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Strengthening effects of coherent interfaces in nanoscale metallic bilayers

Sergey N. Medyanik *, Shuai Shao

School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164, United States

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ABSTRACT

Dislocation nucleation and propagation in a Cu–Ni bilayer with coherent (1 1 1) interface are examined using atomistic simulations. Nanoindentation model is applied to generate dislocations at and near the surface. Mechanisms of interactions between gliding dislocations and coherent interface are investigated. It is found that the interface acts as a strong barrier to dislocation propagation, which results in considerable strengthening of the bilayer. The results are compared to indentation of pure Cu and pure Ni single crystals. It is found that the obtained maximum load for indentation of the Cu–Ni bilayer is higher than for any of the two pure materials. Strain hardening of the bilayer system due to the presence of interface is investigated by analyzing the indentation load–displacement curves.

1. Introduction

The mechanics of deformation at the nanoscale differs significantly from what is typically observed on the macroscale. At such a small scale, due to increased surface-to-volume ratios presence of surfaces and interfaces becomes especially important. As a result, when the layer thickness reduces to the nanometer scale, multilayered materials often exhibit unique mechanical properties, such as ultra-high strength [1–3]. Thus, nanoscale multilayered metallic materials exhibit strength levels up to one half of their estimated theoretical strength [3,4], which is significantly higher than the strength of the individual materials that compose the structure. Commonly, this strengthening has been attributed to the presence of interfaces between dissimilar materials that have a mismatch in various properties, such as elastic modulus, lattice parameter, dislocation core energy, and slip plane orientations [5–9].

Depending on the materials comprising metallic multilayers, interfaces in these systems may be generally classified into three major categories. Coherent interfaces form when the two metals at the interface have the same type of lattice structure, e.g., both face-centered cubic (FCC), and the difference in the lattice parameter is relatively small (on the order of a few percent). Semi-coherent interfaces occur when the type of the lattice is the same, but the mismatch in the lattice parameter is larger. In this case, networks of misfit dislocations form at the interface to accommodate the mismatch. Finally, incoherent (also called weak) interfaces form between materials with different lattice structures, such as, e.g., FCC and BCC (body-centered cubic). It has to be noted that in most systems comprised of materials with the same lattice structure (e.g., FCC–FCC) and a small mismatch in the lattice parameter, both coherent and semi-coherent interfaces may form. In this case, the occurrence of a particular type of interface strongly depends on the thickness of the individual layers comprising the multilayered structure. Loss of coherency occurs when individual layer thickness exceeds some critical value; this phenomenon has been theoretically analyzed by Hirth and Feng [10]. Generally, the mechanical properties of nanoscale metallic multilayers strongly depend on the type of interfaces between the layers comprising the system.

The mechanical properties of nanoscale metallic multilayers also strongly depend on the individual layer thickness. However, this dependence is not completely understood yet. A Hall–Petch

* Corresponding author. Tel.: +1 509 335 7386.
E-mail address: medyanik@wsu.edu (S.N. Medyanik).

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effect [11,12], which is based on the dislocation pile-up mechanisms, is considered to be the main contributor to the strengthening of nanoscale crystalline materials. However, the Hall–Petch model breaks down when individual layer thickness in multilayered systems drops below several tens of nanometers. In that case the strength still continues to increase before it reaches a plateau and then drops in most cases as the layer thickness reduces to one or two nanometers [8,9]. A major role in strengthening of the nanoscale metallic multilayers when the layer thickness is on the order of just several nanometers is attributed to the mechanisms of interactions of *single* dislocations with interfaces.

Atomistic simulations using empirical inter-atomic potentials have been applied to study discrete dislocations and their interaction with grain boundaries and interfaces for a number of pure metallic materials as well as composites. Thus, Hoagland and coworkers have studied coherent (Cu–Ni), semi-coherent (Cu–Ni, Cu–Ag), and incoherent (Cu–Nb) interfaces [6,7]. That work was focused on interactions of single dislocations with interfaces under a tensile (essentially 2d) strain loading conditions and for Cu–Ni systems only cube-on-cube multilayers with {1 0 0} FCC interface planes were considered. Spearot et al. [13,14] and Capolungo et al. [15] investigated tensile deformation and dislocation nucleation from bi-crystal interfaces in copper and aluminum. These studies focused on the interfaces and grain boundaries in bi-crystals comprised of the same material; no interfaces between dissimilar materials have been considered. Recently, Saraev and Miller have studied nanoindentation of copper multilayers [16] as well as copper crystals with nanometer-sized nickel coatings [17]. In the latter work, they considered a bi-crystal with semi-coherent Cu–Ni {1 1 1} interface. In that case, the mechanics of plastic deformation during indentation was dominated by the misfit dislocation networks and strongly depended on the initial position of the indenter with respect to the misfits.

In this work, we study nanoindentation of a Cu–Ni bilayer with a coherent (1 1 1) interface and focus on the effects of the interface on dislocation propagation. To our knowledge, this is the first such study for a fully coherent FCC (1 1 1) interface. It is especially important to model this type of interface because recently manufactured Cu- and Ni-based nanoscale multilayered composites often have layer thicknesses on the order of just a few nanometers when coherent interfaces are more likely to form. We employ nanoindentation model in order to repeatedly generate dislocations at and near the surface and observe their evolution into the bilayer's volume. This approach allows to investigate mechanisms of dislocation–interface interaction under more realistic 3d loading conditions. In addition, the obtained load–displacement curves help to explore the overall strain-hardening behavior and quantify the strengthening effects of interfaces.

2. Computational details

In this work, we perform molecular mechanics simulations using the embedded-atom method (EAM) [18,19] to model interatomic interactions. In the EAM, the total energy of a system of atoms is given as

$$E_{tot} = \sum_i F_i(\rho_i) + \frac{1}{2}\sum_{\substack{ij \\ i\neq j}} \phi_{ij}(R_{ij}), \tag{1}$$

where F_i is the embedding energy which is a function of the atomic electron density ρ_i at atom site i, ϕ_{ij} is a pair potential interaction, and R_i is a distance between atoms i and j. The particular form of the EAM potential utilized in this work is of the type given by Voter and Chen [20,21]. This potential has been previously used for modeling Cu–Ni systems by Hoagland et al. [6], who obtained some physical properties associated with this potential including stacking fault energies (SFEs) for Cu, Ni and interfacial energies for interfaces in Cu–Ni bi-crystals. Previously, the accuracy of this potential for modeling SFEs in Cu and Ni has been tested by Zimmerman et al. [22], who have recommended this potential for use in simulations for both Cu and Ni.

The molecular mechanics simulations employ conjugate gradient procedure for energy minimization and are performed using parallel atomistic simulation program LAMMPS [23,24]. The minimization process is considered to be converged if either the change in energy between two consecutive iterations or the length of the global force vector is smaller than 10^{-14} (whichever occurs first).

In order to study lattice defects in general and dislocation nucleation and propagation in particular we need to reliably locate those defects within the crystal structure. Several different approaches have been commonly used for this purpose based on different criteria, such as, e.g., atomic excess energy or coordination number. In this work, we employ a centro-symmetry parameter, P, introduced by Kelchner et al. [25]. In a perfect FCC crystal, each atom has twelve nearest neighbors. These neighbors can be divided into six pairs that have the opposite positions relative to the given atom. Based on this, the centro-symmetry parameter for a given atom is defined as follows:

$$P = \sum_{i=1,6} |\mathbf{R_i} + \mathbf{R_{i+6}}|^2, \tag{2}$$

where $\mathbf{R_i}$ and $\mathbf{R_{i+6}}$ are the vectors that corresponds to the pairs of the opposite nearest neighbors. A centro-symmetric material, such as FCC metal, tends to preserve its centro-symmetry under homogeneous elastic deformation. Thus, if the material deformation is nearly homogeneous, the value of P is close to zero. However, if the material has defects present where its centro-symmetry is destroyed, P will no longer be zero for the atoms comprising the defects. Instead, the parameter will have a value within the range that corresponds to a particular defect. Thus, values of the centro-symmetry parameter for atoms comprising partial dislocation loops and stacking faults are about 1.6 and 6.4 correspondingly.

The simulated Cu–Ni bilayer is shown in Fig. 1. The dimensions of the modeled atomistic domain are $172 \times 60 \times 172$ Å. The interface between the two materials is parallel to x–z plane. The crystallographic orientation at the interface is the same for both metals – (1 1 1) FCC plane. Fixed boundary conditions are applied in the lateral (x and z) directions while free boundary conditions are used for the top and bottom sides of the domain. A nearly rigid spherical indenter with radius 40 Å modeled using quadratic repulsive force is applied to the center of the top surface. At each

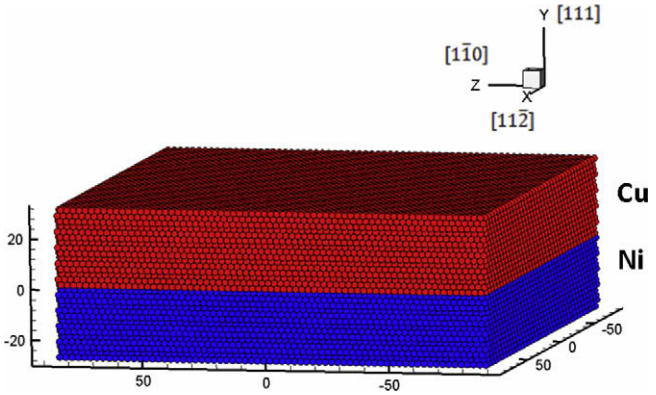

Fig. 1. Initial configuration for a Cu–Ni bilayer. Top layer (red) is copper, bottom layer (blue) is nickel. The interface is FCC (1 1 1) plane for both materials. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)