Chair of Micro Mechanics and Multiscale Materials Modeling | 09599 Freiberg | Phone: +49 3731 / 39-2465 | bernhard.eidel@imfd.tu-freiberg.de IMFD | May 20, 2025