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Molecular dynamics simulation of uniaxial deformation of thin Cu film and Al-Cu heterostructure

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The paper discusses the effect of free surfaces and interfaces on mechanical characteristics of a thin Cu film and an Al–Cu film heterostructure. It is shown that the interface of the cyclically deformed Al–Cu heterostructure evolves from a chessboard distribution with a period dependent on the degree of inconsistency of the material lattice constants to a new more energy-beneficial distribution of hillocks and dimples with spatial scales dependent on the film thickness and specimen dimensions.

Keywords: molecular dynamics, thin films, deformation, uniaxial tension, cyclic loading, interface

1. Introduction

Physical mesomechanics of thin films treats of free boundaries and internal interfaces as important functional subsystems [1]. A series of recent research conducted by Academician V.E. Panin with colleagues [2, 3] points to an interesting phenomenon — structural self-organization of internal interfaces of heterogeneous media in external effective fields. The extremely small spatial scales and thickness of near-surface and interface layers can not allow any longer a complete description of the entire spectrum of observed physical phenomena by continual models. In this context, the use of molecular dynamics simulation, which explicitly accounts for discreteness of a medium, to describe mechanical behavior of similar systems is thus made urgent. In the work, uniaxial deformation of a thin Cu film and a heterostructure formed by interfacing Al and Cu films was simulated. The Cu film was studied for the effect of its structural state and state of its free surface on the stress–strain diagram. The Al–Cu heterostructure was studied for the evolution of its interface under cyclic loading.

2. Molecular dynamics simulation

The interaction of Cu and Al atoms was described by the interatomic interaction potential calculated in the framework of the embedded atom method [4–6]. This many-body potential has been proven efficient in simulation of deformation of metal clusters and heterostructures [7–10]. The particle trajectories were calculated by the LAMMPS parallel molecular dynamic program package [11]. Quasistatic uniaxial tension and compression of the composition was simulated by periodic scaling of the computational cell size in a specified direction with relaxation of the system at intervals between scaling events. In this specified direction, periodic boundary conditions were applied to the system. The rate of increase of the computation cell size was 10 m/s, which is much lower than the velocity of sound in copper and aluminum and corresponds to quasistatic deformation. For numerical integration of equations of atomic motion, the velocity Verlet algorithm was used. For detection of lattice defects, the central symmetry parameter was calculated as follows:

$$P = \sum_{i=1}^{6} \left| \mathbf{R}_i + \mathbf{R}_{i+6} \right|^2,$$

where summation is over the nearest neighbors of a given atom, and $\mathbf{R}_i$ and $\mathbf{R}_{i+6}$ are the radius vectors of the opposite neighbors [12]. The central symmetry parameter P is close to zero for atoms with local coordination of the fcc lattice and markedly increases for surface atoms and with the incipience of a stacking fault.

3. Copper film

3.1. Simulation of the thin Cu film

The single-crystal Cu film was modeled by a parallelepiped ($36 \times 36 \times 18$ nm) containing about two millions of atoms with periodic boundary conditions specified in the

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directions *X* and *Y* parallel to the free surface. The crystallographic orientation of atoms in the parallelepiped was chosen such that the directions [100], [010] and [001] coincided with the coordinate axes. The initial temperature of the Cu film after relaxation was 300 K.

The surface of real materials has a roughness of different scale levels. In this context, it is of interest to analyze the effect of surface roughness on the loading diagram of a thin film whose surface is not perfectly smooth. The surface roughness was modeled by the Fourier filtration method [13, 14] with which the free surface profile of the crystallite was formed. Relaxation of the atomic system at a temperature of 300 K resulted in a thin film whose surface was self-affine on length scales from the lattice constant a = = 0.36 nm to the computation cell size $L_{\max}$ = 36 nm and was of fractal dimension 2.3 and roughness 2.5 nm.

The formation of a polycrystalline film was modeled by quenching from 1 500 K (the molten state) to 300 K (the quenching rate was $1.2 \cdot 10^{13}$ K/s) with subsequent relaxation at 300 K for 40 ns. The relaxation was realized using the Nosé–Hoover thermostat [15]. After 40-ns relaxation at a temperature of 300 K, the film energy continued to decrease slowly. For suppression of the relaxation and grain growth, the system was cooled to a temperature of 200 K, and thereafter its total energy became constant in several nanoseconds. Analysis of the radial distribution function shows that during the relaxation a long-range order in the relative position of film atoms is established [10]. The lattice structure is characterized by the abundance of point and plane defects; the characteristic grain size is about 2 nm. The thickness of the Cu film was 9 nm and its lateral dimension was 18 nm. Periodic boundary conditions were specified in both transverse directions.

3.2. Uniaxial tension of the thin Cu film

Uniaxial tension of the specimen without regard for the effect of grips is characterized by the stress distribution over the entire specimen. The result of this is a rather high (~10 %) elastic limit of the stretched single-crystal Cu film with ideal free surfaces (Fig. 1). The nucleation of an initial stacking fault whose development results in plastic deformation of the film is severely hampered due to the high potential barrier that the atomic system must overcome. Once the first defect arises, the initial symmetry of the system is broken and the stress in the specimen decreases three times. Rendering roughness to one of the free surfaces of the film causes plastic deformation to commence much earlier at ε = 0.05 (Fig. 1). This is indicative of a considerable decrease in potential barrier for a stacking fault to arise near surface irregularities. Once the elastic limit is overcome, plastic deformation proceeds through the development of a system of lattice defects shown in Fig. 2. The further decrease in potential barrier for the transition to plastic deformation was attained by passing to deformation of polycrystalline film with a grain size of ~2 nm. The elastic portion of the σ– ε diagram for the polycrystalline film (ε < <1.5 %) is near the same as the straight elastic portion obtained for the single-crystal film (Fig. 1), and this owes to sufficient isotropy of the elastic properties of copper. A maximum stress of 1.4 GPa is reached, in this case, even at a strain of 2 %, which is a very high yield strength for copper. For comparison the experimental yield strength found for nanocrystalline copper with a grain size of 50 nm is 0.38 GPa [16]. It is obvious that the so high yield strength obtained in calculations is due to the very small grain size.

4. Aluminum–copper heterostructure

4.1. Formation of the Al–Cu heterostructure

An internal interface as an additional subsystem between heterogeneous materials was introduced into consideration by adjoining two single crystals of copper and aluminum with lattice constants $a_{\mathrm{Cu}} = 0.3616$ nm and $a_{\mathrm{Al}} =$ = 0.404992 nm along crystalline planes [100]; thereafter the system relaxed at a constant temperature of 50 K until thermodynamic equilibrium was attained. The Al and Cu crystallites were of dimensions $50\times50\times13\,a_{\mathrm{Al}}$ and $56\times56\times14\,a_{\mathrm{Cu}}$, respectively. Periodic boundary conditions

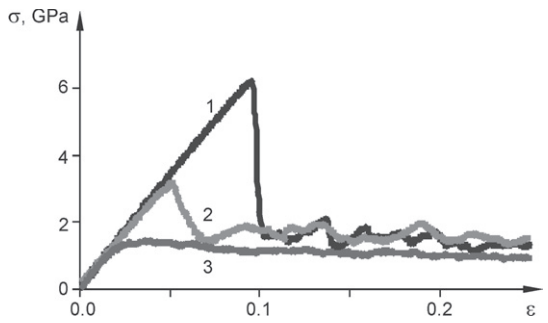

Fig. 1. Stress–strain diagrams of the single-crystal film with ideal free surfaces (*1*), crystallite with a free surface of roughness 2.5 nm and fractal dimension $D_{\mathrm{f}} = 2.3$ (*2*), and polycrystalline film (*3*)

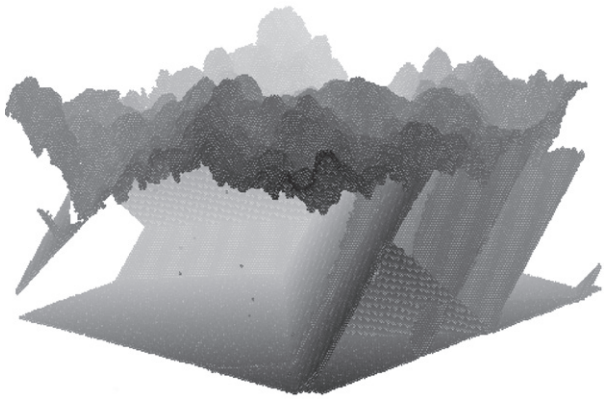

Fig. 2. Deformed crystallite with a free surface of roughness of 2.5 nm and fractal dimension $D_{\mathrm{f}} = 2.3$. Shown in the figure are only atoms with local coordination distinct from the fcc lattice