Graduate Student Research Seminar

Spring 2023

Improving Dislocation Dynamics Mobility Laws through Convolutional Neural Network

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Monday, January 23rd

3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

To stimulate materials innovation for increasingly extreme environments, experts in the field have turned to data-driven solutions over conventional density functional theory analysis. One way to derive laws of physical behavior is via deep machine learning models that can process many data points to uncover hidden correlations in dynamical behavior. To understand the physics governing complex material systems such as high entropy alloys and specialized metal composites, it is critical to utilize robust materials modeling techniques that bridge the microscale structure, mesoscale properties, and macroscale performance. Through specialized defect analysis, conducted via advanced computational methods, one can predict key materials parameters such as the critical resolved shear stress ab initio given a set of interaction potentials for the atomic elements present in a materials system. Current mesoscale techniques struggle to account for thermal effects in material systems, such as thermally activated dislocation motion. These thermal effects are critical for understanding materials response in extreme environments, such as the desirable Tokamak fusion reactor. This presentation outlines how continuum solutions are applied at the mesoscale to replicate configurations generated by molecular dynamics, and how the resultant data can be fed into a convolutional neural network to improve the phenomenological mobility laws governing defect interactions in complex material systems.

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