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Computer Simulation of Interactions between Copper and Aluminum Nano-films

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***Abstract*—Nowadays it has become feasible to simulate the dynamics of molecular systems on a computer. The aim of computer simulations of molecular systems is to compute macroscopic behavior from microscopic interactions. Interactions between closely spaced copper and aluminum nano-films have been carried out by using Lennard-Jones (L-J) potential with Molecular dynamics simulations. The interfacial distance between copper and aluminum nano-films is narrowing from 15 Å to 4Å. The interaction strength firstly keeps almost unchanged in the range of 7 Å to 15 Å. When the distance is less than 7 Å the interaction strength decreases quickly. It is found that the critical distance is around 7 Å. Moreover, the interaction strength increases with the increasing temperature in the range of 4 Å to 7 Å. The interaction also varies with different surface morphologies, the interaction energy of rectangle surface is much more greater than triangle surface at the same spacing. However, it is little affected by the approaching velocity of the two films in the range of 6 Å to 15 Å. When the distance is less than 6 Å, interaction energy decreases sharply. The larger the velocity, the larger the interaction energy. At last, we found that electric field does not affect the interaction energy.**

Keywords- Computer Simulation； Nano-films； Molecular Dynamics； Interaction Strength

I. INTRODUCTION

Thin films have been widely used to improve surface performances in applications such as micro-electromechanical systems (MEMS) [1] [2] [3] [4]. Properties of Cu and Al thin films have been investigated extensively because such films are frequently applied to micro devices. As the size of electronic and mechanical devices shrinks to the nanometre regime, performance begins to be dominated by surface forces. For example, friction, wear and adhesion are known to be central challenges in the design of reliable micro and nano-electromechanical systems. This is because the micro-components have a large surface area to volume ratio. Many interactions that can be neglected at macro-scale are very important at micro-scale because they can affect the stabilities and performances of micro-devices. Therefore, increasing discussions have been carried out on adhesion [5] [6] [7] [8], micro/nano-friction [9] [10] [11] [12] [13] [14], Casimir effects [15] between micro-objects. However, it is difficult to investigate the molecular scale effects directly and accurately using current experimental characterization techniques. Furthermore, it is still not reliably predict the response when two surfaces come into contact at the nano scale. Molecular dynamics (MD) provides a good approach which is widely used for investigations of friction, wear and related processes at the atomic-scale. A lot of work has been devoted to study the properties of thin films and interactions in nano scale by using MD simulations. Iizuka et al [16] focused hardness as one of mechanical properties of sputtered thin films and investigated the relationships between porosity and hardness of Al thin film on the silicon substrate by MD simulations. Tan et al [2] investigated the effects of the film thickness, process pressure and process power on the residual stress of the Cr/Au thin film. Conde et al [3] studied electrostatic actuation of thin-film silicon MEMS using optical and integrated piezoresistive and magnetic detection. Fu et al [4] discussed some critical issues and problems in the development of TiNi thin films, including preparation and characterization considerations, residual stress and adhesion, frequency improvement, fatigue and stability. Harrison et al [10] discussed the mechanical and tribological properties of diamond-like carbon films and self-assembled monolayers by MD simulations. It was also found that MD simulations were able to reproduce the cleavage and flake formation under appropriate conditions during the interaction of a graphite surface with a rigid nanoasperity [13]. However, the interactions between noncontact nano-films are rarely studied in details in most previous studies.

In this work, the noncontact interactions of closely spaced copper and aluminum films are studied. The Lennard-Jones (L-J) potential is used to describe the interactions between copper and aluminum films. The processes are simulated by MD simulation method when the interfacial distance between copper and aluminum nano-films is narrowing from 15 Å to 4Å with different velocities, temperatures, surface morphologies and electric fields.

II. METHODOLOGY

Copper and silicon nano-films are modeled in a periodic unit with lattice parameters a = 72.891Å, b = 36.446Å and c = 1000.000 Å (Fig. 1(a)) in order to eliminate the influence of periodic boundary conditions on the molecular dynamics simulation process [17]. The periodic unit consists of ten layers of copper atoms and seven layers of aluminum atoms, the number of copper atoms is 3605 while the number of aluminum atoms is 2460. MD simulations are performed by using commercial software package Discover. The COMPASS [18] (condensed phase optimized molecular potentials for atomistic simulation studies) force filed based

on PCFF (polymer consistent force field) is used to build the interaction models. The Lennard-Jones-9-6 potential function is adopted by the COMPASS force filed to calculate interactions between copper and aluminum atoms, and it can be calculated by the following expression:

$$E_{ij}=\sum_{i,j}\varepsilon_{ij}\left[2\left(\frac{r_{ij}^0}{r_{ij}}\right)^9-3\left(\frac{r_{ij}^0}{r_{ij}}\right)^6\right] \quad (1)$$

where E_{ij} is a pair potential energy between the atom *i* and atom *j*. The first and the second terms represent all interatomic repulsive and attractive interactions, respectively. ε_{ij} and r_{ij}^0 are the coefficients of well-depth energy and the equilibrium distance. For different types of atoms, the parameters can be obtained by the following equations:

$$\varepsilon_{ij}=2\sqrt{\varepsilon_i\cdot\varepsilon_j}\left(\frac{\left(r_i^0\right)^3\cdot\left(r_j^0\right)^3}{\left(r_i^0\right)^6\cdot\left(r_j^0\right)^6}\right) \quad (2)$$

$$r_{ij}^0=\left(\frac{\left(r_i^0\right)^6-\left(r_j^0\right)^6}{2}\right)^{1/6} \quad (3)$$

where singly subscripted parameters, such as ε_i and r_i^0 depend only on one type of atoms. For all simulations in this paper, the cutoff distance is set as 9.5 Å. The simulation is carried out in the NVT ensemble with temperature equilibrated by the Andersen algorithm [19].

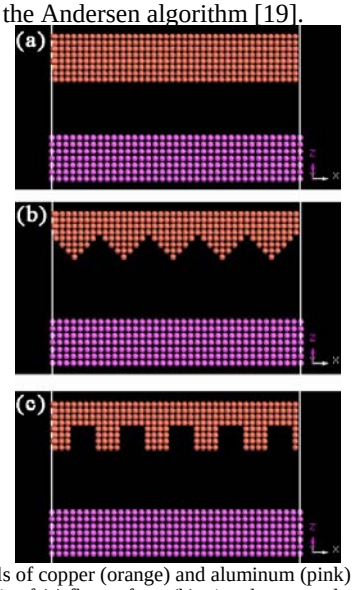

Figure. 1 Models of copper (orange) and aluminum (pink) nano-films. Copper nanofilm is of (a) flat surface, (b) triangle grooved surface and (c) rectangular grooved surface at the initial distance of 15 Å.

For each model, the dynamics processes proceed as follows. The top layer of copper film and the bottom layer of aluminum film are held rigid while the middle layers are free to move without any extra constraints. To achieve the stable state, the equilibration dynamics of 40 ps is carried out with the initial distance of 15 Å. The interaction energy per unit area σ_E in the model is used to estimate the strength of interactions between the two films, and it is calculated by using the following formula:

$$\sigma_E = E_{Inter}/A = \left[E_{total}-\left(E_{Cu}+E_{Al}\right)\right]/\left(a\cdot b\right) \quad (4)$$

where E_{total} is the total energy of the model after molecular dynamics calculations, E_{Cu} and E_{Al} are the total potential energies of copper film and aluminum film after molecular dynamic process, *a* and *b* are the lattice parameters: *a* =72.891 Å, *b* = 36.446 Å.

III. RESULTS AND DISCUSSION

There are two different stages for the interaction when the distance decreases from 15 Å to 4 Å. Fig. 2(a) shows the changes of σ_E as the copper film is moved toward to the aluminum film per angstrom a time at the temperature of 800 K. It is noted that the interaction strength decreases slightly with the decreasing distance in the range of 7 Å to 15 Å. Moreover, when the distance is below 7 Å the interaction energy decreases quickly from -0.088 kcal • mol^{-1} • $Å^{-2}$ to -3.363 kcal • mol^{-1} • $Å^{-2}$. Fig. 2(b) shows the changes of the interactive force upon per unit area *F* with the distance. The force is obtained by the following formula:

$$F=\frac{\Delta\sigma_E}{\Delta d} \quad (5)$$

It is only about -1×10^{-4} nN • $Å^{-2}$ at the distance of 15 Å. The interaction force changes slightly from 7 Å to 15 Å. However, a sharp increase of the force is observed as the two films getting close to each other. The attractive force is -0.128 nN • $Å^{-2}$ at the distance of 4 Å, which is larger than that at the distance of 7 $Å^{-2}$ by 3 orders of magnitude. This result is similar to the behavior of a micro-tip when it is pulled toward a graphitic surface [13]. It is also similar to the results of a copper film getting close to a silicon film [20].

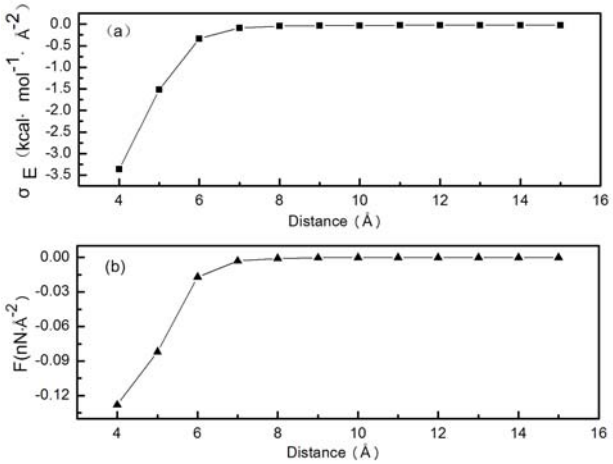

Figure. 2 At the temperature of 800 K, (a) the interaction energy per unit area σ_E and (b) the interaction force per unit area F.

The temperature can significantly affect the interaction between nano-films. Fig. 3 illustrates the simulation results of Fig. 1(a) under the temperatures of 10k, 298k and 500 K. It is evident that the higher the temperature, the larger the interaction energy. This is because the intensity of atom motions can be influenced by the temperature. At a high

temperature, atoms vibrate intensely and the total energy in the model is very large. Therefore, the interaction between the films increases with the temperature.

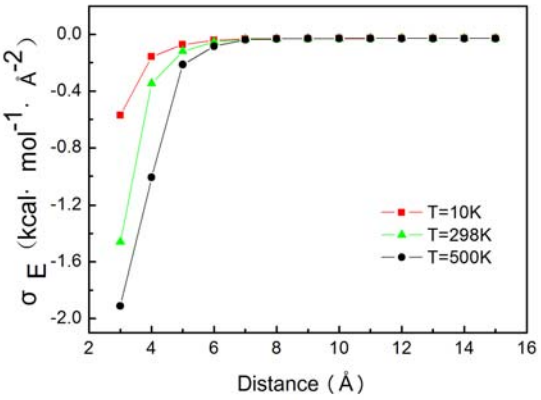

Figure. 3 The interaction energy per unit area σ_E at the temperature of 10 K, 298K and 500K.

It is also found that the films' surface morphology can be changed by modifying the temperature. Photos of the films under different temperatures of 10K, 298K and 500 K are shown in Fig. 4. Each model in the figure has the same distance, which is 4 Å. The most severe changes are observed at the highest temperature, which is in agreement with the experimental findings [21]. This result can be attributed to the enhanced thermal movements of the atoms under higher temperature between the two films at small distances.

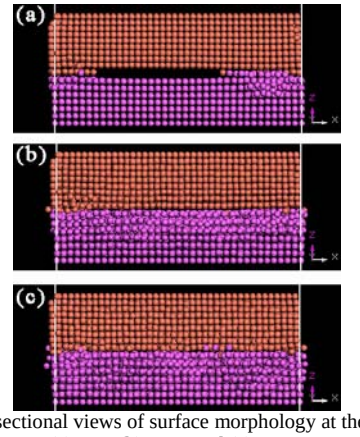

Figure. 4 Cross-sectional views of surface morphology at the temperature of (a)10K, (b)298K and (c)500K.

The velocity is obtained by adjusting both the distance decrement and time step. From Fig. 5 we found that the interaction is little sensitive to the velocity of the two films getting close to each other in the range of 6 Å to 15 Å. When the distance is less than 6 Å, interaction energy decreases sharply. We can also found that when the distance between two films is 4 Å , the interaction energies for velocities of 10 m/s, 50 m/s and 100 m/s are -2.156 kcal • mol^{-1} • $Å^{-2}$, -2.781 kcal • mol^{-1} • $Å^{-2}$ and -2.991 kcal • mol^{-1} • $Å^{-2}$, respectively. This is because the value of impact effected by the velocity. The larger the velocity , the larger the impact. This result can lead to a higher interaction energy.

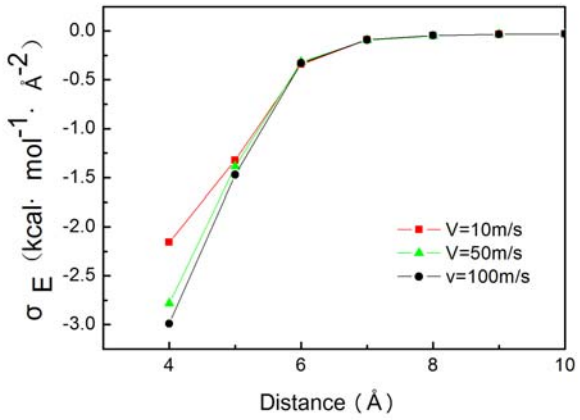

Figure. 5 σ_E with the velocity of 10 m/s, 50m/s and 100m/s at the temperature of 298 K.

The surface morphology can affect the films' interactions. For comparison, two models in Fig. 1(b) and (c) are used, in which the bottom surfaces of copper films have the same roughness but with triangle and rectangular grooves, respectively.

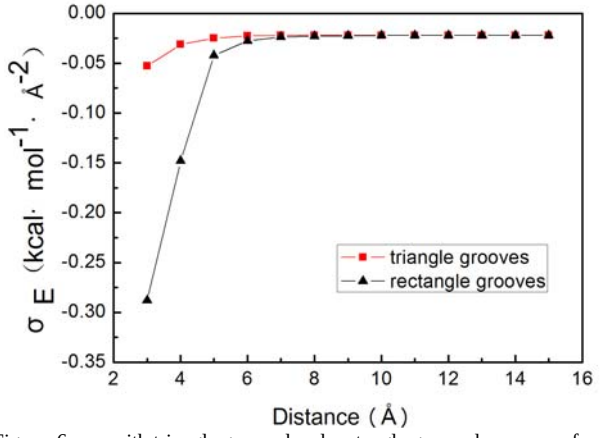

Figure. 6 σ_E with triangle grooved and rectangle grooved copper surface.

The simulation results are shown in Fig.6. The interaction energy is a little larger in the models with grooved copper surface than that with flat copper surface when the distance decreases from 6 Å to 15 Å, which is attributed to the different initial stabilities of atoms in the models. When the distance is below 6 Å, the reduction of the interaction energy for the model with rectangular copper surface is larger than triangle copper surface. At the distance of 4 Å, the interaction energy in the model with triangle copper surface is -0.031 kcal • mol^{-1} • $Å^{-2}$ while the model with rectangular copper surfaces is -0.147 kcal • mol^{-1} • $Å^{-2}$.

The interaction energy is little sensitive to the uniform electric field of the two films getting close to each other from Fig.7. When the distance deceases from 15 to 8 Å, the average interaction energies under the uniform electric field of 0.06 V/ Å, 0.07 V/ Å and 0.08 V/ Å are -0.031 kcal • mol^{-1} • $Å^{-2}$, -0.031 kcal • mol^{-1} • $Å^{-2}$ and -0.030 kcal • mol^{-1} • $Å^{-2}$

^{2}, respectively. We can also know that at the distance of 4 Å, the interaction energies σ_E are -0.556 kcal • mol^{-1} • Å^{-2}, -0.556 kcal • mol^{-1} • Å^{-2} and -0.555 kcal • mol^{-1} • Å^{-2}, respectively.

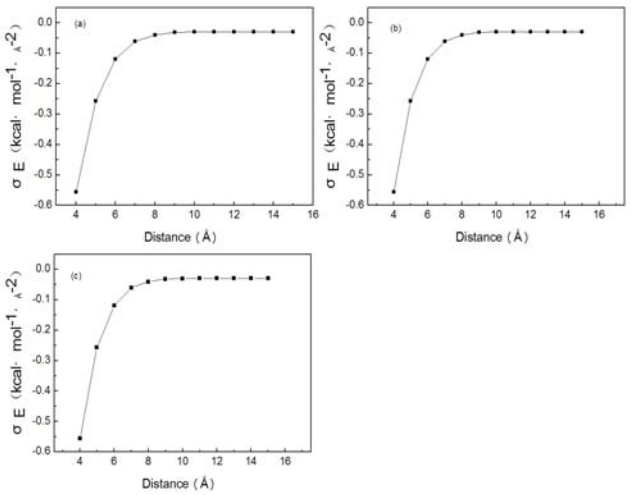

Figure. 7 At the temperature of 298 K (a) σ_E under the uniform electric field of 0.06V/ Å,(b) σ_E under the uniform electric field of 0.07V/ Å, (c) σ_E under the uniform electric field of 0.08V/ Å.

IV. CONCLUSIONS

Dynamic computer simulation is just a branch of computational chemistry and physics in which a mathematical model of the real world is formulated and its consequences for the various physical or chemical quantities are evaluated by numerical methods. The MD simulations of copper and aluminum nano-films are studied to investigate the effects of different distances, temperatures, velocities, surface morphologies and electric field on interaction energy. It is observed that the interaction has two stages when copper film is moved downward to aluminum film from the initial distance 15 Å to the final distance 4 Å. As the distance decreases from 15 Å to 7 Å, the two film's interaction rarely changes. When the distance is below 7 Å, the interaction energy between the films gets stronger with the decreasing distance. The interaction is affected obviously by the temperature as the distance is below 7 Å. It is evident that the higher the temperature, the larger the interaction energy. In addition, different velocities of 10 m/s, 50 m/s and 100 m/s hardly influenced the interaction energy in the range of 6 Å to 15 Å. When the distance is less than 6 Å, velocities influenced the interaction energy a lot. Furthermore the surface morphology can also affect the interaction. Copper films have the same roughness but with triangle and rectangular grooves are studied. When the distance is below 6 Å, the reduction of the interaction energy for the model with rectangular copper surface is larger than triangle copper surface. At last, we found that the interaction energy is little sensitive to the uniform electric field of the two films getting close to each other. This paper shows a new method to investigate the properties of other kinds of interactions between noncontact nano-films.

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