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FRICTION OF FRENKEL-KONTOROVA ATOMISTIC MODEL AT ELEVATED TEMPERATURE

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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 those 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 examined how atmospheric temperature affects the sliding properties in friction and superlubricity regime.

The atomistic friction model, given by

$$H(\{p_i\},\{q_i\}) = \sum_i^N \frac{p_i^2}{2} + \sum_i^N \{\frac{1}{2}(q_{i+1} - q_i - \ell)^2 + \frac{f}{2\pi}\sin(2\pi q_i)\}, \tag{1}$$

is studied. p_i q_i, ℓ, and f stand for the momentum and position of atoms, the mean distance between adjacent atoms, and adhesive interaction. This is one-dimensional Frenkel-Kontorova model with kinetic energy terms. The periodicity length of the sinusoidal potential in Eq.(1) is taken as a unit, while ℓ is assumed to be equal to the golden mean number$\dfrac{1+\sqrt{5}}{2}$, thus obtaining the incommensurate friction system.

The dynamics of friction has been studied after the upper solid surface at the ground state is pushed with initial sliding velocity $P(0)$, that is, the Hamiltonian dynamics conserving

the energy. It has been shown how the position and sliding velocity of mass center change with time. We thus obtained the friction phase diagram, shown in Fig.1, representing atomistic-scale frictional properties in terms of two parameters such as initial velocity $P(0)$ and adhesive interaction f.

Two regimes appear in the diagram as shown in Fig.1. In the superlubricity regime, the superlubric state appears, i.e., two contacting solid surfaces slide without any resistance. The recurrence phenomenon occurs persistently; this regime repeats increasing and decreasing the translational kinetic energy with time. The friction force averaged over the recurrence time exactly vanishes. The sliding distance increases linearly with time. On the other hand, in the friction regime, the energy dissipation occurs; the translational kinetic energy is transferred into the kinetic energy of the internal motions. The upper surface slides but finally ceases to slide for sufficiently large times. The friction occurs in this regime.

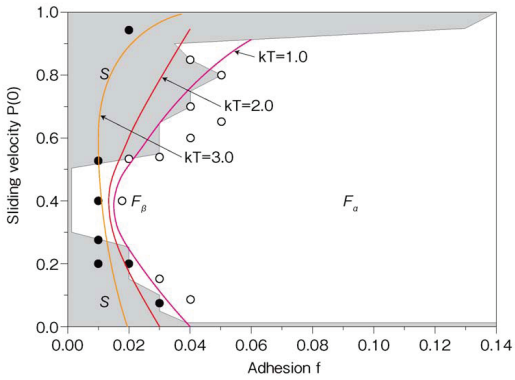

Figure 1 Friction phase diagram at elevated temperature

It has been examined how temperature affects the sliding properties. The extended system molecular dynamics method [3] has been used for controlling the temperature of the atomistic model. The actual atomistic model is contacted against the thermostat, enabling to make the atomistic model at desired temperature. It has been confirmed that the thermodynamic properties of the system can be controlled under desired temperature.

The sliding properties at elevated temperature were also demonstrated. This study will discuss how the friction phase diagram is modified by increasing the system temperature. In superlubricity regime, when increasing temperature, the superlubricity regime is likely to shrink at higher sliding velocity. This can be due to the fact the cancellation of forces acting on atom is unlikely to occur at high temperature and high sliding velocity under adiabatic theorem.

In summary, the sliding properties Frenkel-Kontorova atomistic model has been examined by the extended system molecular dynamics method. It has been confirmed that the molecular dynamics method could successfully control the system temperature. The sliding properties of the model has been shown at elevated temperature, and it has been demonstrated how the friction phase diagram is modified by temperature effect.

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