Graduate Student Research Seminar

Fall 2025

Dependence of Radiation Induced Segregation of Cr on Sink Dimensionality in Fe-Cr Alloys

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Monday, November 3rd

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

Abstract

Radiation-induced segregation (RIS) and chemical redistribution in structural alloys can significantly degrade material performance, ultimately leading to failure. In this study, we investigate how the dimensional characteristics of sinks influence solute concentration distributions and segregation behavior. Specifically, we utilize a kinetic Monte Carlo (KMC) model to simulate atomic-scale diffusion and analyze segregation processes in an Fe–3%Cr alloy. Our analysis includes three representative sink geometries: one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) planar sinks to capture the effects of sink dimensionality on Cr segregation at grain boundaries (GBs). We also found analytical solutions of concentration and segregation profiles for a 3D spherical sink. KMC simulations are performed over a range of temperatures to assess thermal effects on Cr redistribution. The results reveal distinct segregation profiles and concentration gradients, although the dependence with sink density seems to remain linear in all cases with planar sinks. The analytical results show that this is not the case in spherical domains, with a more complex dependence of segregation on sink density. Our finite difference solutions for domains including 2D and 3D planer sinks show promising agreement with corresponding KMC results.

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