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Modeling material interfaces with hybrid adhesion method

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ABSTRACT

A molecular dynamics simulation approach is presented to approximate layered material structures using discrete interatomic potentials through classical mechanics and the underlying principles of quantum mechanics. This method isolates the energetic contributions of the system into two pure material layers and an interfacial region used to simulate the adhesive properties of the diffused interface. The strength relationship of the adhesion contribution is calculated through small-scale separation calculations and applied to the molecular surfaces through an inter-layer bond criterion. By segregating the contributions into three regions and accounting for the interfacial excess energies through the adhesive surface bonds, it is possible to model each material with an independent potential while maintaining an acceptable level of accuracy in the calculation of mechanical properties. This method is intended for the atomistic study of the delamination mechanics, typically observed in thin-film applications. Therefore, the work presented in this paper focuses on mechanical tensile behaviors, with observations in the elastic modulus and the delamination failure mode. To introduce the hybrid adhesion method, we apply the approach to an ideal bulk copper sample, where an interface is created by disassociating the force potential in the middle of the structure. Various mechanical behaviors are compared to a standard EAM control model to demonstrate the adequacy of this approach in a simple setting. In addition, we demonstrate the robustness of this approach by applying it on (1) a Cu-Cu_2O interface with interactions between two atom types, and (2) an Al-Cu interface with two dissimilar FCC lattices. These additional examples are verified against EAM and COMB control models to demonstrate the accurate simulation of failure through delamination, and the formation and propagation of dislocations under loads. The results conclude that by modeling the energy contributions of an interface using hybrid adhesion bonds, we can provide an accurate approximation method for studies of large-scale mechanical properties, as well as the representation of various delamination phenomena at the atomic scale.

1. Introduction

A common complication associated with MD simulations is the definition and selection of interatomic force fields. These force fields provide parameters used to calculate the atom-to-atom interaction behaviors for the simulations. While there are numerous types of force fields available for isolated systems [1], there remains a limited amount of intermolecular capabilities for complex systems. Organizations, such as the National Institute of Standards and Technology (NIST) and the Knowledge of Interatomic Models (KIM), provide researchers with a vast data repository of potentials for use in both MD and ad-initio simulations. However, due to the complex nature of these potentials, the applications of each force field are often limited in scope and can provide unrealistic results if misused. One example is the Embedded Atom Method (EAM) force field, which is a well-defined approach used to simulate structural, mechanical and thermal behaviors of some pure metal structures [2,3]. While this force field is well defined and verified for materials such as pure copper and aluminum, it requires additional adjustments when observing additional atom interactions, such as the effects of surface oxidation [4]. Another approach that is being continuously developed is the Charge-Optimized Many Body (COMB) potential for various metal-oxides. The use of these potentials are typically restricted to temperature-dependent oxidation growth [5,6], low mechanically strained systems or low-temperature interfaces [7]. The issue grows when the scope of the simulation includes additional

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complex interactions, such as those between metals and polymers. The potentials used to model polymers (PCFF, AMBER, CHARMM, etc.) are fundamentally different and incompatible to those used for metallic structures (EAM, MEAM or COMB), this creates a computational challenge when modeling the composite interfaces. With no direct relationship between these force fields, often a new force field relationship must be developed on a material specific basis [8]. As an alternative method, we propose a hybrid adhesion method (HAM) to approximate the mechanical characteristics of surface interactions by linking two or more discrete force fields by an array of adhesive energy bonds.

The principle concept behind the hybrid adhesion method is the simplification of the complex behaviors at a material interface. The theory was developed by combining the principles of classical mechanics used in MD simulations, with those of density functional theory (DFT) in quantum mechanics. The result is a hybrid potential model that enables the use of multiple independent force fields as well as reduces the total computational time by limiting the material interactions to a surface plane at the interface. The method is described in this paper and demonstrated on three different interfaces for application and verification purposes. The first interface is of a standard bulk copper structure modeled with an EAM potential, where the structure is split into layers and the interatomic potentials are discretized to act as independent entities. The second interface is between copper and cuprous-oxide, modeled using the COMB potential. Like the bulk copper structure, the Cu-Cu_2O model is separated into layers of independent force fields and provides a complicated interface structure with multiple atomic interactions. The oxidation of copper surfaces is often observed in electrical components and 3D packaging where it is stacked with thin layers of an epoxy compound [9,10] and provides a good introductory interface for future studies. The final structure is a dissimilar face-centered cubic (FCC) interface of aluminum and copper using an EAM potential. The model introduces the hybrid adhesion method to a misfit dislocation interface. Multi-layered stacking is prone to delamination through fluctuations in environmental conditions, making it an ideal case study for this modeling technique. As such, the application and verification of this method is focused on the mechanical properties and behaviors of each material interface as well as an in-depth study of delamination. To verify the hybrid adhesion method, controlled models using traditional MD techniques were used as baseline structures for comparisons mechanical behavior and response.

2. Theoretical background

The theory behind the hybrid adhesion method originates from the concepts of energy distribution presented by Gibbs and the ideal interface model, Fig. 1. Energy contributions of a two-phase structure consist of a bulk concentration of α-phase, a bulk concentration of β-phase and a surface phase marked by the diffused region at the interface. The energy contribution associated with this surface phase is known as interfacial free energy, or interfacial excess energy [11–13]. A dividing surface can be visualized through a change in energy density profile, normal to the interface, Fig. 1b. The profile displays two constant energy densities for the bulk phases, and a deviating function associated with the contributions of the surface phase region.

With the surface phase layer proportionally thin in comparison with other dimensions [13], Gibbs introduced the concept of a dividing surface where the surface phase is idealized as an interface separating two homogeneous phases. By reducing the interface to an infinitely thin plane, the total energy of the system can be reduced to the sum of the atomic contributions in the two phases in addition to an interfacial free energy, γ. For an ideal two-phase system (Fig. 1c), the corresponding interfacial excess energy can be approximated by:

$$\gamma(T) = \frac{E_{tot} - (N_\alpha e_\alpha + N_\beta e_\beta)}{A} \tag{1}$$

where A is the surface area of the interface, N is the number of atoms in the respected phases and e is the potential energy per atom in the bulk state [16]. The top term, $E_{tot} - (N_\alpha e_\alpha + N_\beta e_\beta)$, is also referred to boundary enthalpy and is often used in MD studies of grain boundaries and applications of mobility [16–19]. The development of the hybrid adhesion method presented in this paper applies the same principles and approximations to apply an adhesive bonding to two, otherwise independent, materials.

2.1. Hybrid adhesion method

The hybrid adhesion method was developed following similar concepts as Gibbs Ideal Interface model, where it discretizes the structure into three partitions: bulk α-material, bulk β-material and an adhesive region. If two bulk materials are defined as independent in both energy and force interactions, the interfacial excess energy and adhesion characteristics can be limited to a

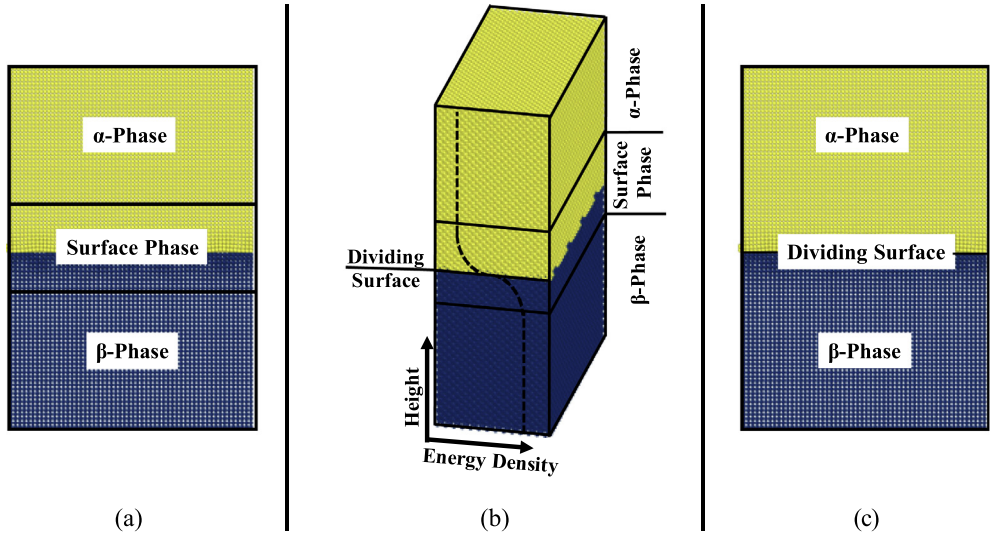

Fig. 1. (a) Real model of two-phase system with a diffused surface region defined [14]. (b) Diffused surface region defined by energy densities [15]. (c) Gibbs Ideal Interface with infinitely thin dividing surface [14].