Graduate Student Research Seminar

Fall 2024

Information Dynamics in Continuum Dislocation Models: Provision and Extraction

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

Abstract

The continuum dislocation dynamics (DD) model is a powerful tool for analyzing mesoscale crystal plasticity, due to its relatively inexpensive computational cost. To inform DD, information needs to be extracted from lower-scale models (Molecular Dynamics) and be applied generally to a continuum framework. This challenge becomes more complex depending on the specific plasticity mechanisms intended for study. In this part of the presentation, the process of extracting solid solution effects from MD and applying them to the DD framework are detailed accompanying compared results of τ_CRSS computation between DD and MD.

The DD framework is based on the non-singular theory developed by Cai et al., whereby a singular dislocation core is rationalized via a spreading parameter. The process of selecting an appropriate dislocation core radius is not trivial, as it traditionally involves computation of the dislocation density tensor and Nye tensor from MD results. It has been shown [5] that spectral analysis of a dislocation line from MD can provide core fitting parameters. In this part of the talk, it is explained how frequency analysis and power spectra can provide insight as to appropriate dislocation core radii in the continuum DD model, and how spectral analysis in DDD can indicate thermal attack frequencies.

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