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Molecular Dynamics Simulation of Contact Process in AFM/FFM Surface Observation

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In order to clarify the contact mechanism between specimen surface and probe tip in the surface observation by the AFM (atomic force microscope) or the FFM (friction force microscope), several molecular dynamics simulations have been performed. In the simulation, a 3-dimensional simulation model is proposed where the specimen and the probe are assumed to consist of mono-crystalline copper and a carbon atom respectively and the effect of cantilever stiffness is also taken into considered. The surface observation process on a well-defined Cu{100} is simulated. The influences of cantilever stiffness on the reactive force images and the behavior of probe tip were evaluated. As a result, several phenomena similar to those observed by the actual surface observation experiment, such as double-slip behavior and dispersion in the stick-slip wave period were observed.

Keywords : AFM/FFM, Molecular Dynamics, Stick-Slip, Friction, Cantilever, Spring Constant

1. INTRODUCTION

AFM is one of the microscopes widely used in the fields of advanced technology, because it can be utilized to any material and possesses an atomic-scale resolution even in air. However, there remain unknown problems, that is, whether a surface image obtained through AFM surface measurement is expressed by a specimen surface atom or periodicity of the specimen surface and the behavior of the specimen atoms in contact point, and so on.

In order to clarify the contact mechanism between specimen surface and probe tip in the surface observation using AFM/FFM, several 3-dimensional molecular dynamics (MD) simulations have been performed by using a simple model where the cantilever stiffness is taken into considered. In this report, the influences of cantilever stiffness on the reactive forces and the behavior of probe tip were evaluated.

2. SIMULATION MODEL

The specimen and the probe are assumed to consist of mono-crystalline copper and rigid diamond, respectively. A Morse potential [1] existed is applied for the description of interaction between a pair of copper atoms. Because the actual potential between a pair of a copper and a carbon atom has not been clarified, then a Morse potential proposed by Inamura et al. [2] is applied here. In order to consider the influence of spring constant of AFM cantilever, an analytical model as shown in Fig.1 is proposed. The probe tip and the supports A, B and C are connected by means of springs in x, y and z directions, their spring constants are k_x, k_y and k_z, respectively. Support A moves at the constant sliding speed V and support B and C move at the same sliding speed as that of the probe tip with keeping the constant distance between the specimen surface. In the friction process, spring forces exert on the probe tip. Now, by taking the mass of the probe tip to be M, its position in the x direction at time t to be $x(t)$, its relative displacement to the support in the y and z directions to be $y(t)$ and $z(t)$, respectively, and the force exerted on the probe tip in each direction to be $F_x(t)$, $F_y(t)$ and $F_z(t)$, respectively, the following equations of motion are obtained.

$$M\ddot{x} = F_x(t) + k_x\{Vt - x(t)\} \quad (1)$$

$$M\ddot{y} = F_y(t) - k_y y(t) \quad (2)$$

$$M\ddot{z} = F_z(t) - k_z z(t) \quad (3)$$

where, $F_x(t)$, $F_y(t)$ and $F_z(t)$ are obtained through the MD calculations. Leap flog method is applied to the integral calculations of Eq.(1)-(3) and Newton's motion-equations.

3. SIMULATION RESULTS AND DISCUSSION

The sliding speed is set at V = 5 m/s. To reduce the noise due to the lattice vibration on the reactive forces, initial temperature is set at absolute zero. To evaluate the influence of the cantilever stiffness on friction behavior its stiffness is set at three types 1, 5, 100 N/m, respectively. These values are selected by referring to that of actual AFM cantilever. Figure 2 shows the sliding/scanning positions and directions.

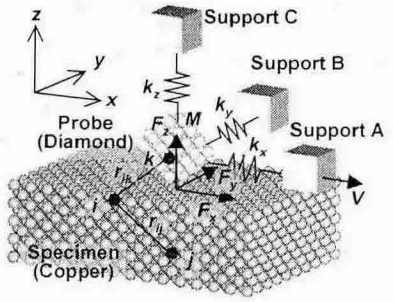


Fig.1 MD simulation model

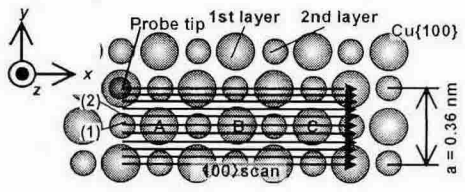


Fig.2 Sliding/scanning positions and directions

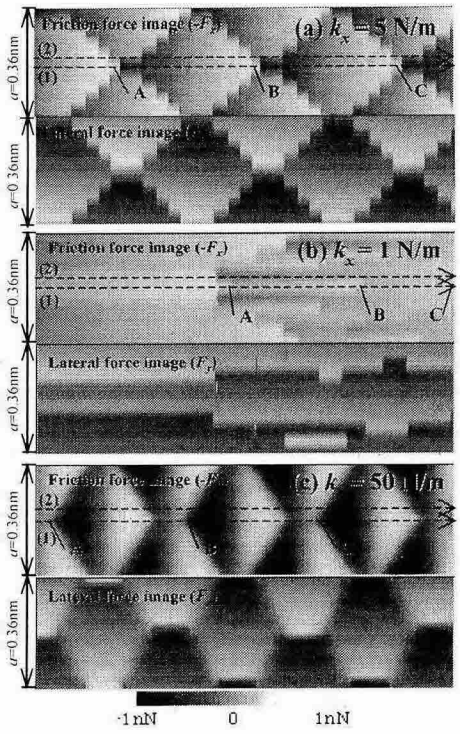
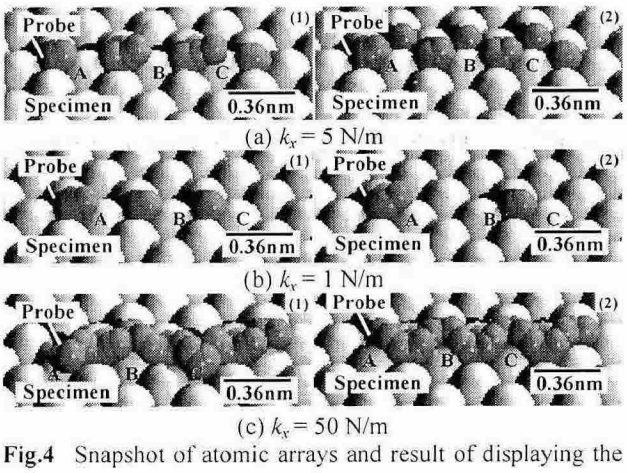


Fig.3 Reactive force images ($k_y = k_z = 5$ N/m)



(a) k_x = 5 N/m

(b) k_x = 1 N/m

(c) k_x = 50 N/m

Fig.4 Snapshot of atomic arrays and result of displaying the position of probe in every 7.5 ps (broken line in Fig.3)

The influences of cantilever stiffness in the scan direction k_x on the reactive forces are described here. Figure 3 shows the obtained reactive force (spring force) images. The horizontal direction of the force images is correspondent to the position of the support in the x-direction. Figure 4 shows the snapshot of atomic arrays and the result of displaying the position of the probe in every 7.5ps, where (1) and (2) show the case of (1) and (2) in Fig.2. Figure 5 shows the variation of the spring force in the sliding direction as a function of the position of support in x-direction. In Fig.3 to Fig.5, (a) to (c) shows the result in the case of k_x = 5, 1, 50 N/m, respectively.

From the comparison between Fig.3(a) and (c), it can be understood that the period of these images is corresponding to that of Cu<100> atomic arrays and the lattice constant of Cu, even though the pattern and the contrast of Fig.3(a) and (c) are different each other. From the comparison between Figs.4(a)(c) and 5(a)(c), it can be understood that the atomic-scale stick-slip phenomenon [3] (2-dimensional [4]) is hardly observed in the case of k_x = 50 N/m, while that is clearly observed in the case of k_x = 5 N/m.

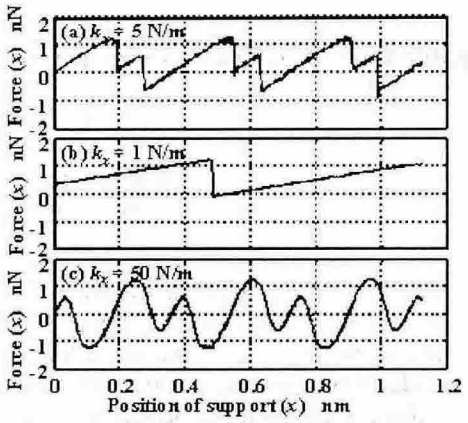


Fig.5 Relationship between friction force (x) and position of the support (x) (in case of Fig.3(2))

The atomic arrays of Cu{001} is hardly recognized from Fig.3(b). This reason is due to the double slip phenomenon [3] in which the probe slides over 2 atomic distances of specimen surface and the dispersion in the period of stick-slip phenomenon (see Figs.4(b) and 5(b)). These phenomena are frequent when the stiffness of the cantilever is relatively low and often observed through actual AFM/FFM experiments [3].

4. CONCLUSIONS

In order to clarify the contact mechanism in the AFM/FFM surface observation, especially the influence of cantilever stiffness on reactive forces, several molecular dynamics simulations have been performed. Conclusions obtained are summarized as follows:

(1) The atomic arrays of surface are hardly recognized from the force images, when the cantilever stiffness is relatively low and the double slip phenomenon and the dispersion in the period of stick-slip phenomenon are often generated.

(2) The molecular dynamics simulation has an advantage for the prediction of period, pattern and contrast of atomic images of solid surfaces in the AFM/FFM observation.

5. ACKNOWREDGEMENT

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