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Atomistic simulation of size effects in single-crystalline metals of confined volumes during nanoindentation

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ABSTRACT

In single-crystalline metals, the sources of size effects depend on the sample length scale. In bulk samples, the interaction of dislocations with each other is responsible for size effects which is commonly termed forest hardening. The Taylor-like hardening models are usually incorporated to capture the forest hardening which states that the strength increases as the dislocation density increases. As an example, the fact that the nanoindentation hardness increases as the indentation depth decreases is justified as an increase in the density of geometrically necessary dislocations. In the cases of small length scales, several experiments on whiskers, wires, and micropillars have demonstrated that the sources of size effects are different from those of bulk material. In the case of nanoindentation of nanoscale samples, it has been experimentally shown that the hardness decreases as the density of geometrically necessary dislocations increases in the region of small indentation depths. It shows that the size effects theory of bulk material cannot be extended to the indentation of nanoscale samples. The present work incorporates the large scale atomistic simulation to investigate the size effects in a nanoscale single crystal Ni thin film during indentation. The results show that the hardness decreases as the dislocation density increases, and the forest hardening model cannot capture the strength size effects during nanoindentation at small length scales. It is observed that the size effects are initially controlled by dislocation nucleation and source exhaustion. As the indentation depth increases, the dislocation length and density increase. Consequently, the number of dislocation sources and their characteristic length increase which decreases the material strength. Finally, increasing the dislocation length and density, the dislocation interaction mechanism also becomes important.

1. Introduction

In bulk metallic systems, size effects are governed by the interaction of dislocations with each other, which is commonly termed forest hardening [1–4]. Taylor-like hardening models are commonly incorporated to capture the forest hardening. As an example, the effects of strain gradient on material strength are modeled using the relation between the dislocation density and strength which is commonly described by the Taylor hardening models [1–3]. There are various types of forest hardening models. However, the models generally state that the strength increases as the dislocation density increases [1–3]. In the cases of nanosize samples, however, several experiments have shown that the sources of size effects are different from those of bulk samples (see e.g. Kraft et al. [5]). Kraft et al. [5], Greer and De Hosson [6], and Greer [4] have reviewed different types of size effects models in metallic samples of confined volumes. Three models of source exhaustion hardening, source truncation, and weakest link theory are usually incorporated to describe these size effects [4]. In the region of small length scales, the samples may lose the dislocation sources due to the source shut down, mechanical annealing, or dislocation starvation [7–9]. Consequently, the reduced mobile dislocation density is insufficient and the applied stress should be increased to sustain the plastic deformation which is termed exhaustion hardening [10,11]. Source truncation occurs when the existing double-ended dislocation sources change into the single-ended ones. Consequently, a new characteristic length of dislocation sources is introduced which increases the strength [12,13]. Cui et al. [14] recently studied the role of single arm sources in microstructural behavior of micropillars using dislocation dynamics. The weakest link theory states that reducing the sample size, the strength of the weakest slip plane present increases which increases the material strength at smaller length scales [15,16].

In recent years, new experimental techniques have been developed to measure the density of geometrically necessary

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dislocations (GNDs) [17–21]. The experimental methods are developed based on the relation between GND density and spatial gradients of plastic slip [22–24]. The experiments have shown new phenomena in metallic samples which cannot be explained using the theories developed for bulk-size material. Demir and his coworkers [20,25] showed that the sources of size effects at small length scales are different from those of the bulk materials during nanoindentation and microbending of metallic samples. Demir et al. [20] conducted nanoindentation of Cu single crystal and measured the GND densities at various indentation depths. It was observed that as the indentation depth decreases the hardness increases [20]. According to the forest hardening models, the GND density should increase [1–3]. However, the results showed that the GND density decreases as the indentation depth decreases [20]. It implies that the hardness decreases as the GND density increases. Moreover, only GNDs were measured during the experiments and not all the dislocation content which includes both GNDs and SSDs (statistically stored dislocations) [20]. Hence, it may have affected the final conclusion. Demir et al. [25] also investigated the size effects in microbending experiment on the Cu single crystal. Again, the results showed that the mean-field behavior of the dislocations breaks down at small length scales [25].

Nowadays, using very powerful supercomputers and efficient and massively parallel codes, the samples in the order of 0.1 μm can be simulated using Molecular dynamics (MD) [26]. To study the relation between the dislocation density and hardness using molecular dynamics, the dislocation information should be extracted from the MD outputs. Various methods of defect visualization have been developed including energy filtering, centrosymmetry parameter analysis, bond order analysis, Voronoi analysis, adaptive common neighbor analysis, and neighbor distance analysis (see Stukowski [27]). Stukowski [27] implemented these methods and compared the obtained results. Stukowski and his co-workers [27–30] developed the Crystal Analysis Tool to obtain the dislocation length and Burgers vector from atomistic simulation outputs. Hua and Hartmaier [31] proposed a method to quantify the Burgers vectors of dislocations from MD results. They calculated densities of GNDs and SSDs using the developed methodology. Begau et al. [32] simulated the nanoindentation of a copper single crystal indented by a spherical indenter using MD. They qualitatively studied the dislocation density variation as the indentation depth increases. However, they did not compare the results to any theoretical models or experiments. Gao et al. [33] tried to compare the dislocation length obtained by atomistic simulation of nanoindentation with that of the theoretical models. However, the dislocation length obtained from MD simulation cannot satisfactorily capture the theoretical models for dislocation length. Recently, Gao et al. [34] studied the plastic zone size of single crystal metals indented by spherical indenter during MD simulation. Voyiadjis and Yaghoobi [26] studied the relation between the dislocation density and hardness during nanoindentation of metallic samples. However, none of the previous works have studied the sources of size effects in the studied cases.

In the current study, the size effects in nanoscale thin films are studied during indentation using large scale atomistic simulation. A Ni single crystal thin film is indented using a conical indenter with a spherical tip. First, a geometric model is derived to predict the GNDs length and density during nanoindentation with a spherical tip. The precise geometry of the indenter is incorporated in the developed model. The obtained results are then compared with the predictions available in the literature. The dislocation length calculated from the theoretical predictions is then compared to the one obtained from MD simulation during nanoindentation. Next, the dislocation density is obtained for various plastic zone sizes using MD. The final step is to investigate the size effects sources using the microstructural information obtained from MD simulation.

2. Simulation details and methodology

To investigate the sources of size effects during nanoindentation, a Ni thin film is simulated using the classical molecular dynamics. The sample dimensions are 120 nm, 120 nm, and 60 nm along $[1\,\bar{1}\,0]$, $[1\,1\,\bar{2}]$, and $[1\,1\,1]$ directions, respectively, which consists of 79,473,309 atoms. A part of the generated sample is represented in Fig. 1. The indenter geometry is selected according to the nanoindentation experiment performed by Demir et al. [20] which is a conical indenter with an angle of $\theta = 60^\circ$ and a spherical tip with the radius of $R = 10$ nm (Fig. 2). Along $[1\,\bar{1}\,0]$ and $[1\,1\,\bar{2}]$ directions, the boundary conditions are set periodic. At the sample bottom, the boundary conditions are free. The required force is applied at each step to all atoms to inhibit the translational movement which is described in detail in [26,35–37]. The parallel MD code LAMMPS is used to perform the simulations [38]. The time step of 2 fs is chosen and the integration algorithm is velocity Verlet. The sample is relaxed for 200 ps prior to the indentation process [26,37]. The relaxed sample is indented with a velocity of 10 m/s along the $[1\,1\,1]$ direction at 300 K. The velocity has been widely used in previous works [26,33,34,37,39,40]. The NPT ensemble is used to simulate the nanoindentation [38]. The EAM interatomic potential E^{EAM} is selected to model the Ni–Ni atomic interaction which is defined as follows

$$E^{\mathrm{EAM}}(r_{ij}) = \frac{1}{2}\sum_{i,j} V(r_{ij}) + \sum_i F(\rho_i), \quad \rho_i = \sum_{i\neq j} \varphi(r_{ij}) \tag{1}$$

where $V(r_{ij})$ and $F(\rho_i)$ represent the pair interaction and embedding potentials, respectively, and $\varphi(r_{ij})$ is a function of the electron density [26,37]. The EAM potential developed by Mishin et al. [41] is used to model the Ni–Ni atomic interaction [42].

The interaction between the indenter and Ni atoms is described as follows [38]:

$$E^{\mathrm{ind}}(r) = \varepsilon(r - r_c)^2 \quad r < r_c \tag{2}$$

where ε, r, and r_c are the specified force constant, distance from particle to the indenter surface, and cutoff distance, respectively. The parameters ε and r_c are chosen as 1 eV/Å^2 and 0.3 nm, respectively. The triangulation method is incorporated to calculate the contact area A which is described in detail in [26,37]. The true indentation depth (h) of a spherical tip, which is slightly different from the tip displacement (d), is calculated using the obtained contact area [37]:

$$h = R - \sqrt{R^2 - a_c^2} \tag{3}$$

where $a_c = \sqrt{A/\pi}$ and R is the radius of the tip (Fig. 3). In the case of the conical part of the indenter, h can be obtained as follows:

$$h = \frac{(a_c - a_0)}{\tan(\theta/2)} + h_0 \tag{4}$$

where h_0 is the indentation depth at which the transition occurs in the indenter geometry from the spherical tip to the conical shape and a_0 is the contact radius at h_0 (Fig. 3). In order to study the effects of temperature, rate of indentation, and selected boundary conditions, a molecular static study, i.e. zero temperature and static indentation, is presented in Appendix A in which the sample is placed on the Si substrate. The Crystal Analysis Tool is used to extract the dislocation information from MD outputs [27–30]. The dislocations are visualized and processed using the software OVITO [43] and Paraview [44].