

Graduate Student Research Seminar

Spring 2023

Modeling Dislocation Glide in Concentrated Random Alloys

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Monday, March 27th
3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

The discoveries of novel material properties in high entropy alloys (HEAs) have drawn a lot of attention from the material science community. However, the vastness of the HEA design space limits our ability to explore this new type of alloys. To further explore this field, there is a dire need for research into the fundamental physics behind HEAs properties. Solid solution strengthening in HEAs is one of the critical physics concepts that needs a deeper understanding. Although small scale simulations, such as density functional theory and molecular dynamics, are being widely used to study these concepts, the nature of these simulations limits our ability to explore meso-scale phenomena. To overcome this, our current study aims to implement the effect of solid solution strengthening in mesoscale dislocation dynamics models. The strengthening effect in concentrated random alloys can be modeled using statistical frameworks that allow us to extract statistical properties of lattice sites hosting different atomic species characterized by atomic misfit due to their size difference. The stress field emerging from this effect introduces an additional energy barrier for a dislocation to overcome to continue its glide motion. We intend to capture the motion of gliding dislocations in the dislocation dynamics simulation, which provides information about the plasticity mechanisms in these systems.



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