Simulation of nanoindentation via interatomic potential finite element method

Ting Zhu [a,*], Ju Li [b,d], Krystyn J. Van Vliet [c], Sidney Yip [b,c], Subra Suresh [c]

[a] *Department of Mechanical Engineering,* [b] *Department of Nuclear Engineering, and* [c] *Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[d] *Department of Materials Science and Engineering, Ohio State University, Columbus, OH 43210, USA*

Abstract

Nanoscale contact of material surfaces provides an opportunity to explore and better understand the elastic limit and incipient plasticity in crystals. In the present study, nanoindentation is simulated via the interatomic potential finite element method (IPFEM). This method differs from the conventional finite element approach which postulates a constitutive relation thought to be appropriate for the problem of interest. Instead, the constitutive relations is derived from the crystal calculation based on the interatomic interactions. The efficiency of the finite element method allows for simulations at comparatively larger length scales, while maintaining atomistic resolutions. The IPFEM calculation is validated by a detailed comparison study with molecular dynamics (MD) simulations for 2D cylindrical indentation of single crystal copper.

Keywords: Nanoindentation; Finite element; Molecular dynamics; Cauchy–Born elasticity; Finite deformation; Instability; Dislocation

1. Introduction

Nanoscale contact of material surfaces provides an opportunity to explore and better understand the elastic limit and incipient plasticity in crystals [1]. Recent in situ experiments by Gouldstone et al. [2] via the Bragg–Nye bubble raft analogue clearly demonstrated that nanoindentation of a two-dimensional crystal leads to homogeneous nucleation of dislocations within the crystal. The homogeneous nucleation of a dislocation beneath a nanoindenter is a phenomenon corresponding to nonlinear elastic instability of perfect crystals at finite strain. Several direct atomistic (molecular dynamics) simulations have been carried out to investigate nanoindentation-induced dislocation nucleation [3,4]. However, due to the computational cost associated with keeping track of large number of atoms, the physical length scale and time scale for molecular dynamics simulations are often unrealistically small. In the present paper, nanoindentation is simulated via the interatomic potential finite element method (IPFEM). This method differs from the conventional finite element approach which postulates a constitutive relation thought to be appropriate for the problem of interest. Instead, the constitutive relation is derived from the crystal calculation based on the interatomic interactions. Since the constitutive relation is obtained directly from atomistics, key properties of the crystal such as crystalline anisotropy, lattice periodicity and nonlinear elastic effects are incorporated automatically. The efficiency of the finite element method allows for simulations at comparatively larger length scales and for realistic boundary conditions. Thus, IPFEM qualifies as a multiscale approach to study defect nucleation at practical length scales large compared to atomic dimensions, while maintaining atomistic resolutions.

2. Formulation

The interatomic interactions are incorporated into the constitutive relations through the Cauchy–Born rule [5], which states that every point in a continuum corresponds to an infinite region at the atomic scale and the local stress at that point can be obtained by deforming the underlying crystal lattices according to the local uniform deformation gradient. From the Cauchy–Born rule, the strain energy density of the continuum is just the energy per unit volume of uniformly distorted lattices and can be computed using

* Corresponding author. Tel.: +1 617 253 7316;
E-mail: zhut@mit.edu

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the interatomic potential. Within the framework of the embedded-atom method (EAM), the energy per atom $\hat{\Psi}$ is

$$\hat{\Psi} = \frac{1}{2}\sum_i V(|\mathbf{r}^i|) + U(\rho) \tag{1}$$

where V is the pair potential, ρ is the ambient electron density and U is the energy required to embed an atom into the corresponding electron density ρ. The index i runs over all atoms within a specified cut-off radius, $|\mathbf{r}^i|$ is the interatomic distance.

Given the energy of the crystal, the constitutive relations are obtained within the framework of hyperelasticity theory in continuum mechanics. Cauchy stress is given by

$$\boldsymbol{\sigma} = \frac{1}{\Omega}\sum_i \left[\frac{1}{2}\frac{\partial V}{\partial r} + \frac{\partial U}{\partial \rho}\frac{\partial \rho}{\partial r}\right]\frac{\mathbf{r}^i \otimes \mathbf{r}^i}{|\mathbf{r}^i|} \tag{2}$$

where Ω is the volume of the current primitive cell. The tangential material modulus is momentarily equal to

$$\begin{aligned}\mathbf{C} = \frac{1}{\Omega}\Bigg\{\sum_i \Bigg[&\frac{1}{2}\left(\frac{\partial^2 V}{\partial r^2} - \frac{1}{|\mathbf{r}^i|}\frac{\partial V}{\partial r}\right) \\ &+ \frac{\partial U}{\partial \rho}\left(\frac{\partial^2 \rho}{\partial r^2} - \frac{1}{|\mathbf{r}^i|}\frac{\partial \rho}{\partial r}\right)\Bigg]\frac{\mathbf{r}^i \otimes \mathbf{r}^i \otimes \mathbf{r}^i \otimes \mathbf{r}^i}{|\mathbf{r}^i|^2} \\ &+ \frac{\partial^2 U}{\partial \rho^2}\left(\sum_i \frac{\partial \rho}{\partial r}\frac{\mathbf{r}^i \otimes \mathbf{r}^i}{|\mathbf{r}^i|}\right)\left(\sum_i \frac{\partial \rho}{\partial r}\frac{\mathbf{r}^i \otimes \mathbf{r}^i}{|\mathbf{r}^i|}\right)\Bigg\}.\end{aligned} \tag{3}$$

The localization criterion [6,7] is applied to detect dislocation nucleation. The acoustical tensor $\mathbf{Q}(\mathbf{n})$ is defined as $\mathbf{Q}(\mathbf{n}) \equiv \mathbf{nLn}$, where $\mathbf{n}$ is the slip plane normal and $L_{ijkl} = C_{ijkl} + \sigma_{il}\delta_{jk}$. The onset of localization occurs when the acoustical tensor becomes singular. That is,

$$\det[\mathbf{Q}(\mathbf{n})] = 0. \tag{4}$$

The constitutive model of Cauchy–Born elasticity describes well the crystal behavior, as long as the spatial variation of continuum deformation field is slow on the atomic scale, and it will break down near the defect where non-local effects become significant. In the context of the more general continuum-atomistic framework of quasicontinuum method [5], Cauchy–Born elasticity is a full-continuum model and represents its local limit. However, for the current approach on nanoindentation-induced elastic instability, the deformation is approximately uniform at the atomic scale, so Cauchy–Born elasticity is adequate to describe the crystal behavior accurately. Furthermore, compared to the quasicontinuum method, the constitutive model of Cauchy–Born elasticity can be easily incorporated into any general-purpose FEM package without significant effort to code and implement. The quantitative prediction on defect nucleation can be furnished with the aid of an accurate and reliable defect nucleation criterion, given by Eq. (4), within the framework of Cauchy–Born elasticity.

Cauchy–Born elasticity described above is implemented in the finite element program ABAQUS/Explicit by writing a "user material" subroutine. In the dynamic, explicit computational procedures, the nonlinear response is obtained incrementally, given the internal forces created by the stress in the element, as well as the applied external forces at the start of an increment, time t. Finite element procedures solve for the acceleration at the start of the increment by solving the discretized local equations of motion. The velocities at time $t + \Delta t/2$ and the displacements at time $t + \Delta t$ are updated by a simple central difference time-integration procedure. The deformation gradient for each integration point at time $t + \Delta t$ is then calculated based on the updated displacement field. Knowing the deformation gradient, a constitutive equation subroutine is required by ABAQUS in order to calculate the stress in the element at time $t + \Delta t$. In the implementation of stress calculation based on Cauchy–Born elasticity, each material point is represented by a set of face-centered cubic (FCC) lattices which deform according to the local continuum deformation gradient. That is, at the beginning of the calculation ($t = 0$), a set of neighboring atoms is created to represent the atomic environment of a material point. The lattice spacing is taken such that the corresponding material point stress is zero. For each time increment, those neighboring atoms update their positions according to the local deformation gradient. Then $\boldsymbol{\sigma}$ and $\mathbf{C}$ are calculated by substituting the deformed positions of neighboring atoms into Eq. (2) and Eq. (3), respectively. Thus, material properties depend exclusively on the atomistic description of the system. The efficiency of finite element calculations allows for the simulation of larger systems while the computation remains faithful to atomistic interactions at large strains. As such, IPFEM qualifies as a multiscale approach.

3. Nanoindentation simulations

Nanoindentation is simulated for a frictionless cylindrical indenter pressed into the (111) surface of single crystal Cu along the $[1\bar{1}0]$ direction. IPFEM calculations will be verified by comparing with direct molecular dynamics (MD) simulations using the same interatomic potential [8].

ABAQUS/Explicit(2001) is implemented to simulate indentation on a small system size, 200×100 Å, for direct comparison with MD calculations. The coordinate system is oriented such that the x_1 and x_2 axes correspond with the $[11\bar{2}]$ and $[111]$ directions, respectively. The out-of-plane x_3 axis is along the $[1\bar{1}0]$ direction. Because of mirror symmetry of the lattices with respect to the $x_1 - x_2$ plane, prior to symmetry breaking induced by dislocation nucleation, the resulting displacement field is only a function of in-plane coordinates and has no variation in the out-of-plane x_3 direction. Therefore, this is a quasi-2D problem. The plane strain linear, triangular elements are used with each element representing a homogeneously deformed crystallite. The boundary conditions are fixed at the bottom, free on the top surface and fixed in the x_2 directions on two

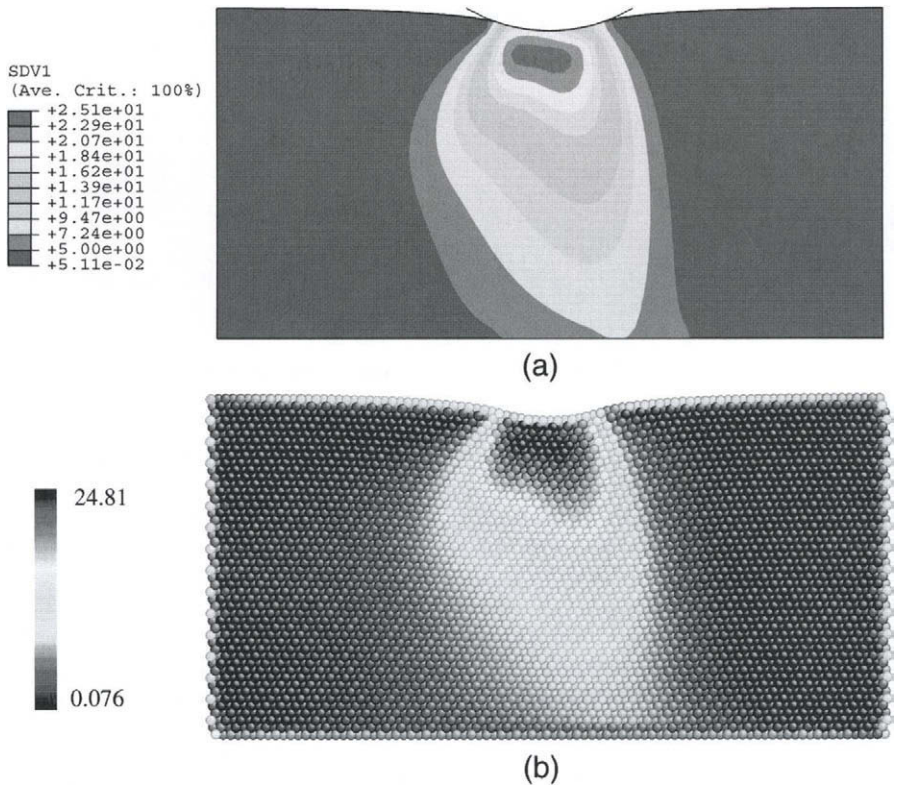

Fig. 1. Contours of Mises stress (in GPa) for cylindrical indentation: (a) IPFEM and (b) MD simulations.

sides. The frictionless cylindrical indenter is defined by an analytic rigid surface with a radius R of 50 Å. The quasistatic solution is approximated by requiring that the kinetic energy is less than 1% of the internal energy of the system.

MD simulations at the temperature 1K are performed to compare with IPFEM calculations. The same in-plane boundary conditions as IPFEM simulations are used and periodic boundary conditions (PBC) are applied for the out-of-plane x_3 direction. The indenter is regarded as an external repulsive potential interacting with copper atoms at the surface. The indentation proceeds in displacement-control at a speed about 0.01 Å/ps.

Fig. 1(a) and (b) show the contours of Mises stress calculated from IPFEM and MD simulations, respectively. The indentation depth is 6.65 Å, corresponding to the moment right before the dislocation nucleates. It can be seen that the IPFEM calculation agrees well with the MD simulation. The calculated nanoindentation response is given in Fig. 2. The IPFEM load versus displacement response is in good agreement with that predicted by the MD simulation. Note that the MD response shows a sharp drop in load at an indentation depth 6.65 Å, which indicates the onset of homogeneous nucleation of dislocation within the crystal. This load drop was not captured in the IPFEM simulation because the 2D setting constrains the out-of-plane displacement mode that the homogeneously nucleated dislocations takes, as shown in the MD simulation. However, the instability criterion given by Eq. (4) can be applied to predict when and where

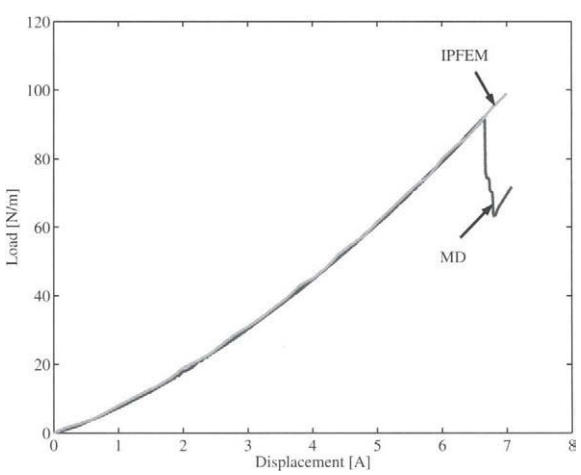

Fig. 2. Load versus displacement curves for cylindrical indentation by IPFEM and MD simulations.

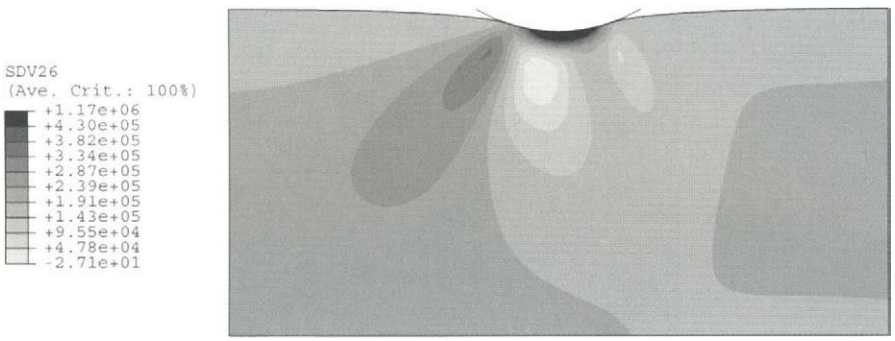

Fig. 3. Contour of det[**Q**(**n**)] by IPFEM simulation.

the dislocation will nucleate. Fig. 3 shows the contour of det[**Q**(**n**)] from IPFEM calculations at an indentation depth of 6.68 Å, when the onset of dislocation nucleation is first detected at one integration point. The critical indentation depth predicted by IPFEM calculation agrees well with that by MD simulations. In calculating det[**Q**(**n**)], the modulus **L** is normalized via the elastic constant of Cu ($C_{44} = 75.4$ GPa). It can be seen from Fig. 3 that the interpolated values of det[**Q**(**n**)] within the light color region are small negative values, which indicate the site of a homogeneously nucleated dislocation. The position of nucleation site is 14.25 Å below the surface and 5.75 Å on the left of x_2 axis.

Fig. 4(a) shows the embryo of a homogeneously nucleated dislocation via MD simulation. Atoms are color-encoded by coordination number N. Perfectly coordinated atoms, $N = 12$, are color-encoded as light gray, and other colored atoms indicate $N \neq 12$. The atoms with charcoal gray color beneath the surface indicates nucleation of a

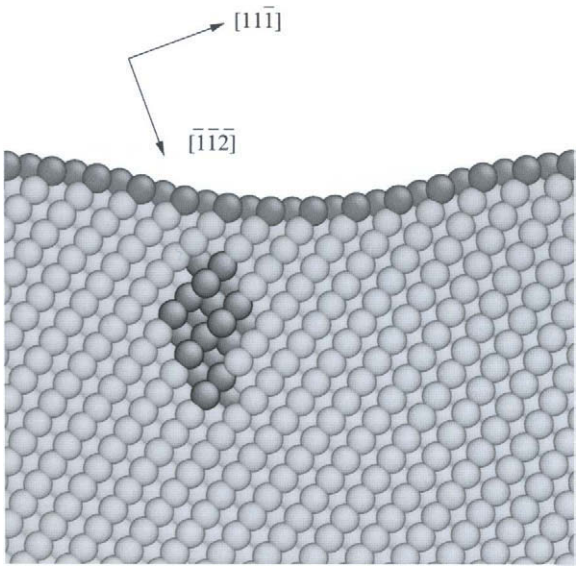

Fig. 4. Atomic structure of homogeneously nucleated dislocation: Shockley partial slip on the (11$\bar{1}$)[12$\bar{1}$] slip system

Shockley partial slip along the [12$\bar{1}$] direction within the (11$\bar{1}$) slip plane. The center of dislocation core as shown in Fig. 4 is about 16.66 Å below the surface and 5.16 Å on the left of x_2 axis. Thus, FEM prediction on nucleation site agrees well with the MD simulation to one atomic lattice spacing.

4. Conclusions

Nanoindentation-induced homogeneous dislocation nucleation in single crystal Cu has been analyzed through IPFEM calculations. The predication on dislocation nucleation is verified by MD simulations. The efficiency of IPFEM permits the simulation of significantly larger systems than would otherwise be possible. We have demonstrated that IPFEM can give quantitative predications on 3D nanoindentation-induced dislocation nucleation at realistic length and time scales, the regime not achievable by MD simulations [9–11]. We conclude by noting that, though the present work only applies IPFEM to study defect nucleation within FCC bulk crystals, further extension of IPFEM can be made to study other type of lattices and/or homogeneous defect nucleation at surfaces and interfaces. Such extensions will further demonstrate the general applicability of predictive calculations of IPFEM to study a wide range of phenomena in small volume structures at the continuum level while maintaining explicitly the atomistic interactions which govern the mechanical response.

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