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Atomistic simulation study on the shear behavior of Ag/MgO interface

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ABSTRACT

Metal-oxide composites with advanced mechanical properties play an important role in many practical applications, and failure of the metal-oxide interface is directly related to service life of related structures. In order to understand interface failure mechanism, study on atomic-scale separation of metal-oxide interface is significant. In this work, shear behaviors of Ag/MgO (0 0 1) coherent interface and semi-coherent interfaces are studied by employing molecular mechanics method, and some interesting size and defect effects are found. The simulation results show that interface shear stress and displacement appear periodic characteristics with loading. For coherent interface, the interface shear stress and displacement both increase first in each period, then the shear stress drops abruptly after reaching ideal shear strength, and the shear displacement jumps by a unit cell length. The shear strength keeps a constant for all periods. Atomistic simulations of interface systems with different thicknesses show size-independent shear strength and intrinsic interface adhesive energy, but needed loading displacement for the first jump of interface displacement is larger for the thicker systems due to the larger energy consumed by bulk materials. For both 1D and 2D semi-coherent interfaces with dislocations, the shear strength is more than one order of magnitude lower than the ideal shear strength, and the interface displacement changes more continuously with decreased period, which is attributed to different shear mechanism related to dislocation gliding. Comparing 2D semi-coherent interface with 1D case, the shear strength and energy barrier of dislocation motion are both higher due to pinning effect of dislocation intersections.

1. Introduction

In many technological applications, such as thermal barrier coatings (TBCs), catalysts, and composite materials, the mechanical properties of metal/oxide interfaces affect the functionality of the systems [1–4]. In general, interface fracture or slipping under complex loading conditions is the important origin of macroscopic failure. A prominent example is in TBCs, when the residual or loading stress exceeds the critical value, interface crack initiates and crack propagation will eventually lead to the delamination between ceramic top coat and metallic bond layer, which is closely related to micro-scale separation mechanism of the interface. Therefore, it is significant to investigate the failure mechanism of metal/oxide interface at atomistic scale.

Compared with interface tensile fracture, interface shear slipping is more complicated considering the effect of loading condition, interface structure and deformation of the constituent bulk materials. A great deal of experimental [5,6] and theoretical studies [7–9] on the shear behavior of nanoscale metal/ceramic interface systems have been carried out. Through shear and normal compression experiments on CrN/metal-interlayer/Si systems, Zhang et al. revealed that the metal/ceramic chemical interface served to weaken the metal layers near the interface mechanically [5]. Guo et al. found that the shear deformation of Ni/Al_2O_3 interface took place by a successive breaking and re-bonding process of the Al-O bond based on the density function theory (DFT) calculation [8].

Though the development of high resolution transmission electron microscopy (HRTEM) and in-situ instrumented micro/nano scale mechanical testing capabilities make it possible for direct atomic observations as well as quantitative analysis for metal/oxide interfaces [5], it is still quite challenging to study atomic behaviors at and adjacent to the interface during interface dynamics, which hinders the understanding of the physics determining the interface mechanical response. On the simulation side, the availability of accurate metal/oxide interface potentials, which are also convenient for large-scale parallel computing, hampers the molecular dynamics study. The pair potentials extracted from ab-initio adhesive or cohesive energies by Chen-Möbius

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inversion method [10,11] prove to be a reasonable description of the metal/oxide interfaces [12].

Owning to the simple epitaxial relationships and negligible chemical and charge transfer contribution to bonding, Ag/MgO(0 0 1) system was often chosen as a model of metal/oxide interface [13,14]. Most of the earlier experimental research investigated the structure and morphology of Ag/MgO interface [15–17], and during in-situ growth of Ag on MgO(0 0 1) surfaces, it was observed that the interface structure transformed from coherent to semi-coherent interface, which was characterized by a square misfit dislocation network oriented along ⟨1 1 0⟩ directions [17]. Actually, fundamental properties of these two types of interfaces, such as shear strength and the energy, are key factors determining mechanical response of real Ag/MgO interface.

In this work, shear behaviors of both coherent and semi-coherent Ag/MgO(0 0 1) interfaces are investigated by using atomistic simulation method to shed light on mechanical response of relevant metal/oxide interfaces. First, a coherent interface model and interatomic potentials are introduced in Section 2. The generalized stacking fault energy (GSFE) profile and interplanar stiffness are calculated and analyzed based on the interface potential. These properties are related to mechanical behaviors of Ag/MgO interface systems. Second, a simulation methodology which contains shear loading method and stress calculation method is introduced in Section 3. Next, calculation results of the coherent and semi-coherent interfaces are shown in Section 4 and Section 5, respectively. Interface shear behavior and induced interface compression are studied in Section 4.1. The effect of model thickness is investigated in Section 4.2. The semi-coherent interface structures, computational models and corresponding interface shear behaviors of both one-dimensional (1D) and two-dimensional (2D) dislocation interfaces are presented in Section 5.1 and Section 5.2, respectively. Finally, the conclusion of this paper is given in Section 6.

2. Coherent interface model and interatomic potentials

2.1. Coherent interface model

The computational model of coherent Ag/MgO interface system is shown in Fig. 1(a). Based on experimental observations [18,19], the preferred interface plane is $[0\,0\,1]_{Ag}||[0\,0\,1]_{MgO}$ (z-axis), and the orientation relationship (OR) between Ag and MgO is $[1\,1\,0]_{Ag}||[1\,1\,0]_{MgO}$ (x-axis), $[\bar{1}\,1\,0]_{Ag}||[\bar{1}\,1\,0]_{MgO}$ (y-axis). Note that the Ag/MgO(0 0 1) interface is a fcc/rocksalt structure, and there are three possible interface matching positions: Ag on O site, Ag on Mg site or Ag on hollow site. Ab-initio calculations [11,20] revealed that Ag on O site corresponded to the lowest adhesive energy of Ag/MgO(0 0 1) interface, thus coherent interface of Ag on O site is studied here. The simulation box is periodic in x, y and z directions, and further check indicates that interface area does not affect the simulation results. In z direction, the upper monolayer (ML) and lower ML are fixed boundaries and enough thick vacuum layer is inserted above the upper ML and under the lower ML. The size of the simulation cells are 20 × 10 × L-L, where 20, 10 and L are the number of unit lattices along x, y and z directions, respectively. The thicknesses (L) of Ag and MgO are kept the same and L changes from 5a to 25a to investigate the effect of model thickness.

Fig. 1(b) shows the interfacial atomic configuration, and it can be seen that Ag atoms sit on O sites. The unit cell length along ⟨1 0 0⟩ crystal orientation (z-axis) is lattice constant a (marked by the yellow dashed square). While along ⟨1 1 0⟩ crystal orientations (x- and y-axis), the unit cell length is defined as $1u = \sqrt{2}a/2$ (marked by the red solid square). Since metal is much softer than ceramic, the lattice constants are both taken as that of MgO (4.32 Å) in this coherent model, i.e., the lattices are forced to match at the interface.

2.2. Interatomic potentials and GSFE profile

Pair potentials have been employed to describe the interatomic interactions of Ag/MgO interface systems in our previous work [21], and the interatomic potentials contain both interface potential and bulk potentials. The interface potential is in the Rahman-Stillinger-Lemberg potential (RSL2) form [11,22]:

$$\Phi_{pair}r = D_0 e^{y\left(1-\frac{r}{R_0}\right)} + \frac{a_1}{1+e^{b_1(r-c_1)}} + \frac{a_2}{1+e^{b_2(r-c_2)}} + \frac{a_3}{1+e^{b_3(r-c_3)}} \quad (1)$$

where $\Phi_{pair}r$ is $\Phi_{Ag-O}r$ or $\Phi_{Ag-Mg}r$. The bulk potential $\Phi_{Ag-Ag}r$ is also in the RSL2 form. As an ionic crystal, the oxide-oxide interactions contain both short-range part $\Phi^{SR}(r)$ and long-range coulomb part $\Phi^{Coul}_{Mg-Mg}(r) = \Phi^{Coul}_{O-O}(r) = -\Phi^{Coul}_{Mg-O}(r) = \frac{Q^2_{eff}}{4\pi\,\epsilon_0\,r}$. For Mg—Mg and O—O interactions, the short-range parts $\Phi^{SR}_{Mg-Mg}(r)$ and $\Phi^{SR}_{O-O}(r)$ are in Morse

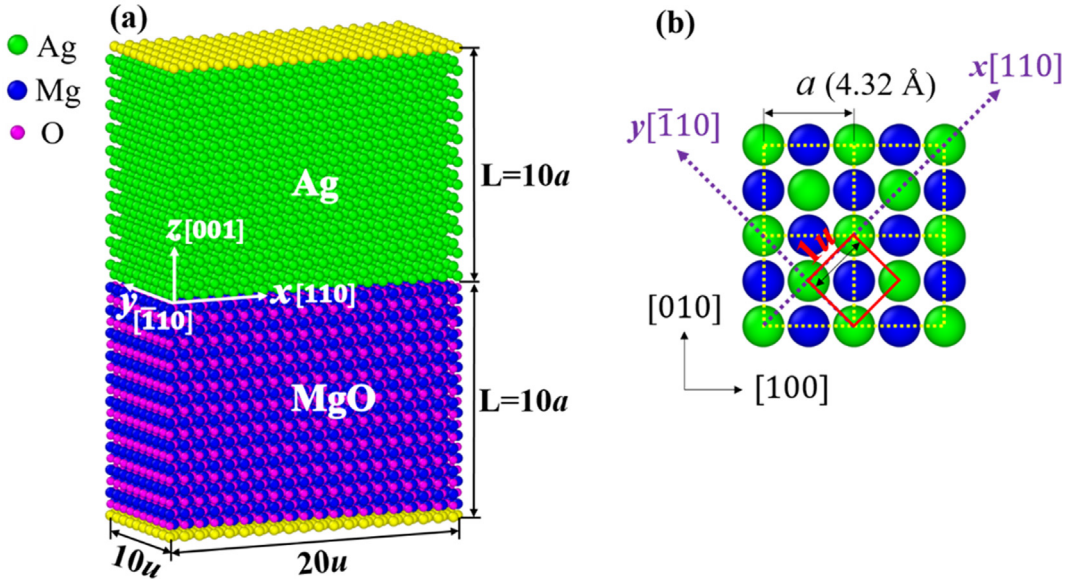

Fig. 1. The computational model of coherent Ag/MgO interface system. (a) Atomic structure of the whole interface model, the top and bottom yellow atoms represent the fixed boundaries. (b) Interfacial atomic configuration showing different unit cells along [1 0 0], [1 1 0] crystal orientations. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)