FFT-based disclination mechanics for solute segregation at grain boundaries inferred from atomistic simulations

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Abstract

This study examines solute segregation at grain boundaries (GBs) in FCC materials with a continuum approach based on the disclination structural unit model (DSUM)1 and elastic dipole tensors2 for modeling GB / solute interactions. In contrast with isotropic elastic analytical solutions3, the fast Fourier transform (FFT) method for field disclination mechanics3 is here applied in the more general context of heterogeneous anisotropic elasticity, to solve the elastic fields of the disclination dipole distributions representing two specific high angle (HA) GBs: Σ29 (5 2 0) (0 0 1) 46.40∘ and Σ149 (10 7 0) (0 0 1) 20.02∘. For the elastic interaction of such interfaces with solute atoms, the elastic dipole tensor contains both the permanent second-rank tensor, which is related to a size effect, and the fourth-rank polarizability tensor2, which is related to a modulus effect by capturing the dependence on the external strain. Numerical comparisons between FFT simulations and Molecular Statics (MS) are performed for three systems: Al, Cu and Ag, with Ag and Ni as solute atoms in substitution. The findings highlight the crucial role of anisotropic elasticity in accurately modeling solute segregation. While FFT and MS calculations show an overall agreement, some discrepancies only occur close to the defect cores attributed by non-linear effects in the atomistic model. Additionally, this study reveals the strong impact of the modulus effect on solute concentration at GBs for some of these particular systems.
References:

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