Nanoindentation simulation on single crystal copper by quasi-continuum method

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A B S T R A C T

Considering that nanoindentation size effect under very small nano scale could not be effectively investigated by traditional experimental methods, this paper proposed to use quasi-continuum (QC) method to establish a multi-scale simulation model for nanoindentation process on single crystal copper at very small depth, below 20 Å. And different-size small indenters were adopted in this paper with their radiuses ranging from 2 nm to 10 nm. The simulation results showed that the contact stiffness did not show indentation size effect, but the values fluctuated on a horizontal line; that the nano-hardness showed obvious indentation size effect.

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1. Introduction

Hardness is an important mechanical property of engineering material. Nanoindentation, also known as depth-sensing indentation technique, is a new technology developed in recent years for hardness test [1–6]. Although nanoindentation has been widely used, the accessible range of experimental studies of nanoindentation is limited by instruments as a typical radius in experimental system is about 1–1.5 μm. Therefore, computer simulation studies of nanoindentation become so important and many simulation methods were proposed as a typical radius in simulation system is about 2–20 nm. Feng et al. [7] proposed a simple closed-form analytical expression for the stress field around an elastoplastic indentation, which gave the physical insight for understanding indentation. Huang et al. [8] also established an analytic model for nanoindentation hardness based on the maximum allowable density of geometrically necessary dislocations. Finite element model is used to by some researchers to simulate nanoindentation process and it can be employed for investigating the stress and strain fields under indenter tip [9–12]. Molecular dynamics method is also a widely-used method to investigate the various characterizations in indentation process, e.g. surface orientation [13], Young's modulus [14], active slip system [15], and contact stiffness [16,17]. As for indentation size effect, one of the first model was proposed by Nix and Gao [18] who used the concept of geometrically necessary dislocations to research the

indentation size effect for crystalline materials. Durst et al. [19] investigated the indentation size effect during indentation testing of crystalline materials in terms of geometrically necessary dislocations using a corrected Nix/Gao model. Lam and Chong [20] described the hardness–depth variation using a strain plastic gradient theory, which differed from that of Nix and Gao [18] where dislocations of the global plastic deformation process are separated. Feng et al. [21] measured the lattice rotations in indentations of different sizes using white beam x-ray micro-diffraction to understand the underlying mechanism of indentation size effect. Budiman et al. [22] grow good quality and thermally stable epitaxial/quasi-single crystal Cu/Nb nanoscale multilayered composite materials, which could help to understand the nanoplasticity mechanisms in the deformation of their nanoscale multilayered materials. Burek et al. [23] produced large grain body-centered tetragonal (BCT) tin nanopillars with 70 nm diameter whose results could help to understand how tin nanostructures behaved during mechanical deformation. Budiman et al. [24] investigated the evolution of dislocation densities during compressive deformation of nanoscale Cu/Nb single crystal multilayers using Synchrotron X-ray micro-diffraction. Kim et al. [25] performed microcompression of Al-Nb multilayer system with bilayer spacing of 5 nm and 50 nm to examine the effect of different bilayer spacings on the deformation behavior of the incoherent multilayer system. Budiman et al. [26] used synchrotron white beam x-ray submicron diffraction to study deformation in Cu/Nb nanoscale single-crystal multilayer pillars, before and after uniaxial compression, and found evidence of statistically stored dislocations (SSD) density increase in the Cu nanolayers caused by the plastic deformation. Budiman et al. [27] studied and confirmed

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the signature behavior of electromigration-induced plasticity in causing a permanent effect on the time to failure (MTF) in the particular set of Cu interconnect samples. The above researches are quite helpful for this paper while this paper will present something a little different.

However, under the condition of nano scale, especially from 2 nm to 10 nm, the classical continuum mechanics may not be applicable, and the molecular-dynamics-based simulation of nanoindentation is limited by computational efficiency. And that is where the quasi-continuum (QC) method adopted by this paper can play a role. The use of QC multi-scale method can not only represent the indentation process, but also facilitate the construction of parameter changes in material characteristics, different boundary conditions and complex material micro-structures without the limitations of experimental conditions. Many characterizations of materials have been investigated by QC method, e.g. the interaction effect of grain boundary and dislocation [28], crack tip modeling [29], contact problem [30].

In this paper, QC method was used to simulate the nanoindentation process on single crystal copper by different-radius cylindrical indenters. A number of loading and unloading curves of load-depth under different-size indenters were obtained in order to further investigate the nanoindentation size effect.

2. Method and simulation model

2.1. Hardness calculation method

By applying force on material through indenters, indentation will occur. Fig. 1 shows a typical nanoindentation loading-unloading curve.

Fig. 2 shows a diagrammatic indentation cross-section of the loading and unloading process by an axisymmetric indenter.

In order to calculate the hardness through load-displacement data, Oliver-Pharr method is usually used [31], and the load-displacement curves of the unloading part can be fitted by the following fitting function:

$$P = B(h - h_f)^m \tag{1}$$

where B and m are the measured fitting parameters.

Elastic contact stiffness can be calculated by:

$$S = \left(\frac{dP}{dh}\right)_{h=h_{max}} = Bm(h_{max} - h_f)^{m-1} \tag{2}$$

Contact depth is calculated by:

$$h_c = h - \varepsilon \frac{P_{max}}{S} \tag{3}$$

where ε is a constant associated with the indenter shape.

Contact area is calculated by:

$$A = 24.56h_c^2 + \sum_{i=0}^{7} C_i h_c^{1/2^i} \tag{4}$$

where C_i adopts different values for different indenters.

Finally, nanoindentation hardness can be calculated by:

$$H = P_{max}/A_c \tag{5}$$

2.2. QC method

QC method, one of the multi-scale simulation methods, was originally developed by Tadmor [32]. It integrates continuum and atoms, which uses atomic-scale solution in dislocation core regions while uses rough description characterized by
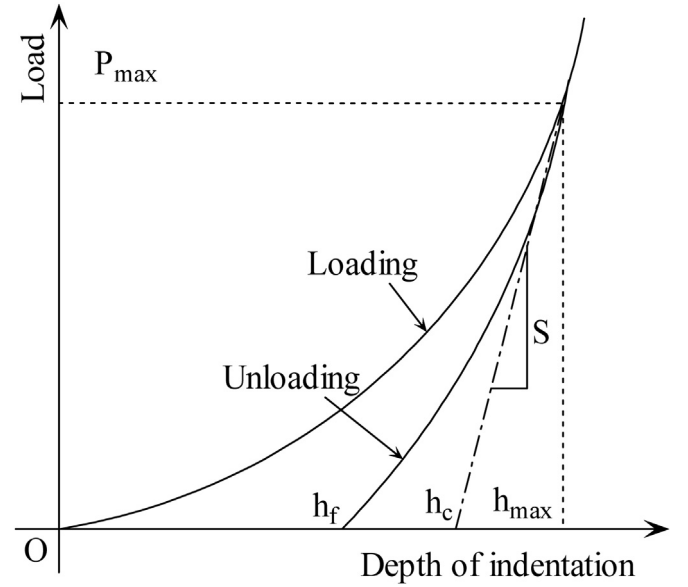

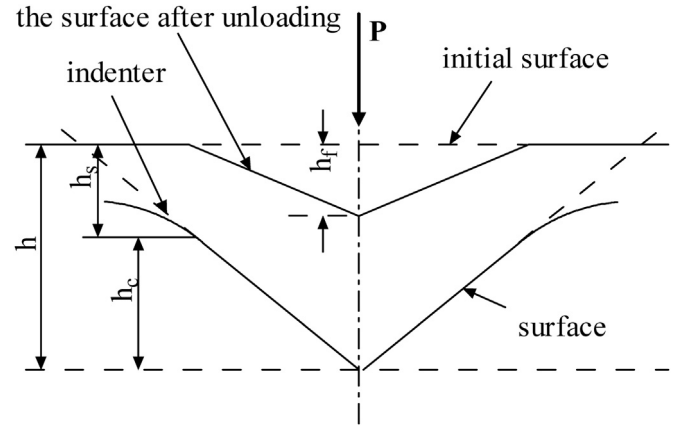**Fig. 1.** Loading/unloading curve of nanoindentation process.

Fig. 2. Material surface during loading and unloading process.

"representative atoms" in the regions far away from core regions.

Fig. 3 demonstrates the basic principle of QC method. The black filled circles in Fig. 3a are the representative atoms and Fig. 3b is the finite element mesh composed of corresponding representative atoms. As shown in Fig. 3b, atoms B, C and D are finite element nodes and atom A is non-representative atom. The displacements of non-representative atoms are derived from the linear interpolation for representative atoms. This purpose can be achieved by using the interpolation equations of finite element method in QC method. In regions where fully detailed atom description is required, we can choose all atoms as representative atoms and reduce the density of representative atoms in regions with smaller deformation gradient. As Fig. 3 shows, we may choose all atoms in the dislocation core region as representative atoms, and reduce the density of representation atoms in regions away from the dislocation core region.

Ideally, in order to calculate the total energy, all the atoms in the domain need to be visited by

$$E_{tot} = \sum_{i=1}^{N} E_i(x_1, x_2, \ldots, x_N) \tag{6}$$

where E_i is the energy contribution from site x_i.