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Dependence of deformation mechanisms on layer spacing in multilayered Ti/Al composite

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ABSTRACT

Molecular dynamics simulations are performed to investigate the effects of layer spacing and temperature on the deformation mechanism of Ti(0001)/Al(111) multilayered composite. The results indicate that the interface rotation driven by local stress concentration dominates the plastic deformation in the sample with smaller layer thickness at both 0.01 K and 300 K. The confined layer slip of dislocations in Al layer is observed, while basal/prismatic interface formation and the transformation of hcp-Ti to fcc-Ti are presented in Ti layer in the samples with larger thickness at 0.01 K. The results also show that the confined layer slip of dislocations and necking in Al layer is the underlying deformation mechanism in the samples with larger layer thickness at 300 K. We have also presented an in-depth discussion of relative deformation mechanisms in this work.

1. Introduction

The incorporation of interface into the crystalline lattice is an effective approach to enhance the metal's properties without changing their chemical composition. Several kinds of interface, such as twin boundary [1–4], low-angle grain boundary [5,6], stacking fault boundary [7,8] and interphase boundary [9–11] have been taken into consideration. As a representative interface, interphase boundaries, in which the interfaces separating two crystals differing in composition, lattice structure or both, are common in multilayered composite. They are generally divided into coherent, semi-coherent and incoherent interface depending on atomic matching degree across the interface. The mechanical behaviour of multilayered composite is affected not only by the atomic coherence degree of the interface, but also by the thickness of the constituent element.

A number of research has been performed on the mechanical behaviour of multilayered composites consisting of face-centered cubic (fcc) and body-centered cubic (bcc), such as Cu/Ni (fcc/fcc) [12–14], Cu/Ag (fcc/fcc) [15], Ag/Ni (fcc/fcc) [16], Cu/Nb (fcc/bcc) [17–20], Cu/Cr (fcc/bcc) [21,22], Al/Nb (fcc/bcc) [23,24], and Cu/V (fcc/bcc) et al. [24] both in experiments and simulations [21–39]. Liu et al. [13] studied the mechanical properties of highly (111) and (100) textured Cu/Ni multilayers experimentally. They pointed out that the hardness of multilayer films increases with decreasing individual layer thickness h_M, and a softening is shown when hardness approaches a maximum at h_M of a few nanometers. In (111) textured Cu/Ni multilayers, nanotwins significantly enhance the mechanical strength and delay the onset of softening. In the simulation, misfit dislocations networks are observed in Cu(001)/Ni(001) interface boundaries due to the mismatch of atomic lattice, which has a significant effect on the interface strength of the Cu/Ni system [31]. McKeown et al. [15] reported that Cu/Ag multilayers have lower peak hardness than Cu/Ni in spite of lower misfit dislocation spacing that is expected to increase the resistance of interfaces to glide dislocation transmission. The reason may be the misfit dislocation core spreading in the interface plane in Cu/Ag. Yuan and Wu [35] simulated the tensile deformation behaviour of Cu/Ag multilayer nanowires (NWs) with interface perpendicular to and parallel with wire axis. In the first structure, the deformation mechanism is changed from interface crossing by dislocations to interface rotation as the layer thickness is decreasing. While for the second structure, the larger total tensile elongation for larger layer thickness could be related to the twinning induced plasticity at the necking position. Ma and his coworkers [33,34] found the interface-induced pseudoelastic behaviour and spontaneous reorientation in multilayer Au-Pd NWs. Misra and his colleagues proposed the Hall-Petch law and confined layer slip model in Cu/Nb multilayers composites and they found that interface stress and interface dislocation arrays on the confined layer slip stress are incorporated in the model to correctly predict the strength increase with decreasing layer thickness [17,18,21]. Meanwhile, Misra's team had performed a number of simulations to investigate the interface properties of Cu/Nb multilayered composites [37–39]. They pointed out that the

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incoherent Cu/Nb interfaces have relatively low shear strength and are referred to as "weak" interfaces. Such interfaces are very strong traps for glide dislocations and, effective barriers for slip transmission. The preferred nucleation sites in the incoherent fcc/bcc interface are not always associated with pre-existing misfit dislocations, and the preferred slip systems are not determined solely by the Schmid factor. Amongst the two or more systems that may be geometrically favored, the activated slip system depends on the structure of the nucleation site.

In conclusion, three different regions of hardness/strength, corresponding to three different deformation mechanisms, are observed with the decrease of individual layer thickness h_M (one half of the modulation period λ) with constant modulation ratio ~1 [25–30]. The first region is the Hall-Petch behaviour. When h_M is at the submicrometer to micro length scales, the yield strength increases with decreasingh_M, following $\sigma \sim h_M^{-0.5}$. The Hall-Petch plays a dominant role due to the pile up of dislocations against the interface [9,25]. The second region is the confined layer slip (CLS) model. As h_M decreases to a few tens of nanometers, the spacing of adjacent layers is too small for the insufficient dislocations to pile up. The Hall-Petch law is invalid. Then single dislocations will glide confined within the layers, which accounts for the slower increase rate of strength with decreasing h_M[22,26]. The third region is the interface barrier strength (IBS) mechanism. When h_M comes to a few nanometer length scales, the dislocation will transmit across the layer interface, and a plateau or softening of hardness/strength is exhibited [27,28]. However, the investigations are mainly focused on fcc and bcc structures. The relative studies on hexagonal close-packed (hcp) metals, such as Ti, Mg, and Zr, still are very rare, despite their industrial importance. Compared with fcc metals, there are limited slip systems for dislocation glide, but profuse twinning systems in hcp metal. Mechanical properties of hcp multilayered composites are not well consist with these three deformation mechanisms [30,40,41]. Therefore, understanding the deformation behaviour in hcp metals becomes extremely crucial. As a typical metal with hcp structure, titanium has attracted increasing interest due to its extensive application and superior mechanical properties [42–46]. However, the deformation behaviour in nanocrystalline Ti with multilayered interfaces is still not well understood so far.

Nowadays, various microstructural characterization techniques (X-ray diffraction, transmission electron microscopy, high resolution transmission electron microscopy, scanning electron microscopy) have been used to investigate the microstructure and mechanical properties of multilayered composites [29,30]. However, systematic investigation of deformation mechanisms of materials using experimental method is still challenging. As an alternative to experiments, molecular dynamics (MD) simulations can serve an important role in understanding the deformation mechanism in multilayered composites [35,36,38,39]. MD simulations have several advantages over experimental investigations and are an invaluable tool for describing the mechanical behaviour and detailed deformation process of materials, especially when experimental observation of nanoscale deformation behaviour is difficult. In this regard, MD has been used to investigate the deformation mechanism of sub-10 nm Ti(0001)/Al(111) multilayered composite at 0.01 K and 300 K in present study. The results indicate that the deformation mechanism is strongly dependent on the individual layer thickness h_M and temperature. The results obtained in our work fill the gap for the three different deformation mechanisms versus layer thickness obtained mainly in fcc/bcc multilayered composites. The general conclusions derived from this work may provide a guideline for the design of high-performance Ti multilayer devices.

2. Simulation model and method

Here, MD simulations are performed to study the deformation mechanism of Ti/Al multilayered composites under tension loading. Schematic of the Ti/Al multilayered composite is shown in Fig. 1, in

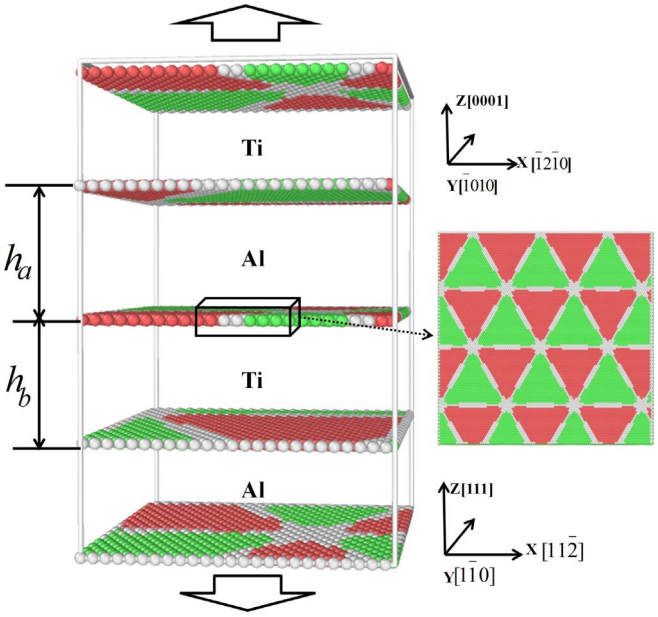

Fig. 1. Schematic of the Ti/Al multilayered composites under tension loading.

which the individual layer thicknesses of Al and Ti are h_a and h_b, respectively. h_a and h_b in the samples are space equaled, resulting in the modulation ratio $h_a/h_b = 1$. The dimensions of the samples in X- and Y- are 7.08 and 7.15 nm. The dimension in Z-increases from 1.41 to 11.23 nm, depending on the thickness of individual layer. The number of the atoms in the simulation ranges from 16,464 to 131,712. Periodic boundary condition is applied in the Z- direction, while X- and Y- are free. In the structure, Al and Ti are all the most close-packed. The stacking sequence of the atomic plane in Al is ABCABC....., while ABABAB..... in Ti. These two structures are usually observed in Ti/Al multilayer films prepared by magnetron sputtering. Mismatch dislocation network is observed in the blow-up section in Fig. 1, owing to the mismatch of atomic lattice in the interface of the Ti and Al. The mismatch degree between Ti and Al is defined as $\delta = (a_{Ti} - a_{Al})/a_{Ti}$, where a_{Ti}, a_{Al} are lattice distances (the distance between neighbouring atoms in the lattice) of Ti and Al, respectively. δ is about 0.03 in Ti(0001)/Al(111) interface, which means the coherent boundary is formed in Ti(0001)/Al(111) interface. (When $0.05 \le \delta \le 0.25$, semi-coherent boundary is formed; $\delta < 0.05$, coherent boundary; $\delta > 0.25$, incoherent boundary).

The EAM potential used here is developed by Wadley and Zhou [47], which describes Ti-Ti, Al-Al and Ti-Al interatomic interaction in the simulation models. All the simulations are performed using the Verlet integration algorithm in a constant time step of 2 fs. The structure is initially equilibrium for 24 ps in NVT ensemble, 30 ps in NPT ensemble to obtain the energetic minimum state before tensile loading. Tensile loading is applied by uniformly adjusting the Z-coordinate of each atom at a constant strain of 0.001. Then the system is relaxed for 1000 time steps to reach a new equilibrium state and a new configuration. All the structure analysis and visualization of atomic configurations are implemented by using the Open Visualization Tool (OVITO) [48]. And the microstructure of the Ti/Al multilayered composite are identified based on common neighbor analysis (CNA) [49], in which the hcp atoms, fcc atoms, bcc atoms and non-structure atoms are colored red, green, blue and white, respectively. Virial theorem [50] is used to calculate the average stress in current study, which is expressed by:

$$\sigma^{\alpha\beta} = \frac{1}{\Omega}\left[-\sum_i m_i v_i^{\alpha} v_i^{\beta} + \frac{1}{2}\sum_i \sum_{j \neq i} F_{ij}^{\alpha} r_{ij}^{\beta}\right] \quad (1)$$