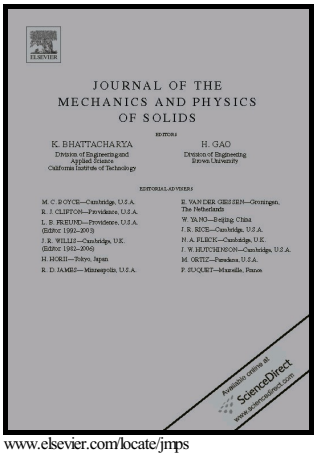

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Multiscale Diffusion Method for Simulations of Long-Time Defect Evolution with Application to Dislocation Climb

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Abstract

In many problems of interest to materials scientists and engineers, the evolution of crystalline extended defects (dislocations, cracks, grain boundaries, interfaces, voids, precipitates) is controlled by the flow of point defects (interstitial/substitutional atoms and/or vacancies) through the crystal into the extended defect. Precise modeling of this behavior requires fully atomistic methods in and around the extended defect, but the flow of point defects entering the defect region can be treated by coarse-grained methods. Here, a multiscale algorithm is presented to provide this coupling. Specifically, direct accelerated molecular dynamics (AMD) of extended defect *evolution* is coupled to a diffusing point defect concentration field that captures the long spatial and temporal scales of point defect motion in the presence of the internal stress fields generated by the *evolving* defect. The algorithm is applied to study vacancy absorption into an edge dislocation in aluminum where vacancy accumulation in the core leads to nucleation of a double-jog that then operates as a sink for additional vacancies; this corresponds to the initial stages of dislocation climb modeled with explicit atomistic resolution. The method is general and so can be applied to many other problems associated with nucleation, growth, and reaction due to accumulation of point defects in crystalline materials.

Keywords: diffusion, accelerated molecular dynamics, vacancy, dislocation

1. Introduction

In many engineering materials, the interaction of mobile point defects (interstitial or substitutional atoms, or vacancies) and extended crystalline defects (dislocations, grain boundaries, voids, interfaces, precipitates) controls the microstructural evolution and mechanical properties of the material. Specific examples across the range of possibilities include precipitate growth, dynamic strain aging, and dislocation climb. These interactions are difficult to model due to the wide range of temporal and spatial scales involved. With regard to timescales, diffusion of point defects in the bulk usually takes nanoseconds to microseconds for each individual hop among atomic sites while diffusion among atomic sites within an extended defect can be orders of magnitude faster due to the non-crystalline environment in the defect. With regard to spatial scales, point defect concentrations are usually low, so that long-range diffusion is required to accumulate point defects around a local defect. Furthermore, the diffusion into the defect is affected by the stress fields

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