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Origin of frictional ageing by molecular dynamics simulation of a silicon tip sliding over a diamond substrate

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ABSTRACT

In this paper, frictional ageing is investigated through simulating a silicon tip sliding over a diamond substrate with a molecular dynamics model. It is demonstrated that contact strengthening in ultra-high vacuum is mainly caused by surface dimerization. With the increase of temperature, tip-substrate contact evolves from incommensurate to commensurate due to the lattice transition from (1×1) to (2×1) lattice ordering. The combination effects of contact strengthening and thermal lubrication lead to a nonmonotonic variation of the mean friction force with temperature rise. However, the friction increase trend induced by the surface dimerization can be suppressed efficiently with the structural lubrication.

1. Introduction

Nanotribology, the study of friction, adhesion, wear and lubrication at the atomic length and time scales, has been of major concern in recent years due to the increasing development of the miniaturization of many technological devices, especially the micro-nanoscale electromechanical systems (MEMS/NEMS) [1–3]. Silicon (Si) is the predominant material in the manufacturing of MEMS/NEMS [3]. Due to the small size and high surface-to-volume ratio of these devices, friction and adhesion forces may display unusual phenomena and play a dominant role in their functioning. Therefore, despite the wide application of Si-MEMS/NEMS, investigations of their fundamental tribological properties at the nanoscale continue to rouse interest today.

Previous literatures on atomic friction showed that friction behavior can be profoundly affected by dynamical factors such as temperature and sliding velocity. It is reported that [4–6] in ultra-high vacuum (UHV) conditions friction decreases with increasing temperature while it increases with scanning velocity. This is termed thermolubricity [7] where thermally activated jumps of the sliding tip lead to reduction of friction. However, some recent experimental findings, performed with an amorphous Si tip sliding over a variety of sample surfaces such as Si wafer, SiC wafer, NaCl crystal, and HOPG surfaces in UHV [8–10], revealed a nonmonotonic variation of kinetic friction with increase of temperature, which is inconsistent with the common paradigm of thermolubricity. Similar surprising observation was made in ambient condition and at around room temperature, where both experimental measurements and numerical simulations have attributed this friction mechanism to frictional strength or frictional ageing [11,12]. It is therein reported that the ageing arises from meniscus condensation between tip and sample, leading to a logarithmic increase of static friction with time while the surfaces are held together. Another grounded reason of friction ageing was addressed to a growth in the contact interface with time due to asperity creep [13–15]. However, MD simulations mimicking ambient environment had been conducted with both amorphous silica surfaces and quartz (001) surfaces [16]. Those studies excluded the hypothesis of meniscus formation and demonstrated that in the absence of deformation creep the mechanism of the frictional ageing is purely due to interfacial chemistry.

In water-free medium and in the absence of stepped roughness such as in atomically flat contact interface, bond formations caused by humidity and/or creep are irrelevant explanations of the observed friction ageing. Some attempts to show evidence of contact ageing in UHV were performed at finite temperature [8] based on the modified mechano-kinetic (MK) model. With the MK model the friction strengthening is shown to be directly related to thermally assisted formation as well as rupture of molecular bonds at the interface. Nevertheless, the physical reason of the origin of the contact ageing revealed by experiments in UHV remains unknown [9] because the thermally assisted bonding should not be responsible to the dramatic change in the friction force.

In this paper, we conduct MD simulations to gain deep insight into the observed experimental frictional ageing in UHV, where the buried frictional interface is fully accessible. We model an atomic force microscope (AFM) experiment through simulating a

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Si tip sliding over an atomically flat (001) surface with a diamond-like carbon structure. Surprisingly, we discover that the ageing leading to an increase of friction arises from dangling bonding of the tip apex atoms, which may form dimer rows on the interface. This surface dimerization is a thermally assisted process. In one hand, it is characterized by long straight dimer rows that cause uniform slip which favor contact ageing. On the other hand, it consists of short dimer rows with antiphase boundaries that induce partial slip and hence, tend to lower the friction force. In addition, we show that this frictional strength caused by tip apex dimerization is sensitive to crystallography orientation. Thus, structural lubricity appears to be a better technique in reducing friction than thermolubricity for Si-based material interactions.

2. Methodology

In the aim to bring evidence to the mechanism of friction ageing in UHV and in the absence of deformation creep we modeled AFM experiments considering an atomically smooth Si (001) asperity sliding on an atomically smooth diamond-like carbon (001) substrate, as shown in Fig. 1. The motivation of the above chosen materials has twofold concerns. First, we want to use the same (Si-based and carbon-based) materials with those in the aforementioned UHV experiments of friction strengthening. Second, beside of its widely use in the microelectronic industry a Si(001) surface displays a variety of amazing phenomena despite of its relatively simple composition [17].

The simulation setup consists of a square-base prismatic Si tip with a size of $5a_{Si} \times 5a_{Si} \times 4a_{Si}$ that corresponds to a contact area of approximately 6.65 nm^2. A $24a_C \times 18a_C \times 3a_C$ carbon (C) substrate with diamond structure is considered with horizontal periodic boundary conditions. a_{Si} and a_C stand for silicon and diamond lattice constants, respectively. Fixed boundary conditions are applied in the diamond substrate and the Si tip by freezing the four bottom atomic layers of the substrate and the four top layers of the tip as reported in Refs. [18,19], respectively. In the tip, each atom in the top four layers are frozen without thermal vibration in the six degrees of freedom but can move along with the tip in the horizontal plane. On the substrate, the bottom four layer atoms are fixed with all the six degrees of freedom in order to restrain the substrate rigid movements along any directions. The four next adjacent layers to the boundary layers in both the tip and substrate are coupled to a Langevin thermostat for temperature control while the remaining layers are subjected to Newtonian dynamics.

For visualization purpose the above enumerated layers are shown sequentially in different colors as displayed in Fig. 1. The Lennard-Jones (LJ) potential function is chosen to model the Si–C atomic interactions, which are short-range van der Waals interactions [20]. Intra-atomic forces within the tip and the substrate, however, are derived from the Tersoff potential type [21,22] since it can reasonably predict the properties of crystal phases for diamond and silicon, respectively [23,24].

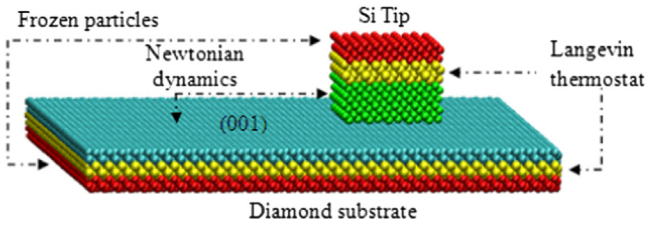

Fig. 1. MD simulation model system of Si(001) tip and diamond-like(001) substrate. Red balls are frozen atoms. They are restricted in any direction for the substrate while they are free to move in the horizontal plane (001) for the tip. Yellow particles are subjected to Langevin thermostat for heat dissipation control. The dynamics of green and cyan particles obey Newtonian motion. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The study is conducted with two MD simulation models. The first model aims at elucidating the mechanism of the frictional ageing in UHV as reported in literature [8–10]. In this regard the same temperature is applied to the tip and to the substrate while it is varied simultaneously from $T = 0$ K to $T = 500$ K. Clearly, the highest temperature is much lower than the melting point of Si determined experimentally by Broughton and Li [25] (1687 K) or calculated by Cook and Clancy [26] (2547 K) from the Tersoff potential. Sliding is performed by pulling the tip top atoms along the [100] direction of the substrate at constant scanning velocity. The second model tries to investigate another friction reduction mechanism that is different from the thermolubricity. In this model, we rotate the substrate in the (001) plane with respect to the tip vertical axis in different angles and then drag the tip sliding over the sample. This allows us to assess the sensibility of ageing on crystallography orientations. Note that the results presented in this letter are quantities average over a period of 100 thousand MD steps after an initial run of 200 thousand MD steps for equilibration.

3. Results and discussion

Results of the mean friction force for a range of temperature are presented in Fig. 2. They are obtained from dragging a Si(001) tip sliding over a diamond-like(001) substrate, of both atomically flat terraces and under a constant normal load of 20 nN. Scannings were simulated at constant sliding velocities V of 3.6 m/s and 5.6 m/s, respectively, showing consistent results. The MD simulations carried out here reveal a nonmonotonic variation of the mean friction force as a function of temperature. This is consistent with experimental observations previously reported [8–10] for amorphous Si tip sliding over a variety of surfaces. Note that, although the global trend is reproduced, two major differences still exist between our numerical experiments and real experiments. One difference lies in the magnitude of the driving velocity of the tip (on the order of m/s in simulations while nm/s in experiments). Another difference appears on the asperity of the contacting surfaces (absence of contamination or roughness at the contact interface in simulations).

As seen in Fig. 2, the average friction exhibits four different regimes that can easily be distinguished. They are labeled as I, II, III and IV as the temperature increases. The fundamental question to be addressed is the dramatic change in the friction behavior, which is usually attributed to friction strengthening in literatures.

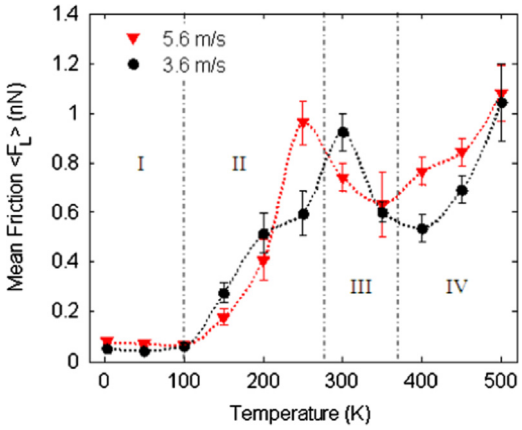

Fig. 2. Average lateral force F_L as a function of temperature from the MD simulation systems. Circular symbols and triangle symbols indicate simulation results for velocity 3.6 m/s and 5.6 m/s, respectively. Dotted lines are spline fits to guide the eye. External load is set at $N = 20$ nN and scan direction along [100].