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Nonlocal instability analysis of FCC bulk and (100) surfaces under uniaxial stretching

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ABSTRACT

The objective of this paper is to examine the instability characteristics of both a bulk FCC crystal and a (100) surface of an FCC crystal under uniaxial stretching along a ⟨100⟩ direction using an atomistic-based nonlocal instability criterion. By comparison to benchmark atomistic simulations, we demonstrate that for both the FCC bulk and (100) surface, about 5000–10,000 atoms are required in order to obtain an accurate converged value for the instability strain and a converged instability mode. The instability modes are fundamentally different at the surface as compared to the bulk, but in both cases a strong dependence of the instability mode on the number of atoms that are allowed to participate in the instability process is observed. In addition, the nonlocal instability criterion enables us to determine the total number of atoms, and thus the total volume occupied by these atoms, that participate in the defect nucleation process for both cases. We find that this defect participation volume converges as the number of atoms increases for both the bulk and surface, and that the defect participation volume of the surface is smaller than that of the bulk. Overall, the present results demonstrate both the necessity and utility of nonlocal instability criteria in predicting instability and subsequent failure of both bulk and surface-dominated nanomaterials.

1. Introduction

Since Hadamard (1903), the notion of instability in continuous solids has been studied by many authors (Hill, 1962; Stroh, 1962; Rudnicki and Rice, 1975; Rice, 1976; Hill and Milstein, 1977; Gao, 1996). In these continuum mechanics-based formulations, as originated by Hill (1962), a small perturbation is applied to an infinite body of a solid, and a material stability analysis is performed to determine whether the perturbation grows unboundedly with time. If it does, the material is considered to be unstable; if it does not, the material is considered to be stable (Belytschko et al., 2002). Furthermore, the material stability analysis depends upon the state of deformation in the material through the determinant of an acoustical tensor, which depends upon both the current state of stress and stiffness in the material. We note that other researchers have extended these concepts to analyze, in a continuum fashion, the stability of surfaces attached to an infinite half space (Srolovitz, 1989; Suo et al., 1992).

Recently, nanomaterials have been extensively studied, and found to exhibit superior mechanical properties (Park et al., 2009), with the particularly salient property of having a strength that has been found to approach a significant fraction of the ideal strength (Zhu and Li, 2010). Because of this, and the related interest in connecting macroscale instability to atomic-scale processes, there has been a burst of activity applying continuum mechanics concepts to study instability in nanomaterials. There have typically been two approaches to this class of problems. The first involves the determination of crystal elastic constants directly from an underlying interatomic potential, which are then directly utilized for a material stability analysis (Milstein and Huang, 1978; Alber et al., 1992; Wang et al., 1993, 1995; Kitamura et al., 2004; Lu and Zhang, 2006). Other researchers have made a multiscale link between interatomic potentials and continuum mechanics, typically using the Cauchy–Born hypothesis, such that finite element calculations of atomic scale instability can be performed at both zero (Li et al., 2002; Vliet et al., 2003; Zhu et al., 2004; Pacheco and Batra, 2008) and finite temperature (Xiao and Yang, 2007).

One key issue that has recently drawn attention is the fact that instabilities at the atomic scale, for example dislocation nucleation, tend to involve the collective motion of a group of atoms, rather than originating with an individual atom. If this is the case, then such instabilities have an inherently nonlocal character. This point was first noted by Miller and Rodney (2008), who demonstrated

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