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ON THE STABILITY OF THE STATE OF SUPERLUBRICITY

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ABSTRACT

Superlubric state was found in a molecular dynamic simulation study of incommensurate Frenkel-Kontorova model [1]. This finding was supported by an experimental study with ultra-high vacuum scanning tunneling microscopy [2]. Recently, superlubric state was experimentally found in friction of tungsten tip sliding on graphite in ambient laboratory air [3]. Since there are likely to be some impurities at the frictional interface in this experiment, the experimental result indicates that the superlubric state is stable against contaminations of impurities. Here we examined this indication by performing a molecular dynamic simulation study of incommensurate Frenkel-Kontorova model with impurities. In case of attractive impurities, the impurities were placed at the peaks of the sinusoidal substrate potential; in case of repulsive ones, they were placed at the bottoms. The concentration of the impurities was set to be 1/1500. The interaction potential between the impurities and the sliding atoms was expressed by Gaussian function. The strength of the interaction was varied from 1 to 3 times of the amplitude of the sinusoidal substrate potential. For each value of the strength of the impurities, motions of the sliding atoms were observed for various initial velocities and amplitudes of the substrate potential. Observing the sliding motions, friction diagrams, which show where in the parameter space friction and superlubric states are, were constructed. If the velocity of the center of mass of the sliding crystal decreased, the sliding motion was defined to be in frictional state. If the center of mass velocity did not decrease, the sliding motion was defined to be in superlubric state. The obtained friction diagrams showed that if the interaction strength between the impurities and the sliding atoms was smaller than 3 times of the amplitude of the substrate potential, the friction diagram remained unchanged. Hence, the superlubric state was shown to be stable against the weak impurities.

1. INTRODUCTION

Superlubric state was found in a molecular dynamic simulation study of incommensurate Frenkel-Kontorova model [1]. This finding was supported by an experimental study with ultra-high vacuum scanning tunneling microscopy [2].

The friction force is the drag against sliding, appearing when two solid surfaces move relatively. Then, the energy is dissipated during sliding. The friction is a problem of how the energy can be dissipated. The data of friction forces usually measured contains many unknown factors: surface roughness, fractures, plastic deformations, poisoning by contaminants, etc. It is difficult, therefore, to study the origin of friction force from the experimental data available at present. More recent experimental studies try to exclude many of the unknown factors by preparing well-defined surfaces.

This study theoretically considers the stability of the state of superlubricity by assuming two clean solid surfaces, which is generated by intrinsic factors, such as molecular interactions between constituent atoms, not by extrinsic factors such as surface asperities or surface contaminants. Friction is formulated as a problem of whether or not given (sliding) kinetic energy for the translational motion dissipates into the kinetic energies for the internal motions during sliding. We shall study the dynamics in friction by using the Frenkel-Kontorova model with kinetic energy terms.

2. EFFECT OF IMPURITIES ON SUPERLUBRIC STATE

Recently, superlubric state was experimentally found in friction of tungsten tip sliding on graphite in ambient laboratory air [3]. Since there are likely to be some impurities at the frictional interface in this experiment, the experimental result indicates that the superlubric state is stable against contaminations of impurities. Here we examined this indication by performing a molecular dynamic simulation study of incommensurate Frenkel-Kontorova model with impurities. In case of attractive impurities, the impurities were placed at the peaks of the sinusoidal substrate potential; in case of repulsive ones, they were placed at the bottoms. The concentration of the impurities was set to be 1/1500. The interaction potential between the impurities and the sliding atoms was expressed by Gaussian function. The strength of the interaction was varied from 1 to 3 times of the amplitude of the sinusoidal substrate potential. For each value of the strength of the impurities, motions of the sliding atoms were observed for various initial

velocities and amplitudes of the substrate potential. Observing the sliding motions, friction diagrams, which show where in the parameter space friction and superlubric states are, were constructed. If the velocity of the center of mass of the sliding crystal decreased, the sliding motion was defined to be in frictional state. If the center of mass velocity did not decrease, the sliding motion was defined to be in superlubric state. The obtained friction diagrams showed that if the interaction strength between the impurities and the sliding atoms was smaller than 3 times of the amplitude of the substrate potential, the friction diagram remained unchanged. Hence, the superlubric state was shown to be stable against the weak impurities.

3. STABILITY OF SLIDING DISTANCE

The friction diagram, specified by the adhesive strength and the sliding velocity, has been investigated while changing the sliding distance of the crystal. It has been found that the area of the superlubric regime in the friction diagram is likely to shrink, but the area is unlikely to disappear by the molecular dynamics simulation.

4. SUMMRY

Main The conclusions are summarized as follows.

1. The state of the superlubricity is stable against the existence of the imperfections such as impurities and the lattice defects.
2. The superlubricity is likely to appear by strengthening the spring constant of the sliding crystal.
3. The durability of the superlubricity is obtaiend at the large the sliding speed.

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