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Velocity-dependent threshold behavior of wearless nano-friction

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Abstract

A law of friction accompanying steady sliding motion between crystal lattices constituting a nano-electromechanical system (NEMS) was revealed by molecular dynamics simulations using simplified models. A threshold phenomenon was predicted as a common feature characterizing dependence of the wearless frictional resistance on the sliding velocity v_{stroke}. The threshold sliding velocity v_{th} linearly depends on the lattice-constant ratio, which was turned out to be a key parameter determining v_{th}. The increased dynamic-frictional force in the case of $v_{\text{stroke}} > v_{\text{th}}$ possibly reflects enhanced rate of energy dissipation via anharmonicity of the interatomic potential due to resonant excitation of phase-matched normal phonon modes in the crystal lattices sliding relative to each other.
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1. Introduction

In order to develop methods of designing artificial materials of desired frictional characteristics for nano-electromechanical systems, a better atomistic understanding of wearless sliding friction is indispensable. Although there have been a number of studies on dynamic friction from the atomistic point of view in terms of theoretical or computational physics, the obtained knowledge is still fragmentary and thus is quite insufficient to apply to design of artificial materials for sub-micrometer size mechanisms and actuators. It is indeed well known that wearless dynamic friction is a typical energy-dissipation phenomenon, where the atoms in the solid execute chaotic trajectories in phase space owing to anharmonicity of the interatomic potential, resulting in ergodic behavior [1]. But the universal features and their atomistic origin of wearless-frictional characteristics of mesoscopic solid materials, e.g. dependence of the frictional force on the applied load and the sliding velocity have not been elucidated yet.

In previous systematic analyses based on molecular dynamics (MD) simulations, we have revealed some features and laws of wearless friction accompanying steady sliding motion between mesoscopic single crystals and nanostructured materials [2–7]. A significant feature is that unlike the frictional characteristics of a macroscopic solid system wearless-frictional characteristics of an isolated mesoscopic system reflect phonon modes of the lattices sliding relative to each other. These studies suggested possibility of designing artificial materials of desired frictional characteristics for sub-micrometer size mechanisms and actuators by the method of "phonon-band engineering" utilizing nano-fabrication technology [4,5].

In this article we present an investigation of threshold behavior characterizing dependence of the wearless-frictional resistance on the sliding velocity.

2. Simulation methods

Molecular dynamics simulations of friction between the atomically flat surfaces of two closest-packed lattices were carried out using a two-dimensional (2D) model illustrated

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in Fig. 1. In this article, particles belonging to the bottom layer of lattice A are referred to as fixed particles. Particles belonging to the top layer of lattice C are referred to as stroking particles. We refer to the other particles as passive particles, the total number of which was in the range 2400–10,880 in the present simulations. Lennard-Jones (LJ) potential was assumed between the particles; this simple potential was chosen since the purpose of this work is to study universal law independent of adiabatic potential of a specific material. Existence of the interface was taken into account by assuming ε_{AC} (the depth of the LJ potential between A and C particles) equal to 1/100–3/10 of ε_{AA} (that between two A particles) and ε_{CC} (that between two C particles). The averaged horizontal lattice constant of crystal A (or C) was set equal to the distance σ_{AA} (or σ_{CC}) that minimize LJ potential between two A (or C) particles. A periodic boundary condition was imposed on the lateral boundaries. The stroking particles were fixed at first until thermalization of the passive particles. The distance L_z between the stroking and the fixed layers was adjusted prior to each experiment of sliding friction so that initial load agrees with desired values. Once adjusted, L_z was kept constant throughout the simulation run. Then, a simulation of steady sliding movement was started at time $t = 0$. The stroking particles were made to move along the interface at a constant sliding velocity v_{stroke} much slower than root mean square of thermal velocity of the passive particles. The same velocity v_{stroke} was also added to the thermal velocity of each passive C particle at $t = 0$. Motion of the passive particles was traced by solving equations of motion numerically using symplectic integrator to the second order. Applied load N and frictional force F_{fr} as functions of time t are obtained by

$$N = (F_{sz} - F_{fz})/2L_x, \quad (1)$$

$$F_{fr} = (F_{fx} - F_{sx})/2L_x, \quad (2)$$

where L_x is the distance between the lateral boundaries. F_{fx} is a parallel component and F_{fz} is a perpendicular component of a resultant of forces exerted on the fixed particles; F_{sx} is a parallel component and F_{sz} is a perpendicular component of a resultant of forces exerted on the stroking particles at the time t. In this article, σ_{AA}, m_A (the mass of an A particle), and ε_{AA} are adopted as units of length, mass, and energy, respectively. ε_{AA} is also adopted as a unit of temperature. MD simulations were carried out systematically for a variety of values of the simulation parameters: σ_{CC}, 0.75–1.25; ε_{CC}, 0.5–100.0; m_C (the mass of a C particle), 0.2–512.0; T (mean temperature), 0.05–1.2; N, −0.5–3.5; v_{stroke}, 0.02–0.65. After each simulation run we ascertained whether wear had taken place or not, and only data under wearless condition are used for analyses in the following sections.

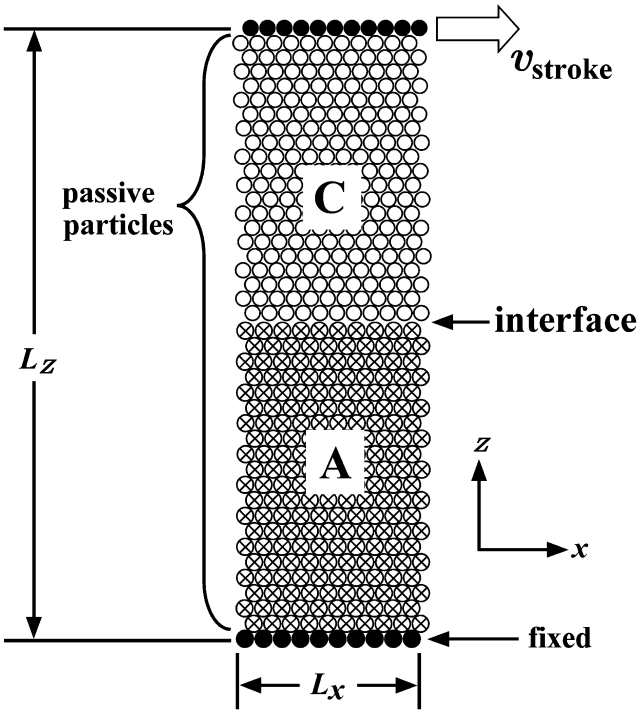

Fig. 1. Two-dimensional MD simulation model used here to study dynamic-frictional characteristics of two single crystals whose atomically flat surfaces are placed in sliding contact. The initial configuration is shown. The total number of the passive particles was in the range 2400–10,880 in the present study.

3. Results

A large number of simulation data were arranged as dependence of the dynamic-frictional force on the sliding velocity v_{stroke}, the applied load N, and the mean temperature T averaged over the passive particles. The results obtained under the experimental conditions that $\sigma_{CC}/\sigma_{AA} = 34/32, 35/32, 36/32$, $\varepsilon_{CC}/\varepsilon_{AA} = 1.0$, $\varepsilon_{AC}/\varepsilon_{AA} = 0.1$, $m_C/m_A = 1.0$ are shown in Figs. 2–4 as typical exam-

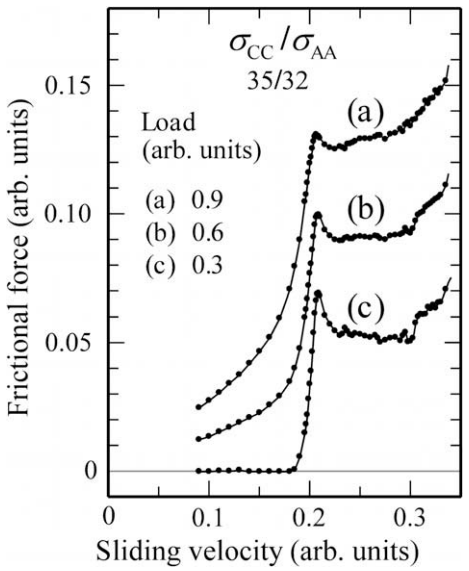

Fig. 2. Typical dependence of the wearless-frictional force on the sliding velocity. The result in the case of the lattice-constant ratio $\sigma_{CC}/\sigma_{AA} = 35/32$ is shown for the applied load $N = 0.3, 0.6, 0.9$.

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