Friction Phase Diagram of Frenkel-Kontorova Atomistic Model

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1. Introduction

The atomistic origin of friction forces stemming from interfacial atomic-interactions has been investigated from both of theoretical and experimental viewpoints [1,2]. By studying frictional properties of nano-structured materials, novel understandings explaining the atomistic mechanisms of static/dynamic friction and that of superlubricity appearing at incommensurately contacting surfaces have been obtained. For applying the superlubricity mechanisms for practical use, it is crucial to determine the conditions for its appearance, describing how we design and synthesize superlubric systems. To this end, we need to develop realistic interatomic potentials of metals and semiconductors, and also develop the tribological molecular dynamics simulation at elevated-controlled temperature. This study has presented the atomic-scale friction simulation at elevated temperature. The friction diagram, specified by the parameters of sliding velocity and adhesive interaction has been investigated. Two regimes such as friction and superlubricity appear and it has been investigated how atmospheric temperature affects the sliding properties in friction and superlubricity regime.

2. Frenkel-Kontorova atomistic model

The atomistic friction model, given by

$$H(\{p_i\},\{r_i\}) = \sum_i^N \frac{p_i^2}{2} + \sum_i^N \{\frac{1}{2}k(r_{i+1} - r_i - \ell)^2 + \frac{f}{2\pi}\sin(2\pi r_i)\}, \quad (1)$$

is studied. p_i, k, l and k stand for momentum, inter-atomic interaction, lattice constant, and adhesive interaction. We obtained the friction phase diagram, shown in Fig.1, representing atomistic-scale frictional properties in terms of two parameters such as velocity and adhesive force.

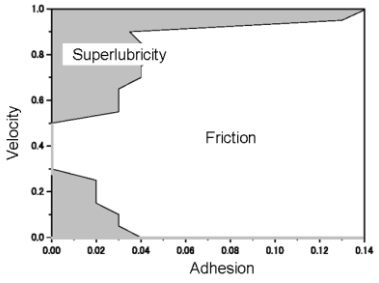

Fig. 1 Friction phase diagram

Two regimes appear in the diagram. In the superlubricity regime, the superlubric state appears, i.e., two contacting solid surfaces slide without any resistance. In the friction regime, on the other hand, the energy dissipation occurs. It has been found that the translational kinetic energy is transferred into the kinetic energy of the internal motions.

3. Frictional properties at elevated temperature

We use the thermostat molecular dynamics method developed by Nosé to control the temperature of the atomistic model. As shown in Fig.2, it is found that we have successively controlled the model temperature at kT=0.1 and kT=0.2, respectively.

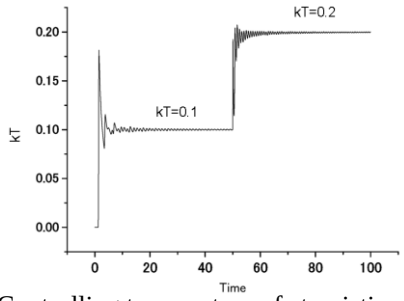

Fig.2 Controlling temperature of atomistic model

Figure 3 shows the calculated frictional properties, representing how the upper body slides after pushing the body at the specified initial velocity. In superlubricity regime, for example, the position of mass center moves at constant velocity. This study also clarifies how the friction phase diagram is modified at elevated temperature.

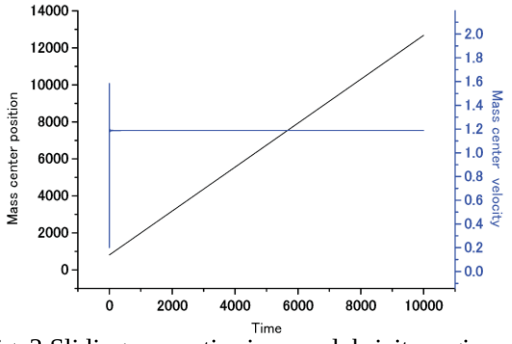

Fig. 3 Sliding properties in superlubricity regime

4. References

[1] A. Erdemir and J. -M. Martin, Superlubricity, Elsevier (2007).
[2] M. Hirano, Atomistics of friction, Surface Science Reports, 60, 8, 159-201 (2006).