Friction between a Ge tip and the (001)-2×1 surface: A molecular-dynamics simulation

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(Received 20 February 2001; revised manuscript received 21 May 2001; published 31 August 2001)

In order to investigate the friction between a Ge tip and its (001)-2×1 surface by molecular-dynamics (MD) simulation, two schemes are adopted. In the first scheme the tip advances over the substrate each MD step while in the second scheme the tip advances every 1000 MD steps. It is found that if the tip and the substrate approach each other closely enough, for both schemes wear occurs via a slip-stick mechanism, but their details are quite different. We present a detailed explanation for this phenomenon and conclude that the second scheme is more appropriate for the description of experimental situations. In additions, we find that the friction properties of the nanomaterials are related to sliding direction.

DOI: 10.1103/PhysRevB.64.113313 PACS number(s): 81.40.Pq, 46.55.+d, 61.82.Rx, 61.82.Fk

The dynamical interaction between a tip and a substrate involves cohesion, wear, adhesion, friction, diffusion, etc. It is closely related to indentation processes and interfacial phenomena in nanomaterial science. It has been widely explored both theoretically and experimentally.[1–12] However, in recent theoretical works there exists an obvious weakness, i.e., due to the limitation of computer resources the speed the tip advances over substrate is greater than 1.0 m/s, and in some cases as large as 100.0 m/s.[1–5] Experimentally, the velocity is only in the range μm/s to mm/s.[5–11] Thus the experimental and the simulation velocities are quite different. For this reason, we may question the conclusions from those simulations. In order to investigate this problem, as an example, we simulate the interaction of a Ge tip and the (001)-2×1 surface of Ge by a molecular-dynamics method. Our aim is to present a reasonable method to describe the friction phenomenon of nanomaterials theoretically.

In the simulations, the computational cell consists of a Ge tip which is placed above a Ge substrate. The substrate is a thick slab and constructed with 17 Ge (001) atom layers. Each layer contains 100 atoms. The tip is constructed with 13 Ge (111) layers, including 3 atoms in the bottom most layer, and 30 atoms in the top layer. The total number of atoms in this computational cell is 1873. Periodic boundary conditions are used in the two dimensions parallel to the surface plane. In the third dimension, fixed boundary conditions are established by static atoms in the bottom most five layers of the substrate and the top most three layers of the tip. The positions of the static atoms are fixed at their bulk lattice sites. There are ten and twelve dynamic atom layers in the tip and in the substrate, respectively. The interatomic potential is the Tersoff potential.[13] The potential provides an approximate and computationally efficient description of the essential physics of the interatomic interactions in semiconductors C, Si, and Ge.[13]

In this work two methods are used. In the first method, the static atoms of the tip are displaced by a MD time step in the direction of sliding and the dynamic atoms are relaxed simultaneously. This is a traditional method and has been widely used in the study of a tip-substrate system.[1–5] In the second method, the tip is fixed over the substrate while its dynamic atoms are relaxed for 1000 time steps. Then the static atoms of the tip advance 0.1 Å (or 0.05 Å) along the direction of sliding. The process is repeated. For all of the simulations, the temperature of dynamic atoms is controlled by a Hoover thermostat.[14] The numerical integration of the equation is done by a velocity Verlet algorithm,[15,16] with a time step $\Delta t = 3.0 \times 10^{-15}$ s in the integration algorithm. The initial simulation temperature is set at $T = 50$ K, and this value is maintained throughout the simulations by implementing the Hoover thermostat. Before the simulations are performed for the system by MD, a conjugate gradient method has been used to relax the tip and the substrate of the system, respectively. For the substrate we obtain a dimerizing (001)-2×1 reconstructed surface. The bond length of the dimer is 2.43 Å and slightly smaller than the nearest neighbor distance of Ge (2.45 Å). In all of the cases we simulate a constant height scan of a tip over a substrate. In order to do a clear comparison of the two methods the tip is kept close to the substrate. The scan height of the tip is 1.132 Å above the surface of the substrate.

We first perform MD simulations for the tip-substrate system by the first method. With this method, we perform three simulations. In the three simulations, the displacing velocities of static atoms of the tip, with reference to the substrate, are 50.0, 5.0 and 2.5 m/s. The corresponding total number of time steps are 20 000, 120 000 and 160 000, respectively. These simulations take 2, 12, and 16 days on an 600 MHz alpha workstation, respectively. The sliding directions are all chosen along the *X* axis. The *X*, *Y*, and *Z* directions of the substrate are [110], [$1\bar{1}0$], and [001] while the *X*, *Y*, and *Z* directions of the tip are [$0\bar{1}1$], [$2\bar{1}1$], and [111], respectively. For convenience, hereafter we shall call the three simulations 1-I, 1-II, and 1-III, respectively. We have plotted three sets of snapshots for the three simulations, and all are found to be similar to each other. As an example, only two of the snapshots are shown in Fig. 1, one snapshot from simulation 1-I(a) and one from simulation 1-II(b). From the three sets of snapshots, it is obvious that a wear has occurred in all of the three simulations and some atoms of the tip have transferred into the substrate. This is not difficult to understand. The tip has a far larger ratio of surface area to bulk volume than the substrate has. This makes the surface energy

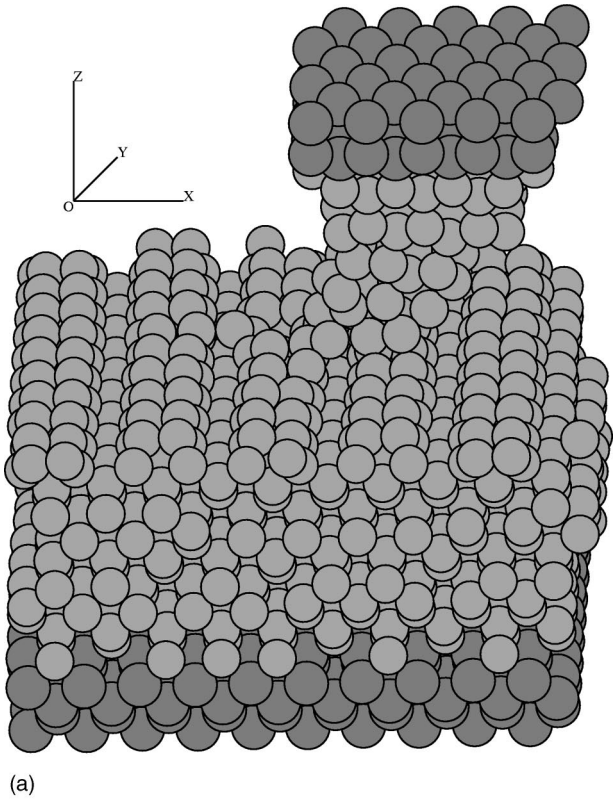

FIG. 1. Snapshots of a Ge (111) tip on a Ge(001)-2×1 substrate. They are taken when the tip arrives at the position of 8 Å from the same start point on the substrate, for (a) simulation 1-I and (b) simulation 1- II.

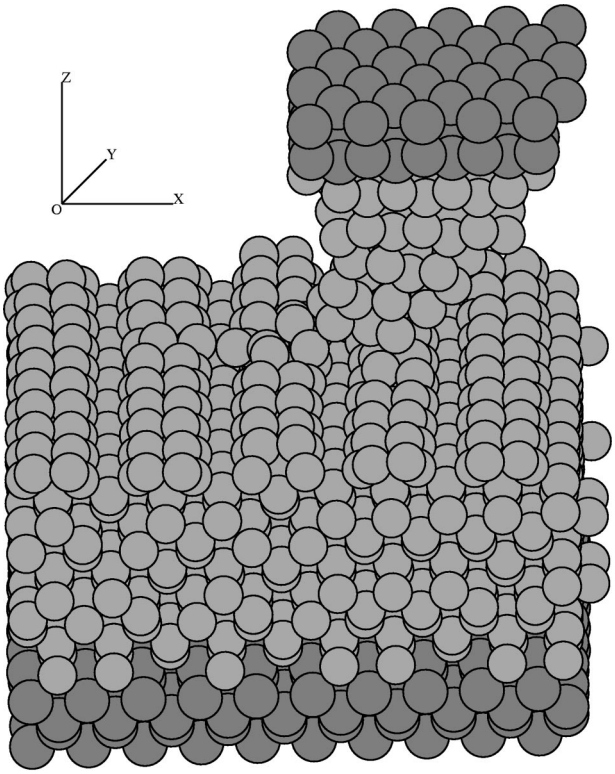

FIG. 2. The same as Fig. 1, but, for simulation 2-I.

of the tip higher than that of the substrate. Thus some atoms in the tip are attracted by the substrate more strongly than by the tip and transfer to the surface of substrate. From the three sets of snapshots, we also see that an atom is ''kicked'' out from a dimerizing row and into a trough between two dimerizing rows for all three simulations. This causes that an atom row of the dimer row loses an atom and the trough obtains an atom (for example, see Fig. 1). In the Ge(001)-2×1 surface this damage is permanent, at least by this first simulation procedure. From these computational results, it should be noted that although the difference of the tip's velocities in simulation 1-I and 1-II (or simulation 1-I and 1-III) is of one order (or more than one order) of magnitude, the atomic configurations during friction for this three simulations are very similar.

Using the second method we perform two additional simulations. In simulation 2-I the tip advances 0.1 Å every 1000 time steps, while in 2-II the tip advances 0.05 Å every 1000 time steps, corresponding to an average velocity of 3.33 and 1.666 m/s. In the two simulations the total number of time steps are 120 000 and 240 000, respectively. Snapshots for simulation 2-I and 2-II are found to be similar to each other. As an example, we show one snapshot from simulation 2-I in Fig. 2. As in set 1, wear can clearly be observed. However, we find that the results of simulation 2 are quite different from those of simulation 1 in the atomic configurations. Although a dimerizing row has been destroyed, an atom from the tip has been embedded in the dimerizing row in simulation 2-I and 2-II. This leads to the partial recovery of atom structure of the dimerizing row in simulations 2-I and 2-II. In simulation 1-I, 1-II, and 1-III a

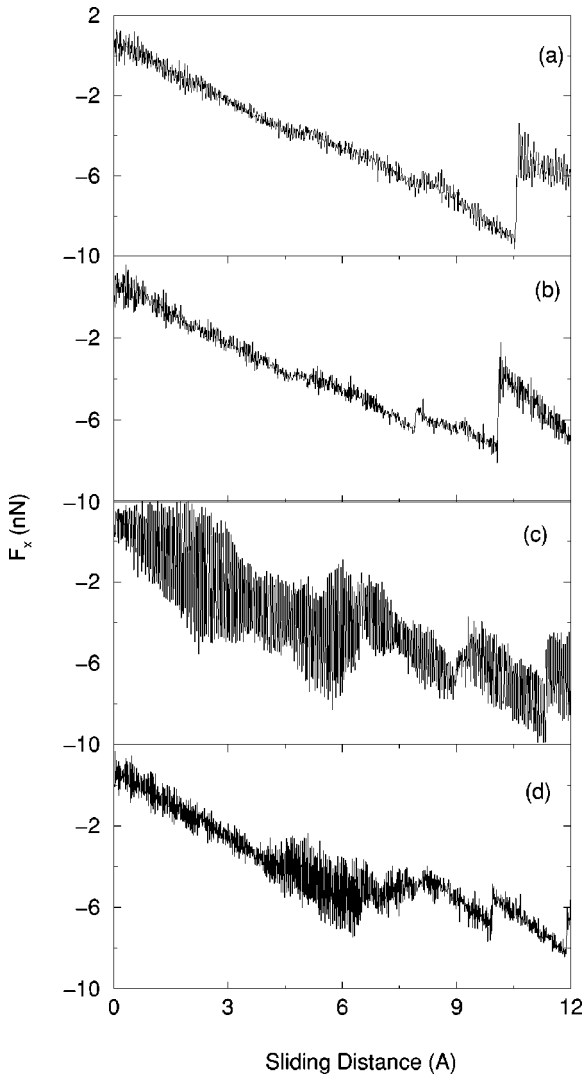

FIG. 3. The friction force F_x on the tip as a function of the sliding distance. Simulation (a) 1-II, (b) 1-II I, (c) 2-I, and (d) 2-II.

single atom row of the dimerizing row loses an atom permanently (see Fig. 1).

The atomic configurations of the first method are different from the ones of the second method, the friction properties are also different in detail. These properties can be seen from the friction force as a function of sliding distance. Because the shape of curve of the friction force versus sliding distance of simulation 1-I is almost the same as that of simulation 1-II (or 1-III) and the shape of the curve of simulation 2-I is similar to one of 2-II, as an example, we plot the friction force F_x in Fig. 3 for simulation 1-II, 1-III, 2-I, and 2-II. The friction force F_x is calculated as the sum of the X components of the forces on all atoms in the tip. From the figure it may be seen that the variation of the friction force versus sliding distance has the well-known saw-tooth shape, and F_x varies between larger and smaller values. This corresponds to the sliding and stick and slip motion. The friction force F_x is built up during the elastic stages, until yielding occurs and the force suddenly drops. The variation of the force with the sliding distance increases. This indicates that a wear occurs in the sliding process as shown in Figs. 1 and Fig. 2. Note that the saw-tooth shape of friction force versus sliding distance from the present simulations is also observed in experiments and previous theoretical simulations for a tip-substrate system.[2,7] Likewise, the amplitudes of fine oscillations in the force are larger in Fig. 3(c) than in Fig. 3(d). This is probably an effect of phonons. Finally, from Fig. 3, we can see that the the shapes of the curve of F_x versus sliding distance from 1-I, 1-II, and 1-III are different from the ones from 2-I and 2-III.

Why are the atomic configurations and the friction properties of the first method quite different from the ones of the second method, although the equivalent speed of the tip in simulation 2-I (3.33 m/s) is the same order of magnitude as the one in the simulation 1-III (2.5 m/s)? And why are the configurations and the friction properties of simulation 1-I almost the same as the ones of simulation 1-II and 1-III, although the difference of the their tip's speeds is larger than one order of magnitude? This may be explained as follows.

It is well known that the velocity of atomic thermal movement (ATM) of Ge spans the range from several m/s to several of hundreds m/s at the room temperature.[17] In experiments the advancing speed of the tip with respect to the substrate is at the range from several μm/s to several mm/s.[5–11] This velocity is very much slower than the velocity of the ATM. This means that when the tip is moving, due to the ATM, the dynamical atoms have enough time to adjust themselves to approach a quasiequilibrium state. In other words, in the experiments the tip-surface system is at a quasiequilibrium state all along when the tip is moving. However, in the first method the velocity of the tip is at the range of the velocity of ATM. In other words, the distance a dynamical atom walks by the ATM is approximatively equal to the distance the tip moves. In this case, the dynamical atoms do not have enough time to arrive at a quasiequilibrium state when the tip is moving. Thus the first method is unsuitable for the description of a friction process with the present computer resources. In the second method, the tip advances 0.05 Å every 1000 time steps, and the average component velocity of ATM of Ge atom at 50 K is equal to 75 m/s. Therefore, within 1000 time steps, a dynamical Ge atom may walk an average distance of ATM of 2.25 Å along the direction of sliding. It is a far longer distance than the distance of 0.05 Å the tip moves. This means that the tip-substrate system has enough time to reach a quasiequilibrium state when the tip advances 0.05 Å every 1000 time steps. Thus, the second method should be closer to the experimental situation than the first method. Moreover, a force that an atom ''feels'' in a quasiequilibrium state is quite different from one in a nonequilibrium state, and the atomic configuration and the friction properties are determined by the force field. Therefore, the atomic configurations and the friction properties of the first method are different from ones of the second methods, although the order of magnitude of the average speed of the tips is nearly the same in simulations 1-II and simulation 2-I. The difference of the velocities of simulations 1-I and 1-II is one order of magnitude, but both velocities are in the range of the velocity of ATM. This means that the tip substrate cannot reach a quasiequilibrium state whether the tip moves

at the speed of 50 or 5 m/s. Perhaps, this is the reason that the atomic configurations and the friction properties of simulation 1-I are almost the same as ones of simulation 1-II (or 1-III).

It should be emphasized that different from the first method, at large mean tip velocity (several m/s) the second method may be used to simulate the process of a quasiequilibrium state to another quasiequilibrium state, thus, using the second method to simulate a tip-substrate system has become possible. Note that, according to our experience, in order to simulating a quasiequilibrium process the distance the tip advances should be smaller than 0.1 Å. We also add a simulation more using the second method using equivalent velocity 16.66 m/s (tip moves 0.05 A per 100 time steps). In this simulation, we find that the atom configurations agree with the results in Fig. 1 very well, and they are different than the results in Fig. 2. This indicates that the second method is indeed similar to the first method when tip's velocity is over 16 m/s. Therefore, using fewer time steps, say, 100 steps, the second method will can not simulate a quasiequilibrium state.

We repeat all above simulations by considering a different sliding direction, i.e., now the tip moves along the *Y* direction. We obtain similar conclusions (the results are not shown here). In addition, it is found that there are more zigzag subpeaks in the curve of friction force versus sliding distance when the tip moves along the $[2\bar{1}\bar{1}]$ (*Y* direction) than along the $[0\bar{1}\bar{1}]$ (*X* direction). This is due to the fact that the sliding of atoms is easier along the $[2\bar{1}\bar{1}]$ direction than along the $[0\bar{1}\bar{1}]$ direction in the (111) face of the tip. When the tip advances along the $[2\bar{1}\bar{1}]$ direction we do not find a permanent damage in the substrate for both procedures. Since sliding may inhibit a process of building up a larger force exerting on an atom, the atomic configuration is destroyed more easily when the tip moves along the $[0\bar{1}\bar{1}]$ than along $[2\bar{1}\bar{1}]$.

Finally, we should also stress that in order to simulate the tip-substrate system more realistically the computational cell should be large. By considering this situation, the research on nanofriction using a parallel algorithm is under way in our group at present. In addition, we also did the same calculations for a Si tip-surface system. We obtained the similar conclusions to the present. The results will be published elsewhere.

In summary, to investigate the consequences of the dynamical interactions between the tip and the substrate we have performed MD simulations, employing Tersoff potential for Ge. We use two methods to simulate the system. In the first scheme the tip advances over the substrate each MD time step (the traditional method) while in the second scheme the tip advances every 1000 MD steps. We find that for small separations of the tip and the substrate a wear occurs in these simulations and the atoms of the tip transfer into the surface of the substrate. In the two methods, the friction properties, including friction force versus sliding distance and the atomic configurations, are quite different from each other in detail. In addition, it is found that the frictional properties depend on a sliding direction in the interactions between nanomaterials. From our numerical simulations we conclude that the second method is more appropriate for the description of tribology between solid and solid materials than the traditional method under the present computer resources. Using the present method simulation of a tip-substrate system has become possible.

We thank Dr M. Machholm for her reading through this manuscript with helpful suggestions. This work was supported by a Singapore-MIT Alliance Research Grant.

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