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Three-dimensional phase-field model of dislocations for a heterogeneous face-centered cubic crystal

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Abstract

A central aim of current materials studies is to develop a predictive modeling that incorporates dislocation-based plastic activity and microstructural evolution. Phase-field method has emerged as a powerful tool for addressing this issue, providing us with a versatile variational framework able to describe the movement of dislocations in interaction with underlying microstructures. In this article, a three-dimensional phase-field model of dislocations (PFMD) is developed with a discretization scheme that explicitly captures the face-centered cubic (FCC) geometry. Within this framework, continuous fields are discretized in a way that allows to consider strongly heterogeneous materials and sharp interfaces (free surfaces, stiffer precipitates, pores...) without generating numerical artifacts. The PFMD exposed in this work reproduces dislocation activity in FCC geometry, their reactions, and a particular attention is devoted to the dislocation core behaviors in order to remove effects present in prior generic PFMDs that can appear to be spurious for micron-scale applications. This allows us to rigorously reproduce the dislocation's velocity with respect to experimental friction coefficients. The model is discussed and illustrated by applications standing at different space-scales that show how dislocations operate with microstructural heterogeneities such as free-surfaces (cylindrical nanopillar) and voids (pore under isostatic pressure).

Keywords: Dislocations, Phase-Field, Numerical Modeling, Nanopillar, Pore

1. Introduction

The macroscopic mechanical behavior of heterogeneous metallic alloys results from the evolution of its microstructure (solid precipitates, pore network...) generally coupled to microscopic phenomena (dislocations, microcracks...). Numerically however, at a space and time-scale of the industrial processes, it is impossible to reproduce this behavior without introducing constitutive laws that partially lack physically based justifications [1, 2]. As a consequence, these models can fail to accurately describe and predict the evolution of a given system under specific mechanical loads [3].

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