Thin Solid Films 520 (2012) 4934–4940

Contents lists available at SciVerse ScienceDirect

Thin Solid Films

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

Effect of surface step on nanoindentation of thin films by multiscale analysis

Huaibao Lu, Yushan Ni *

Department of Mechanics and Engineering Science, Fudan University, Shanghai 200433, China

ARTICLE INFO

Article history:
Received 15 June 2011
Received in revised form 2 March 2012
Accepted 7 March 2012
Available online 14 March 2012

Keywords:
Multiscale
Nanoindentation
Surface step
Indenter size
Step height

ABSTRACT

Nanoindentation simulations on flat and stepped surfaces are respectively investigated using the quasicontinuum method based on the embedded-atom method potential. Effect of surface step considering indenter size and step height is studied. Results show that the critical load for the first dislocation emission will be decreased with the increase of step height. However, the effect of surface step will be weakened if the indenter size continues to increase. Initial atomistic structures after dislocation nucleation and emission are discussed systematically. The initial dislocations are not quite identically nucleated under the stepped surface. Stress distribution analysis reveals that the shear stress in the slip planes close to the step is much larger than the shear stress in the slip planes far from the step for nanoindentation on the stepped surface. The multiscale simulation results are consistent with experimental results and analytic solutions. The conclusions about step effect considering indenter size and step height are helpful for understanding the microscopic mechanism of nanoindentation tests on thin films with surface step.

1. Introduction

With the rapid development of technology and the intensive study of the microstructure of materials, surface steps of thin films have been the topic of substantial research, attracted by their physical importance in the growth process of epitaxial thin films [1]. The crystal vapor surface of such epitaxial films is typically a highly structured near-facet plane consisting of multiple terraces and steps [2]. The surface steps have been observed to affect the yield stress measured by nanoindentation distinctly in experiment and atomic simulations. Using interfacial force microscopy in the nanoindentation experiment, Kiely et al. [3] have investigated the effect of surface step on the initiation of plastic yield by performing nanoindentations as a function of separation between the probe and neighboring steps. The mean stress at yield was 30%–45% lower at a step than in regions free of surface defects, which shows a strong effect of surface step on nanoindentation. However, it is difficult to directly examine the dislocation activities and atomic structures under the step by experiments. One of the available methods is the atomic scale simulation to identify microscopic mechanisms, and to put insights into microscopic behavior such as molecular dynamics (MD) that can effectively simulate the dynamic behavior of nanoscale materials. Zimmerman et al. [4] employed MD method to examine nanoindentation of a Au (111) crystal both near and far from a surface step. The effect of surface step on critical load of initial dislocation nucleation was not as great as seen experimentally.

Although MD simulation can reflect atomic level information, effectively simulate the dynamic behavior of nanocrystalline materials and offer insights into microscopic behavior, it cannot depict large scale systems due to the computational intensity of the problem and cannot overcome the boundary effect caused by the relatively small computational spatial size. Therefore, it is necessary to develop a multiscale method bridging atomistic and continuum approaches. The quasicontinuum (QC) method is one multiscale methods proposed by Tadmor et al. [5] in 1996, which can directly investigate the process of dislocation nucleation and emission, study the microscopic mechanical properties of thin films during nanoindentation and effectually avoid the boundary effect encountered in MD simulation.

Using QC method, Shan et al. [6] studied the effects of surface step on the first dislocation emission in nanoindentation on thin copper film. But their conclusion about the role of step height did not reveal the intrinsic effect of step height on the plastic threshold in nanoindentation. As we know, the measured hardness by indentation tests is related with indenter size [7–9]. But nanoindentation on stepped surface with various indenter sizes has not been studied. The above discussions motivate us to further study the effect of surface step on nanoindentation by multiscale method. In the present work, we perform a series of nanoindentation simulations of an Al (110) crystal with different indenter widths to investigate the role of indenter width on the effect of surface step. We also study the influence of step height on the first dislocation emission in nanoindentation. The multiscale simulation results are consistent with experimental results and analytic solutions in published literatures. Based on the simulation results, atomistic mechanism of plastic deformation during nanoindentation on thin films with surface step is illustrated. The

* Corresponding author. Tel.: +86 21 55665173.
E-mail address: niyushan@fudan.edu.cn (Y. Ni).

0040-6090/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.tsf.2012.03.019

conclusions about the interrelation between surface step and indenter size and effects of step height on nanoindentation are shown to be significant on the microscopic mechanism of nanoindentation tests on nanoscale materials.

2. Quasicontinuum method and nanoindentation model

2.1. Quasicontinuum method

QC method [5] is a viable multiscale approach to simulate the mechanical response of crystalline materials at zero temperature, which permits the treatment of long-range fields in a computationally efficient manner while resolving non-linear regions of the configuration space atomistically. It is established that discrete atomic description is only necessary at highly deformed region and in the vicinity of defects or interfaces. As shown in Fig. 1, representative atoms are divided into local atoms and non-local atoms. The local atoms capture the deformation behavior of atoms that undergo only a near homogeneous deformation, whose energies are computed from the local deformation gradients based on Cauchy–Born continuum approximation, while the non-local atoms are treated by discrete atomistic lattice statics in the areas where defect cores or severe plastic deformation occurred, whose energies are computed by an explicit consideration of all its neighbors. During QC simulation, a mesh adaption strategy, including both mesh refinement and mesh coarsening, is adopted to automatically reduce the degrees of freedoms without losing atomistic detail in regions where it is required [10,11]. Therefore, compared with a single scale atomistic method, such as standard lattice statics (LS) and MD approaches, QC method is capable of implementing large-scale atomic system simulations without the limitations of fixed or periodic boundary conditions and save considerable computing time while maintaining accuracy and convergence. Tadmor et al. [12] studied the incipient plasticity during nanoindentation with both rectangular and cylindrical indenter based on QC method on simple crystal films. Smith et al. [13] extended the method to handle complex crystal structures. Knap and Ortiz presented a streamlined and fully three-dimensional version of the QC method [14], and they applied the streamlined theory to investigate the effect of indenter-radius size [15]. Very recently, QC method has been applied to study the mechanical response of atomic processes and to elucidate detail of deformation mechanisms of nanocrystalline metals, such as the nucleation and collective interaction of dislocations [16,17], nanoindentation [18–23], nanoscale contact [24–28], fracture [29–31], mechanical behavior of grain boundary [32,33], nanovoid cavitation [34,35] and phase transformation [36].

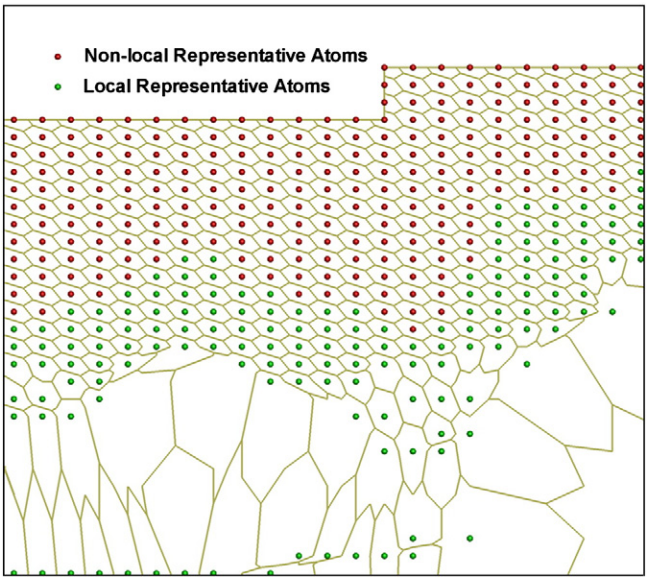

Fig. 1. Schematic representation of non-local and local representative atoms.

2.2. Nanoindentation model

To examine step effect considering indenter size and step height, QC simulations of nanoindentation at zero temperature are performed on flat surface and stepped surface, respectively. Fig. 2 shows the schematic representation of nanoindentation model. As shown in Fig. 2, the computational overall size of Al film investigated in this simulation is 1500 Å thick, 3000 Å wide and infinite in the out-of-plane direction with periodical boundary. Compared with the single scale atomistic simulation, the model size used in QC simulation is larger by an order of magnitude [37,38], which can effectively prevent the boundary effects and more accurately capture the detail of collective dislocation activities during nanoindentation. The distance between the indenter and the step is 4.66 Å; the crystal orientation is $x[111]$, $y[\bar{1}10]$ and $z[\bar{1}\bar{1}2]$, respectively. A rectangular indenter is pushed into the $(\bar{1}10)$ plane. Because the pushing direction is parallel to Burgers vector, dislocation nucleation and emission can be clearly observed. During the whole simulation, free boundary conditions are applied on the top, left and right surface of Al single crystal film, while fixed boundary conditions are used on the bottom surface which is fixed on a rigid support. For the sake of simplicity and easier control, the indenter used in the present investigation is modeled as a rectangular rigid body. In order to investigate the interrelation between surface step and indenter size, six indenters (i.e. $D1$, $D2$, $D3$, $D4$, $D5$, and $D6$) are used with a width of $6a_0$, $10a_0$, $14a_0$, $18a_0$, $22a_0$ and $26a_0$ (a_0 is the lattice spacing between the adjacent (111) slip planes, 2.33 Å), respectively. The friction-free and perfect stick contact conditions are assumed between the indenter and the top surface of Al thin film. The rectangular indenter is controlled to be down step by step with a value of 0.1 Å without friction. At each loading step, a quasi-Newton solver is used to iteratively minimize the total energy and to indentify the new stable equilibrium configuration of the system in the new load step boundary conditions. As we know, the results of atomistic simulations are depended heavily upon the interatomic potentials used to define the interaction forces between atoms, and thus a proper potential description must be required. Since EAM (embedded-atom method) potential which originally developed by Daw and Baskes [39] can describe well many metal properties such as the lattice constants, cohesive energy and elastic constants, it is now widely used to simulate the mechanical response of nanocrystalline metals. In the present work, the Ercolessi–Adams potential [40] is used for the simulation of face-centered cubic Al thin film. The elastic constants and effective isotropic properties for Al obtained from QC simulations based on Ercolessi–Adams EAM potentials and experimental results [40] are given in Table 1, where a, b, C, G and ν are the lattice constant, Burgers vector module, elastic constants, shear modulus and Poisson's ratio, respectively. For the shear modulus (G) and Poisson's ratio (ν), they are estimated by the following Voigt average method [41],

$$G = (C_{11} - C_{12} + 3C_{44})/5 \tag{1}$$

$$\nu = (C_{11}/2 + 2C_{12} - C_{44})/(2C_{11} + 3C_{12} + C_{44}) \tag{2}$$

As Table 1 demonstrates, it can be seen clearly that the calculated material's parameters from QC simulations with Ercolessi–Adams EAM potentials agree well with experimental results. This means that Al EAM potential utilized in this work can well reproduce the mechanical behavior of nanoindentation on Al film.