SIMULATION ANALYSIS OF CONTACT PROCESS IN AFM SURFACE OBSERVATION

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SUMMARY
In order to dynamically clarify the contact mechanism between specimen surface and probe tip in the surface observation, by using atomic force microscope (AFM) or friction force microscope (FFM), 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 rigid diamond, respectively. The atomic-scale stick-slip phenomenon is also taken into considered there. The surface observation process on a well-defined Cu{100} crystal is simulated. From the simulation results, it is verified that the surface images and the 2-dimensional atomic-scale stick-slip phenomenon just as observed through the real AFM/FFM surface observation can be detected from spring force acting on the cantilever. From the evaluation of the behaviour of specimen surface atoms, the importance of the consideration of specimen stiffness in deciding the cantilever properties is also understood. Influence of the probe tip shape on the force images is also evaluated. From these results, it is verified that the behaviour of the specimen surface as well as the solid surface images in the AFM/FFM surface observation can be understood by the molecular dynamics simulations by using the model presented here.

Keywords: AFM, molecular dynamics, stick-slip, friction, cantilever, 2-dimensional friction phenomenon

1 INTRODUCTION
So many surface analyses have been performed on the atomic scale with the appearance of the new surface measurement instruments, such as scanning tunnelling microscope (STM) and atomic force microscope (AFM). Especially, AFM is one of the microscopes widely used in the fields of advanced technology, because it can be utilised to any material and possesses an atomic-scale resolution even in air. The atomic-scale stick-slip phenomenon was discovered by Mate et al. [1] through the AFM or FFM (friction force microscope) surface measurement for the first time. It is a unique phenomenon in such friction process at an atomic level. Recently, many researchers have been making efforts to clarify the atomic-scale friction mechanism using AFM or FFM, and some worthwhile insights are reported so far [2, 3].

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 behaviour of the specimen atoms in contact point, and so on. Komiyama et al. [4], have been simulated on AFM surface image with or without point defect by using Morse potential function and investigated on possible resolution limit of AFM. However, they have never taken into account of the cantilever and the specimen stiffness. Sasaki et al. [5] or Hölscher et al. [6], have been analysed on image pattern of FFM by using 3-dimensional model where the cantilever stiffness is taken into considered, even though never taken into account of specimen stiffness. Many researchers have also been simulated on contact process between a slider or probe of AFM/FFM and a specimen surface by using the molecular dynamics method [7-11]. As a result, they have been reported on various interesting phenomena such as the atomic-scale stick-slip phenomenon, and have been clarified on the atomic interaction in the contact process or the surface images to some extent. However, they have also never taken into account of cantilever stiffness, even though taken into account of the specimen and probe stiffness there.

The parts of the authors had been simulated on the atomic-scale stick-slip phenomenon by using 2-dimensional molecular dynamics simulations [12]. In this paper, to dynamically clarify the contact mechanism between specimen surface and probe tip in the surface observation using AFM/FFM, especially, the clarification of detecting mechanism of force images and the influence of the probe tip shape on force images, several 3-dimensional molecular dynamics simulations have been performed by using a simple model where the cantilever stiffness is taken into considered. In the simulations, the force images due to the variation of the spring forces, the dynamics of the specimen surface atoms as well as that of the probe tip are investigated. Various phenomena, such as the existence of the 2-dimensional atomic-scale stick-slip phenomenon [2] even in the 1-dimensional sliding process and the influence of probe tip shape on the force images are discussed.

2 SIMULATION MODEL
The specimen and the probe are assumed to consist of mono-crystalline copper and rigid diamond, respectively. The scanning direction of the probe is taken as $x$ axis and direction perpendicular to the sliding direction is taken as $y$ axis. The $x$-$y$ plane corresponds to specimen surface. The direction perpendicular to the specimen surface is taken as $z$ direction. They are chosen according to a right hand coordinate system. A Morse potential [13] exists 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. [14] is applied here. 723 copper atoms are subject to the simulations. In order to consider the influence of spring constant of AFM cantilever, an analytical model as shown in Figure 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 \(t\) is \(x(t)\), 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.

\[
M \ddot{x} = F_x(t) + k_x \left[ y(t) - x(t) \right]
\]

\[
M \ddot{y} = F_y(t) - k_y y(t)
\]

\[
M \ddot{z} = F_z(t) - k_z z(t)
\]

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 (MD calculations), here.

### 3 IDEAL REACTIVE FORCE IMAGE

Ideal reactive force images are obtained by displaying the reactive forces acting on the probe assuming the stiffness of the spring to be infinite and the probe as well as the specimen to be perfect rigid bodies respectively, in Fig.1. Here and in the simulations, the \(x\), \(y\) and \(z\) axes correspond to \([100]\), \([010]\) and \([001]\) of copper respectively, and \([001]\) of copper corresponds to the specimen surface of well-defined in an atomic level. The scan (sliding) positions or directions of the probe are set as shown in Figure 2 \((a \times 3a)\). (1) and (2) in Fig. 2 are the cases where the probe slides just on top of the surface atoms or on the position shifted in \(a/10\) \((a\) is lattice constant of copper: \(a = 0.36\) nm) from top of the surface atoms, respectively. In order to investigate the influence of the difference of probe tip shape on force images, a carbon atom and a diamond lattice are selected as the probes, as shown in Figure 3.
forces are positive when the spring forces affect the probe in the positive direction of the y and z-axes (\(F_y, F_z\)), respectively.

The difference between Fig.4 and Fig.5 is remarkable.

\begin{figure}[h]
\includegraphics[width=0.5\textwidth]{friction_image}\caption{(a) Friction force image}
\end{figure}

\begin{figure}[h]
\includegraphics[width=0.5\textwidth]{lateral_force_image}\caption{(b) Lateral force image}
\end{figure}

\begin{figure}[h]
\includegraphics[width=0.5\textwidth]{normal_force_image}\caption{(c) Normal force image}
\end{figure}

Figure 5: Ideal force images by a diamond lattice probe

In Fig.4, the reactive force images by the each specimen surface atom has been clearly expressed, and the position of the each specimen surface atom can be clearly also grasped. On the other hand, in Fig.5, the pattern of which reactive force images by each atom is complicated, and the phase of the images is retarded in \(a/2\) comparing with Fig.4. However, the specimen surface atom interval can be grasped from the periodicity of the images.

4 SIMULATION RESULTS AND DISCUSSION

Table 1 shows the simulation parameters applied here, respectively. To reduce the noise due to the lattice vibration on the reactive forces, initial temperature is set at absolute zero. The cantilever stiffness is set at 5 N/m in both x, y and z directions referring to that of actual AFM cantilever.

4.1 In case of a carbon atom probe

Figure 6 shows the variation of the spring forces as a function of the position of support in x-direction, and Figure 7 shows the snapshot of atomic arrays and the result of displaying the position of the probe in every 7.5 ps, where (a) and (b) show the case of (1) and (2) in Fig.2.
In Fig. 6, the friction force (spring force) is positive when the spring $k_x$ in Fig. 1 is extended ($-F_x$), on the other hand, the lateral and normal forces (spring forces) are positive when the spring $F_y$ and $F_z$ in Fig. 1 are compressed ($F_y$, $F_z$), respectively.

In Fig. 6(a), generation of 3 stick-slip waveforms are confirmed and the state that the probe tip slides on top of 3 specimen surface atoms are understood from friction and normal forces. This behavior is also understood by seeing Fig. 7(a). This means that the atomic-scale stick-slip phenomenon can be detected from the spring force acting on the cantilever by using proposed model. The stick-slip wave period is equal to the copper lattice constant $a = 0.36$ nm, or it is proven that the simulation can reproduce the stick-slip phenomenon on the atomic-scale just like observed through AFM (FFM) surface observation [1]. Still, the atomic-scale stick-slip phenomenon which is an elementary process of the friction can be also fundamentally explained according to the model of Tomlinson [15].

On the contrary, the generation of 2-dimensional atomic-scale stick-slip can be grasped by comparing the friction and the lateral forces in Fig. 6(b) and snapshot of Fig. 7(b). In this case, the probe tip sticks by avoiding the atoms in the specimen surface primary layer. That is, the generation of wraparound of the probe tip and the 2-dimensional friction process even in 1-dimensional sliding process [2] are confirmed. The probe tip does not rest and slips at comparatively low speed even through in the stick process. The reason why is caused by the stick-slip behavior of specimen surface atom due to their elasticity as shown in Fig. 8.

Figure 9 shows the reactive force (spring force) images by using a carbon atom probe. The horizontal direction of the force images is correspondent to the position of the support in the x-direction.

In the variation of the friction force image, the rapid change from the thin gray to the thick gray shows the slip. On the other hand, the change from the thick gray to the thin gray shows the stick. From the change of the friction and lateral forces, the generation of 2-dimensional stick-slip phenomenon even in 1-dimensional sliding process as well as the discrimination of specimen surface atoms can be confirmed. On the contrary, the discrimination of specimen surface atoms becomes relatively hard by seeing the normal force.
image because its change is smaller than those of the friction and lateral forces. This indicates the importance of choosing the stiffness of the cantilever dependent on the elasticity of the specimen.

4.2 In case of a diamond lattice probe with flat tip

Figure 10 shows the variation of the spring forces as a function of the position of support in x-direction, and Figure 11 shows the snapshot of atomic arrays and the result of displaying the position of the probe in every 7.5 ps, where (a) and (b) show the case of (1) and (2) in Fig. 2.

The stick-slip waveforms in the friction force in both Figs. 10(a) and 10(b) are different from those in the case of single-atom probe tip (see Fig. 6). The 2-dimensional friction process in the lateral force in Fig. 10(b) is weakened than that of Fig. 6(b), as well. In the change of the normal force in both Figs. 10(a) and 10(b), the state in which the probe tip slides on the ups and downs due to the specimen surface atoms is not observed. It is different from the result due to the single-atom probe tip (see Fig. 6). In this case, it seems that the contact surface of the probe is consisted of multiple atoms (5 atoms), so that the atomic arrays hardly take that of the potential energy minima. These phenomena can be easily grasped by seeing Fig. 11, as well.

Figure 12 shows the reactive force (spring force) images by using a carbon atom probe. The horizontal direction of the force images is correspondant to the position of the support in the x-direction.

It is proven that the force images in Fig. 12 is retarded in a/2 in comparison with Fig. 9. The pattern of friction and lateral force images in Figs. 9 and 12 resemble well each other, however, the difference between both can be grasped by seeing the stick-slip wave form on which a small stick-slip wave is superposed when the probe slides on top of the specimen surface atoms and the fact that the normal force keeps a constant value much bigger than that when a mono-atom probe tip is applied (Fig. 10(a)).

Figure 11: Snapshot of atomic arrays and the result of displaying the position of the atom P in Fig. 3 in every 7.5 ps (in case of a diamond lattice probe)
5 CONCLUSIONS

In order to dynamically clarify the contact mechanism in the AFM/FFM surface observation, especially the influence of the probe tip shape on the surface images, 3-dimensional molecular dynamics simulations have been performed by using a simple model on cantilever stiffness effect. Conclusions obtained are summarised as follows:

- 2-dimensional atomic-scale stick-slip phenomenon even in 1-dimensional sliding process can be analysed through the molecular dynamics simulation by using present model.
- The importance of choosing the stiffness of the cantilever dependent on the elasticity of the specimen is confirmed.
- Though the friction and lateral force images by mono-atom probe and a lattice probe often resemble each other by originating from the periodicity of the specimen surface, it is locally different.
- The fluctuation of the reactive forces by using a lattice probe is smaller than those by using mono-atom probe.
- The normal force image greatly changes by the probe tip shape. The probe tip shape can be distinguished referring to the matter described in (3) to here.
- The molecular dynamics simulation considering stiffness of the cantilever has an advantage in estimating the various phenomena in AFM/FFM surface observation.

6 ACKNOWLEDGEMENT

This research was partially sponsored by the Grant-in-Aid for Encouragement of Young Scientists (No.13750113) from the Japan Society for the Promotion of Science, and the Sasakawa Scientific Research Grant of the Japan Science Society.

7 REFERENCES