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A study of conditions for dislocation nucleation in coarser-than-atomistic scale models

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Abstract

We perform atomistic simulations of dislocation nucleation in defect free crystals in 2 and 3 dimensions during indentation with circular (2D) or spherical (3D) indenters. The kinematic structure of the theory of Field Dislocation Mechanics (FDM) is shown to allow the identification of a local feature of the atomistic velocity field in these simulations as indicative of dislocation nucleation. It predicts the precise location of the incipient spatially distributed dislocation field, as shown for the cases of the Embedded Atom Method potential for Al and the Lennard-Jones pair potential. We demonstrate the accuracy of this analysis for two crystallographic orientations in 2D and one in 3D. Apart from the accuracy in predicting the location of dislocation nucleation, the FDM based analysis also demonstrates superior performance than existing nucleation criteria in not persisting in time beyond the nucleation event, as well as differentiating between phase boundary/shear band and dislocation nucleation. Our analysis is meant to facilitate the modeling of dislocation nucleation in coarser-than-atomistic scale models of the mechanics of materials.

I. Introduction

Homogeneous dislocation nucleation (HDN) has been studied experimentally [1] [2] [3] and through modeling in many papers. Attempts have been made to formulate a nucleation criterion [4] [5] [6] [7] that can be used in larger length-scale analysis to predict the nucleation event. Ideally, the criterion should predict the precise location and instant of instability. It should also be able to predict the line direction and the Burgers vector associated with the nucleating dislocation loop. The simplest attempt to predict nucleation was based on atomic level shear stress, called Schmid stress, which was proven insufficient, when tested through numerical simulations. Rice and co-workers [8] [9] also proposed a nucleation condition for dislocation emission from crack tips, based on the notion of γ-surface given by Peierls and Nabarro [10] [11], and Vitek [12]. This γ-surface approach has been shown to be very useful in analysis of nucleation near crack tips [8] [9]. However, this approach fails qualitatively for homogeneous dislocation nucleation [7]. Li et al. [6] introduced the Λ criterion, which was based on Hill's analysis [13] of stability of plane waves in a deformed crystal. Miller and Acharya [5] proposed a stress gradient based approach to predict HDN.