Quasicontinuum Study of Nanoindentation into Nanocrystalline Aluminum Thin Film

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ABSTRACT: Quasicontinuum simulations are performed to examine the mechanical response of nanocrystalline aluminum thin film under nanoindentation. The simulations are conducted by driving the flat indenter into the (111) face of one grain in the aluminum film, two load drops have been found during the indentation process, evidence indicates that these load drops are related to the stacking fault emitted from the grain boundary. The effect of indenter width on nanoindentation response is also studied through three simulations with different indenter sizes. A rule is discovered that larger load is needed to initiate the first load drop for the wider indenter; however, this rule is not followed by the second load drop.

KEYWORDS: nanoindentation; quasicontinuum method; nanocrystalline materials; aluminum

0 Introduction
Nanocrystalline materials show unique mechanical properties under applied load. Many experiments and simulations have been carried out to study the mechanical properties of nanocrystalline materials. Nanoindentation, a small-scale contact experiment, was established to test the hardness, elastic modulus, strain hardening exponent and other important mechanical parameters of small volumes of materials[1]. And it is very suitable to investigate the plastic deformation of nanocrystalline metals. The indenter size can be selected to be either significantly smaller or significantly larger than the average grain diameter so different aspects of the deformation can be revealed[2]. Yang and Vehoff observed that when the indenter size was smaller than the grain size, the dislocations nucleated below the indenter tip interact directly with the surrounding grain boundaries (GBs) for grains below 900nm[3]. Dupont and Sansoz’s quasi-2D atomistic simulation indicated that when the indenter was several times larger than the grain size, the GB networks cause softening effects at the tip/surface interface and the deformation mechanisms are GB movement as well as deformation twins[4].

In this study, the simulation of nano-indentation into nanocrystalline aluminum under zero temperature was performed using a quasicontinuum (QC) model. The width of the indenter was kept much less than the average grain diameter. We obtained the load-displacement curve for the nanocrystalline aluminum and we compared it with the nanoindentation response of single crystalline aluminum. Simulations using another two indenters of different size were also performed in order to find out how the mechanical response depends on the indenter width.

1 Computational model
The quasicontinuum method is a multi-scale method combining atomistic and continuum simulations [5]. In a quasicontinuum simulation, the critical region subjected to large deformation gradients are treated by molecular dynamics (MD) and the other regions are treated using the finite element method (FEM). Thus the computational effort is significantly reduced. This technique is performed by energy minimization under zero temperature, and the result is provided as the equilibrium atomic configurations.

A 2D quasicontinuum model with the dimensions of 200nm×100nm was created. The crystalline orientation of the crystal is illustrated in Fig.1(a). The flat knife-like indenter was assumed rigid and it had no interfacial interaction with the sample. The bottom of the sample was fixed and a periodic boundary condition was applied to the out-of-plane direction. The other sides were kept free. Regions under the indenter and the GBs were refined down to the atomic scale, while the other part of the crystal was

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coarsely meshed. A closer look of the region under the indenter was shown in Fig.1(b). The sample was considered to contain only five grains: the indented grain, its three neighbors and the left part of the crystal. The left part of the crystal was treated as a single crystal grain because the indenter was relatively small and was thought to merely affect the indented grain and its neighbors. The grains were numbered as shown in Fig.1(b). Grains 2, 3 and 4 have geometry of regular hexagon with the edge length of 4.33nm. Grain 1, named indented grain, is a half hexagon. The grain boundaries between grain 1 and grains 2, 3, 4 were all pure <110> tilt GBs. The orientations of grains 1 to 4 were set as follows: Grain 1 has the same orientation as the global crystal orientation shown in Fig. 1(a); grains 2 to 4 were rotated along the [1 \bar{1} 0] direction from the global crystal orientation to 5 degrees, 5 degrees and -3 degrees respectively.

Fig.1 Quasicontinuum model of a nanocrystalline aluminum thin film indented by a flat indenter.

(a) Full view of both finite element and atomistic regions
(b) Close view of the region under the indenter. Bold lines were added to highlight the GBs.

The sample was first relaxed to accomplish minimized energy. Then the indenter was driven into the (111) face of the sample with the step of 0.2 Å until the indentation depth reached 8 Å. Before every step, energy minimization was carried out to adjust to the new boundary conditions. The embedded atom method (EAM) potential for FCC Al used in our simulation was developed by Ercolessi and Adams [6]. Within the EAM model, the total energy E for a system can be written as,

\[ E = \sum_{i} F_{i}(\rho_i) + \frac{1}{2} \sum_{i,j} V_{ij}(R_{ij}) \]  

where the summations extend over the total number of atoms \( N \) in the system, \( F_{i} \) is the embedding function, \( \rho_i \) is the electron density at atom \( i \), \( V_{ij} \) is a pair interaction function and \( R_{ij} \) is the distance between atoms \( i \) and \( j \).

2 Nanoindentation Response of Polycrystalline Aluminum

The flat indenter used here was 20 Å. The computed load-displacement curve is presented in Fig.2 in a solid line. The load was calculated by dividing the force exerted on the nods by the interplanar spacing of the [1 \bar{1} 0] planes. The curve starts from a negative value because of the initial relaxation [7]. Then the curve rises in a linear pattern until point A. At point A the load drops from 12.94N/m to 11.52N/m, and then the curve rises nonlinearly to point B where the load drops again from 16.97N/m to 11.65N/m. After point B, the curve continues going up until the indentation depth reaches 8 Å.

The result for the single crystalline aluminum under the same condition is also shown in Fig.2 in a dashed line. This single crystal simulation was initially carried out by Tadmor and Miller [7], and we repeated the simulation by changing the indenter width to 20Å. The load applied to the single crystal increases linearly with the increasing indentation depth, and is larger as compared to the polycrystal simulation at any indentation depth.

It is indicated in previous literature that in this particular crystal orientation, the dominant deformation mechanism of single crystalline aluminum thin film is deformation twinning [8]. In our study of
nanocrystalline aluminum thin film, deformation twinning as well as dislocation movement were both observed.

Fig.3 shows the atomic configuration at point A. Two phenomena were observed. First, a twin (Fig.3(a)) was formed near the surface. Its twinning plane is (11̅1), and the twinning direction is [112]. The existence of the twin is further evidenced by plotting the atomic displacement along the Y and Z axes (Fig.4). Second, a stacking fault (Fig.3(b)) with the dislocation core at approximately (15,-30) was found near the grain boundary of grain 1 and grain 3. After careful observation, this stacking fault is believed to be separated from the grain boundary and moved leftward to the place where it was found.

Fig.2 Load-displacement curve for nanoindentation into a (111) face of single crystalline aluminum (dashed line) and polycrystalline aluminum (solid line).

Fig.3 Atomic configuration at point A. Red dashed lines indicate boundaries of grain 1.
(a) Twin formed near the surface. (b) Stacking fault near the grain boundary of grains 1 and 3.

Fig.5 shows the mechanism of the second load drop at point B. Fig.5(a) is the atomic configuration just before point B. The twin formed at point A propagated along the [112] direction and its front arrived at approximately (0,-30). The stacking fault mentioned above traveled leftward with its core reached nearly the same position. Fig.5(b) demonstrated the result of the interaction of the twin and the stacking fault. The twin disappeared and another stacking fault was form with its core near (0, -25).

On the basis of the above, the load drop is related to the grain boundary. The stacking fault separated from the grain boundary can interact with twins and thus cause change in mechanical response.

Fig.4 Displacement experienced by the atoms along the Y and Z axes
(a) UY contour plot. (b) UZ contour plot
3 Effects of Indenter Width on Nano-indentation Response

Three indenters with different widths of 10Å, 15Å and 20Å were used in this study. The results were plotted as shown in Fig.6. It is indicated in the figure that the mechanical response under nanoindentation is very sensitive to the indenter width. As the indenter becomes wider, the first load drop occurs at a larger indentation depth and the corresponding load is also larger. However, when the hardness (mean contact pressure) instead of force is considered, the widest indenter is corresponding to the smallest hardness. Hardness of 10.13GPa, 7.68GPa and 6.47GPa were obtained for the 10Å, 15Å and 20Å indenters respectively. This is consistent with the literature that significant increase in hardness was observed with reduced indenter size.

However, the second load drop does not obey the same rule as found for the first load drop. The loads to initiate the second load drop are 13.66N/m, 9.95N/m and 16.97N/m for the 10Å, 15Å and 20Å wide indenters respectively. No monotonicity is observed here.

4 Conclusions

Quasicontinuum simulations of nano-indentation into the (111) face of one grain in nanocrystalline aluminum thin film were performed. The different nanoindentation response of polycrystalline and single crystalline aluminum was studied. And the effect of indenter width on nanoindentation response was observed through three simulations with different indenter sizes. The major conclusions of this work can be summarized as follows:

(1) At the same indentation depth, the force needed to hold the indenter is smaller for the polycrystal as compared to the single crystal.

(2) Two load drops were observed on the nanoindentation response curve for nanocrystalline aluminum thin film.

(3) As the first load occurs, both mechanical twinning and stacking fault were found.

(4) The second load drop is attributed to the twin-stacking fault interaction.
The first load drop is sensitive to the indenter size. A rule is found out that, as the indenter becomes wider, larger indentation depth and larger load is required to initiate the first load drop. A smaller hardness was observed with the wider indenter. However, the second load drop does not follow the same rule.

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