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A multiscale method for dislocation nucleation and seamlessly passing scale boundaries

Jinghong Fan [a,*], Ross J. Stewart [a], Xiangguo Zeng [b]

[a] Kazuo Inamori School of Engineering, Alfred University, Alfred, NY 14802, USA
[b] Department of Engineering Mechanics, Shichuan University, Chengdu 610065, PR China

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ABSTRACT

In the concurrent multiscale analysis, it is difficult to have truly seamless transition between the atomistic and continuum scale. This situation is even worse when defects pass through the boundary between different scales. For example, there is a lack of effective methods to handle the dislocation passing through scale boundaries which is important to investigate plasticity at the nanoscale. In this paper, the generalized particle (GP) method proposed by the first author is further developed so that a seamless transition and dislocation passing between different scales can be realized. Specifically, the linkage between different scales is through material neighbor-link cells (NLC) with scale duality. This indicates that material elements can be high-scale particles through a lumping process and can also be atoms via decomposition depending on the needs of the simulation. At the interface, the information transfer from bottom scale-up or from top scale-down is through the particles or atoms in the NLC. They are with the same material structure, all possess nonlocal constitutive behavior; thus, the smooth transition at the interface between different scales can be attained and validated to avoid non-physical responses. To save degrees of freedom, atoms are lumped together into a generalized particle in the domain in which the deformation gradient is near homogeneous. On the other hand, when defects such as dislocations in the atomistic domain are near the particle domain, the particles along dislocation propagation path and its surrounding region will be decomposed into atoms so dislocations can freely pass through the scale boundary and propagate inside the model just as it propagates in the deformed atomistic crystal structure. The method is verified first for seamless transition of variables at the scale boundary by a one-dimensional model and then verified for dislocation nucleation and propagation passing through scale boundaries in two cases, one is near the free surface and the other is inside of the copper nanowire. All the validations are through comparisons with fully atomistic analyses under same conditions. The comparison is satisfactory.

1. Introduction

Dislocation nucleation and evolution are fundamental mechanisms of plasticity. Understanding of these physical mechanisms through analysis and computational simulation is still a major scientific task and it is the reason why multiscale analysis of plasticity, involving dislocation nucleation and scale boundary passing, is so important. Extensive reviews on state of the art for multiscale analysis are given in Fan (2009, 2010), here we only highlight some work important to the background, significance, category, shortcomings, and existing works related to dislocations in multiscale analysis.

* Corresponding author. Tel.: +1 607 8713781; fax: +1 607 8712348.
E-mail address: fanjing@alfred.edu (J. Fan).

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Recently, discrete dislocation analysis shows grain size dependence on the flow strength of polycrystals (Balint et al., 2008) and interprets plasticity size and surface effects for freestanding FCC thin films (Espinosa et al., 2006). The analysis based on continuum dislocation theory can also show some typical material behavior such as the Bauschinger effect of translational work hardening and a size effect typical to problems of crystal plasticity (Kochmann and Le, 2008; Kaluza and Le, 2011). The length scale effect of plasticity is incorporated through the explicit coupling of the density of geometrically necessary dislocations with the crystallographic slip rule (Liang and Dunne, 2009). Dislocations have their origin in atom motion and they can be simulated by atomistic analysis. Recently, a review on atomistic modeling of fatigue is given by Horstemeyer et al. (2010). By atomistic simulations, it shows that dislocation substructures were observed to develop in the atomic lattice during cyclic loading in copper bicrystals. It showed that the reversible plastic slip along the active crystallographic directions at the crack tip was responsible for advancing the crack during applied cycling. These simulation results may help to explain the same behavior observed in the macroscopic scale for fatigue.

In an attempt to study the effects of dislocations on the larger scale and for some complicated physical mechanisms such as fatigue (Curtin et al., 2010), influence of non-glide stresses on plastic flow (Vitek et al., 2004), shock compression (Shehadeh et al., 2005), and dislocation boundary effects (Khan et al., 2004; Shehadeh et al., 2005) multiscale analysis of plasticity was developed. The classification of the multiscale modeling method is still under discussion and development and different categories can be defined based on the methodology, feature and usage of the methods (Fan, 2010). From a methodology point of view, multiscale analysis can be basically classified into hierarchical (sequential) and concurrent (parallel) methods. The former is basically a one way coupling from a lower scale to adjacent upper scale (Park, 2008). A typical one includes a two-scale model to get the overall stress–strain response of the polycrystalline material by Taylor averaging on the stress response of each grain (Potirniche et al., 2007). Recently Wang and Beyerlein (2011) developed a three-dimensional discrete dislocation dynamics (DD) simulation model to understand the relationship between dislocation glide behavior and macro-scale plastic slip behavior in single crystal BCC Ta. For the first time, it is shown that non-Schmid effects on screw dislocations of both {1 1 0} and {1 1 2} slip systems must be implemented into the DD models in order to predict the strong plastic anisotropy and tension–compression asymmetry experimentally observed. They concluded that incorporation of fundamental atomistic information is critical for developing a physics-based, predictive meso-scale DD which has been used to investigate individual dislocation glide behavior and macro-scale plastic slip behavior in single crystal BCC metals. Aoyagi et al. (2007) studied multiscale crystal plasticity modeling based on geometrically necessary crystal defects and simulation on fine-graining for polycrystals.

The second category is the concurrent (or parallel) method (Rudd and Broughton, 2000; Liu et al., 2004) in which both lower and upper scale behavior and their coupling are simultaneously accounted for. Two of these concurrent multiscale methods are the quasicontinuum (QC) method (Tedmor et al., 1999; Knap and Ortiz, 2001) which couples the atomistic simulation with a larger finite element continuum and the CADD method, short for the Coupled Atomistics and Discrete Dislocation method. The QC method is the one with a relatively long history. Ten findings by using this method have been summarized recently (Fan, 2010). For investigating dislocation propagation in the continuum domain, the QC method can change the finite element meshes into atomistic domains through a re-mesh technique. It, however, is complicated for applications.

Recently, a new classification of concurrent multiscale methods was proposed (Seather et al., 2009) which is based on how the atoms in the atomistic domain of molecular dynamics (MD) are connected to the continuum domain. In this classification, approaches that relate atoms and finite element (FE) nodes in a one to one manner, or through a form of interpolation, will be referred to as direct coupling (DC) methods. According to this definition, most of the existing multiscale methods including the QC and CADD method belong to the DC methods. Non-DC methods have just appeared. The method of ESCM, short for the embedded statistical coupling method, is a non-DC method which is proposed by Seather et al. (2009). This method uses statistical averaging over selected time intervals and atomic subdomains at the MD/FE interface to determine nodal displacement boundary conditions for the continuum FE model. These enforced displacements then generate interface reaction forces that are applied as constant traction boundary conditions to the localized MD subdomains; thus there is no need for the direct connection between atoms and FE nodes in a one-to-one manner.

While DC methods are straightforward, there is difficulty for truly seamless transition along the boundaries between the atomistic and the continuum domain. Curtin and Miller (2003) reviewed most of the DC multiscale models for static analysis. They concluded that almost all the DC models have difficulty producing truly seamless transition along the boundaries between the atomistic and the continuum scales. Intrinsic incompatibility causes non-physical phenomena including ghost forces. The incompatibility originates from the material constitutive behavior of the continuum that is local; that of atoms, however, is non-local in nature. Local behavior indicates that the force (stress) of a material point depends only on the deformation gradient (strain) at the same point. Non-local constitutive behavior indicates that the force at any atom also depends on the atoms not in direct contact but within its neighborhood through interatomic forces. Recently, a benchmark test of 14 different types of DC multiscale methods were conducted (Miller and Tadmor, 2009). It uses a common framework as a platform to test the accuracy and efficiency of the 14 methods on a test problem. While this test is significant, the quantitative criterion for accuracy comparison uses the global error which covers all atoms in the simulation system. Thus, it is difficult to make a judgment for how accurate the DC method is in describing material local behavior. In fact, it was found in the benchmark test that slight error in global energy estimation can lead to profound effects on the resulting dislocation motion.

Another two shortcomings of DC methods have motivated the development of the ESCM non-DC method. The first DC shortcoming is that in most cases the finite element size has to be near the interatomic distance at the atomic/continuum