Journal of the Mechanics and Physics of Solids 88 (2016) 35–49

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Multiscale modeling of crack initiation and propagation at the nanoscale

Behrouz Shiari [a,*], Ronald E. Miller [b]

[a] Center for Wireless Integrated MicroSensing and Systems WIMS^2 University of Michigan, Ann Arbor, MI, USA
[b] Department of Mechanical and Aerospace Engineering Carleton University, Ottawa, ON, Canada

ARTICLE INFO

Article history:
Received 30 May 2015
Received in revised form
5 November 2015
Accepted 14 December 2015
Available online 17 December 2015

Keywords:
Multiscale
Nanoscale
Crack
Dislocation

ABSTRACT

Fracture occurs on multiple interacting length scales; atoms separate on the atomic scale while plasticity develops on the microscale. A dynamic multiscale approach (CADD: coupled atomistics and discrete dislocations) is employed to investigate an edge-cracked specimen of single-crystal nickel, Ni, (brittle failure) and aluminum, Al, (ductile failure) subjected to mode-I loading. The dynamic model couples continuum finite elements to a fully atomistic region, with key advantages such as the ability to accommodate discrete dislocations in the continuum region and an algorithm for automatically detecting dislocations as they move from the atomistic region to the continuum region and then correctly "converting" the atomistic dislocations into discrete dislocations, or vice-versa. An ad hoc computational technique is also applied to dissipate localized waves formed during crack advance in the atomistic zone, whereby an embedded damping zone at the atomistic/continuum interface effectively eliminates the spurious reflection of high-frequency phonons, while allowing low-frequency phonons to pass into the continuum region.

The simulations accurately capture the essential physics of the crack propagation in a Ni specimen at different temperatures, including the formation of nano-voids and the sudden acceleration of the crack tip to a velocity close to the material Rayleigh wave speed. The nanoscale brittle fracture happens through the crack growth in the form of nano-void nucleation, growth and coalescence ahead of the crack tip, and as such resembles fracture at the microscale. When the crack tip behaves in a ductile manner, the crack does not advance rapidly after the pre-opening process but is blunted by dislocation generation from its tip. The effect of temperature on crack speed is found to be perceptible in both ductile and brittle specimens.

1. Introduction

During the last decade, there have been many numerical simulations carried out to study the fundamental physics of fracture mechanics at different scales, including tools such as first principle calculation (Abraham et al., 1998), molecular dynamics (MD) (Bitzek et al., 2015), and the finite element (FE) method (Fries and Belytschko, 2010). Although the continuum picture of plasticity does properly incorporate the conservation of energy and the increase of entropy, it lacks a

* Corresponding author.
E-mail address: bshiari@umich.edu (B. Shiari).

http://dx.doi.org/10.1016/j.jmps.2015.12.003
0022-5096/

description of the microscopic lattice structure and the defects present in crystals. A complete understanding of plasticity can only emerge from models incorporating the nucleation, propagation, interaction, and annihilation of crystal defects. On the other hand, many fracture phenomena still cannot been understood thoroughly using only a single length-scale or time-scale tool. For example, continuum mechanics fails to predict that a mode-I crack propagates at super-Rayleigh speed, while atomistic simulations are able to support the experiments results on this dynamic fracture feature (Buehler, 2008). Fracture of FCC metals is another example of multiple interacting length-scales and time-scale (Hai and Tadmor, 2003), where the interplay between dislocations, twinning and long-ranged crack tip elastic fields becomes relevant. With respect to time-scale, the evolution of a plastic zone around a crack happens over extremely long times compared to the vibrations of crack tip atoms which occur on the time-scale of the Debye frequency. In general though, fracture at macroscopic length-scales (several hundred micrometers) and time-scales (seconds) occurs as a result of a series of smaller failures at micro length-scale (nanometers) and time-scale (nanoseconds). Furthermore, the exact mechanism of how these micro length and time scales affect the propagation process of cracks remains unclear, and as such attention has also been directed towards coupled or multiscale methods that can bridge the gap between the continuum and atomistic scales (Shiari et al., 2005a).

A major category of multiscale simulations is the class of so-called concurrent multiscale models (Curtin and Miller, 2003). These approaches link methods appropriate at each scale together in a combined model, where the different scales are able to exchange information through coupled or matching interfaces. Most of concurrent multiscale models utilize molecular dynamics (MD) at the fine-scale and finite elements (FE) at the coarse-scale. It is a central aim of concurrent methods to provide an accurate coupling between the respective atomistic and continuous model, such that an ideal coupled model will offer the same accuracy as the full atomistic system. In reality, all concurrent multiscale methods apply an approximate coupling condition which introduces a coupling error, in addition to the numerical discretization error. These errors are manifested, for instance, in the so-called *ghost forces* observed in some methods for static problems (Miller and Tadmor, 2009), and in phonon reflections for dynamic problems (Shiari et al., 2008). Dynamic concurrent methods experience spurious reflection of high frequency waves or phonons at the atomistic/continuum interface which can be attributed primarily to two aspects of the approximate model: (a) the dynamic mismatch created by the change in constitutive behavior of the model across the interface and (b) the change in the scale refinement of the model as it extends out from the fine scale region (Shiari et al., 2007). This reflection of high frequency waves at the interface overheats the atomistic zone, and as such it becomes critical to develop methods that take away the reflected in order to maintain the correct temperature in the atomic region (Shiari et al., 2008). These difficulties can, to a great extent, be overcome in so-called "zero temperature" dynamic simulations[1] through the use of special history-dependent non-local boundary conditions for the atomistic problem (Tadmor and Miller, 2012). However, these techniques are quite expensive to use for three-dimensional problems because of the involvement of many atoms at the interface. As well, they are not necessarily straightforward to extend to systems at constant finite temperature.

To investigate crack propagation, the concurrent multiscale method must work at both the level of the material description (by incorporation of both elastic continuum regions and atomistic regions) and also at the level of defects, in that the dislocations are treated differently depending on the region in which they reside. A few dynamic multiscale methods such as the quasicontinuum (QC) method (Dupuy et al., 2005), embedded statistical coupling method (ESCM) (Yamakov et al., 2014), and the coupled atomistic-discrete dislocation method (CADD) (Shiari et al., 2005a, 2005b; Qu et al., 2005; Pavia and Curtin, 2015) are capable of modeling nucleation and motion of dislocations during the simulation. In QC, this is achieved by adaptive refinement of the model to track the dislocations, in ESCM the dislocations are allowed to pass out of the atomistic region but are not explicitly modeled in the continuum. In CADD, dislocations are converted to elastic defects and treated using a discrete dislocation framework.

In this paper, the dynamic CADD method is used to investigate crack tip propagation in aluminum and nickel crystals. The method contains four main elements: a scheme to mechanically couple an atomistic region with a continuum region containing discrete dislocations, an algorithm to detect dislocations near the atomistic/continuum interface, an algorithm to pass dislocations from the atomistic region to the continuum region, or vice versa, and a thermostating system inside the atomistic region to absorb high frequency phonons and prevent spurious wave reflections. The method is able to treat dynamic loading from remote boundaries and the interaction of the stress waves with the crack tip. After briefly summarizing the model, which has been published elsewhere (Shiari et al., 2005b), in Section 2, Section 3 describes the propagation of ductile and brittle cracks due to dynamic loads on the remote boundaries of the model. We investigate the resulting dislocation propagation, nano-void nucleation and stress distribution during the crack tip propagation in edge-cracked single crystals of nickel and aluminum. We use these simulations to characterize the crack propagation process and failure mechanisms based on the dislocation and stresses around the crack tip at different temperatures.

2. Model description

Dynamic CADD (Shiari et al., 2008, 2007, 2005a, 2005b), an extension of the original static version (Shilkrot et al., 2004a,

[1] Zero-temperature dynamics refers to simulations that are started from an equilibrium, zero temperature system at rest, so that only a relatively small local temperature rise occurs as the system evolves.