

# Velocity-Dependent Threshold Phenomenon of Nano-Friction Predicted by Non-Equilibrium Molecular Dynamics Studies

Keiji Hayashi, Taiga Mori, Ryouhei Taniguchi, Keisuke Nakamura and Daimu Tajima

Graduate School of Engineering, Kanazawa Institute of Technology  
7-1 Ohgigaoka, Nonoichi, Ishikawa 921 - 8501, Japan

## ABSTRACT

A law of friction accompanying steady sliding motion between crystal lattices constituting a nano-electromechanical system (NEMS) was revealed by non-equilibrium molecular dynamics simulations. A threshold phenomenon was predicted as a common feature characterizing dependence of the wearless-frictional resistance on the sliding velocity  $v_{\text{stroke}}$ . The threshold sliding velocity  $v_{\text{th}}$  linearly depends on the lattice-constant ratio, which was turned out to be a key parameter determining  $v_{\text{th}}$ . 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.

**Keywords:** phonon-band engineering, nanotribology, complex system, non-equilibrium molecular dynamics

## 1 INTRODUCTION

In order to develop methods of designing artificial materials of desired frictional characteristics for nano-electromechanical systems (NEMS), 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]. One of the significant

features is threshold behavior characterizing dependence of the wearless-frictional resistance on the sliding velocity [3]. Unlike the frictional characteristics of a macroscopic solid system, wearless-frictional characteristics of a mesoscopic system reflect phonon modes of the lattices sliding relative to each other, for the case where coupling between the dynamic-frictional system and a heat bath is weak. These studies suggested possibility of designing artificial materials of desired frictional characteristics for NEMS by the method of “phonon-band engineering” utilizing nanofabrication technology [4, 5].

In this article we present an investigation of the threshold phenomenon under the stationary condition.

## 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 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 2400-10880 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  $\varepsilon_{AC}$  (the depth of the LJ potential between A and C particles) equal to 1/100 - 3/10 of  $\varepsilon_{AA}$  (that between two A particles) and  $\varepsilon_{CC}$  (that between two C particles). The averaged horizontal lattice constant of crystal A (or C) was set equal to the distance  $\sigma_{AA}$  (or  $\sigma_{CC}$ ) 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  $v_{\text{stroke}}$  much slower than root

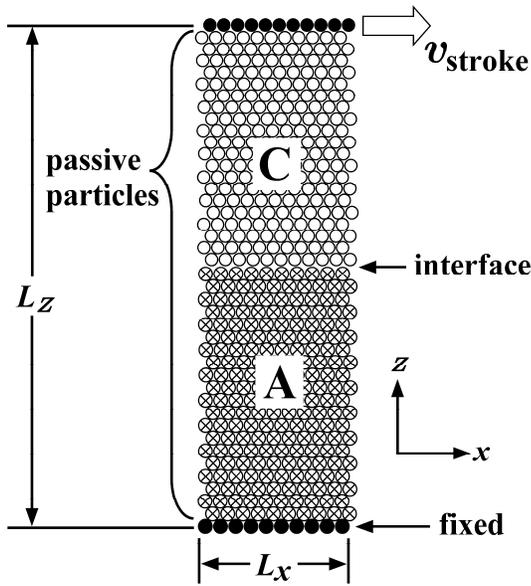


Fig.1. Two-dimensional MD simulation model used here to study dynamic-frictional characteristics of two single crystals whose atomically flat surfaces are placed in sliding contact. The initial configuration is shown. The total number of the passive particles was in the range 2400 - 10880 in the present study. The Nose-Poincaré thermostats were used to maintain a local quasi-temperature of the passive particles neighboring the stroking and the fixed layers without drift during a simulation run.

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. The Nosé-Poincaré thermostat [8] was used to maintain a local quasi-temperature [2] of the passive particles neighboring the stroking and the fixed layers without drift during a simulation run. The applied load  $N$  and the frictional force  $F_{fr}$  are obtained by

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

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

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,  $\sigma_{AA}$ ,

$m_A$  (the mass of an A particle), and  $\varepsilon_{AA}$  are adopted as units of length, mass, and energy, respectively.  $\varepsilon_{AA}$  is also adopted as a unit of temperature. MD simulations were carried out systematically for a variety of values of the simulation parameters:  $\sigma_{CC}$ , 0.75 - 1.25;  $\varepsilon_{CC}$ , 0.5 - 100.0;  $m_C$  (the mass of a C particle), 0.2 - 512.0;  $T$  (the mean temperature, *i.e.* the total thermal kinetic energy divided by the number of all the passive particles), 0.01 - 0.16;  $N$ , -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.

### 3 RESULTS

A large number of simulation data under the stationary condition were arranged as dependence of the dynamic-frictional force on the sliding velocity  $v_{stroke}$ , the applied load  $N$ , and the average of the local quasi-temperature over the passive particles around the interface. 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 examples. The solid lines in these figures are fits to the data. The frictional force as a function of  $v_{stroke}$  in the case of  $\sigma_{CC}/\sigma_{AA} = 35/32$  is shown in Fig. 2 for  $N = 0.3, 0.6, 0.9$ . The number of the passive particles was 5360. Almost the same  $v_{stroke}$  dependence of the frictional force was obtained also by MD simulations using a similar model without the Nosé-Poincaré thermostats [7]. Frictional force dramatically increases as  $v_{stroke}$  exceeds a certain threshold  $v_{th}$  [3]. Based on the systematic search for the dominant experimental parameters determining  $v_{th}$ , we found that  $v_{th}$  depends most strongly on the lattice-constant ratio  $\sigma_{CC}/\sigma_{AA}$ . Figure 3 compares the velocity-dependent threshold behavior at  $N = 0.6$  for  $\sigma_{CC}/\sigma_{AA} = 34/32, 35/32, 36/32$ . The plots of  $v_{th}$  as a function of  $\sigma_{CC}/\sigma_{AA}$  (Fig. 4) indicates, furthermore, linearly proportional relationship between  $v_{th}$  and  $\sigma_{CC}/\sigma_{AA} - 1$ .

### 4 DISCUSSION

This simple relationship is possibly explained from the theoretical point of view in terms of the atomistic energy-dissipation mechanism. Frictional power should be equal to rate of the energy-dissipation process; this process completes itself in two steps. In the first step, the lattices A and C are forced to vibrate at the washboard frequencies

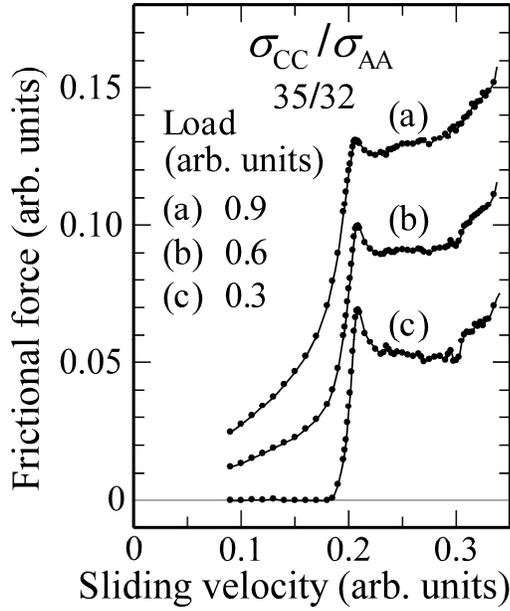


Fig.2. Typical dependence of the wearless-frictional force on the sliding velocity. The result in the case of the lattice-constant ratio  $\sigma_{CC}/\sigma_{AA} = 35/32$  is shown for the applied load  $N = 0.3, 0.6, 0.9$ .

$v_{\text{stroke}}/\sigma_{CC}$  and  $v_{\text{stroke}}/\sigma_{AA}$  respectively, by weak interaction between them at the interface. This step leads to coherent excitation of normal vibrational modes. Then, in the second step, this vibrational energy disperses to all the normal modes in each lattice owing to anharmonicity of the interatomic potential. This incoherent dispersion of vibrational energy results in thermal distribution of phonons. The second step is the rate-determining stage in the energy-dissipation process for the case where coupling between the nanometer-scale wearless-frictional system and a heat bath is weak. Without the second step, the energy transfer in the first step soon terminates when the amplitude of the vibration mode reaches the steady value. It should be noted that the effects of the anharmonicity of the interatomic potential are noticeable in the second step only under the experimental conditions where amplitude of oscillatory change in the interatomic distance has grown comparable to its equilibrium distance in the first step. One of them is the condition that the washboard frequency agrees with the renormalized eigenfrequency of one or some of the normal vibrational modes satisfying the phase-matching condition. Then, the resonance causes vigorous increase in amplitude of such mode(s) in the lattice A or C, resulting in high dissipation rate and thus strong frictional resistance. The fundamental phase-matching condition is given by

$$k_x = \sigma_{CC}^{-1} - \sigma_{AA}^{-1}, \quad (3)$$

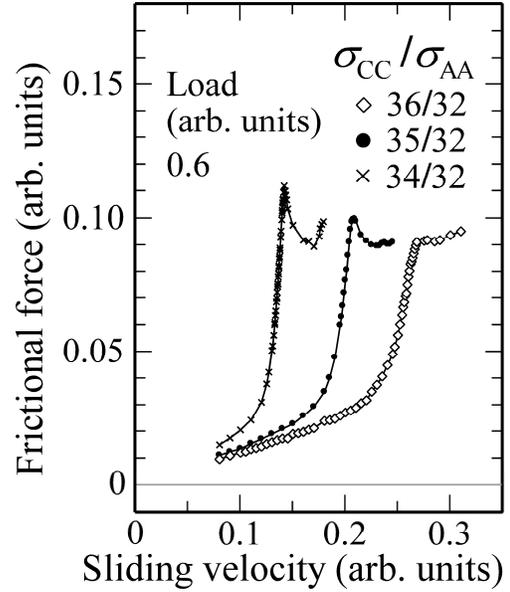


Fig.3. Comparison of the threshold characteristics among the MD models of deferent lattice-constant ratio  $\sigma_{CC}/\sigma_{AA} = 34/32, 35/32, 36/32$ . The wearless-frictional force at the applied load  $N = 0.6$  is plotted as a function of the sliding velocity.

where  $k_x$  is the moving-direction component of the wavenumber vector  $(k_x, k_z)$  of the relevant normal vibrational mode. The resonance condition is given by

$$v_{\text{stroke}}/\sigma_{CC} = f_A(k_x, k_z), \quad (4)$$

or

$$v_{\text{stroke}}/\sigma_{AA} = f_C(k_x, k_z), \quad (5)$$

where  $f_A(k_x, k_z)$  is the eigenfrequency of the mode in the lattice A and  $f_C(k_x, k_z)$  is that in the lattice C. We assume approximately linear dispersion relations

$$f_A(k_x, 0) = c_A |k_x| \quad (6)$$

and

$$f_C(k_x, 0) = c_C |k_x| \quad (7)$$

for the range of  $1/17 \leq |k_x| \leq 1/9$ . Although not described here, based on further MD analyses of spatial distribution of the local quasi-temperature we believe that the relevant normal vibrational modes are longitudinal ones regarding their  $x$  component and that the heat generation at the interface preferably occurs in the lattice A or C, according

as  $\sigma_{AA} < \sigma_{CC}$  or  $\sigma_{AA} > \sigma_{CC}$ . Thus, we conclude that the threshold sliding velocity  $v_{th}$  is originally

$$v_A = c_A \left| \sigma_{AA} - \sigma_{CC} \right| / \sigma_{AA} \quad (8)$$

in the case of  $\sigma_{CC} / \sigma_{AA} > 1$ , or

$$v_C = c_C \left| \sigma_{AA} - \sigma_{CC} \right| / \sigma_{CC} \quad (9)$$

in the case of  $\sigma_{CC} / \sigma_{AA} < 1$ . Figure 4 clearly demonstrates that the dependence of  $v_{th}$  on  $\sigma_{CC} / \sigma_{AA}$  obeys the simple Eq. (8).

## 5 CONCLUSIONS

Artificial modification of threshold velocity  $v_{th}$  is a necessary fundamental step toward establishment of the method of “phonon-band engineering”. The purpose of the present investigation based on MD simulations adopting a simplified 2D model was to clarify the nature of  $v_{th}$ . The experimental parameter mainly determining  $v_{th}$  was turned out to be the lattice-constant ratio  $\sigma_{CC} / \sigma_{AA}$ . We proposed a possible atomistic mechanism of energy dissipation underlying the simple linearly proportional relationship between  $v_{th}$  and  $\sigma_{CC} / \sigma_{AA} - 1$ , lying emphasis on the resonance and the phase matching.

Based on this 2D study, we paid attention to  $v_{th}$  in three-dimensional MD analyses of wearless-frictional characteristics, through which the simple relationship similar to the 2D case was obtained between  $v_{th}$  and the lattice-constant ratio. Recently, we applied these results to design of lateral strained-layer superlattices; details will be described elsewhere.

## ACKNOWLEDGEMENT

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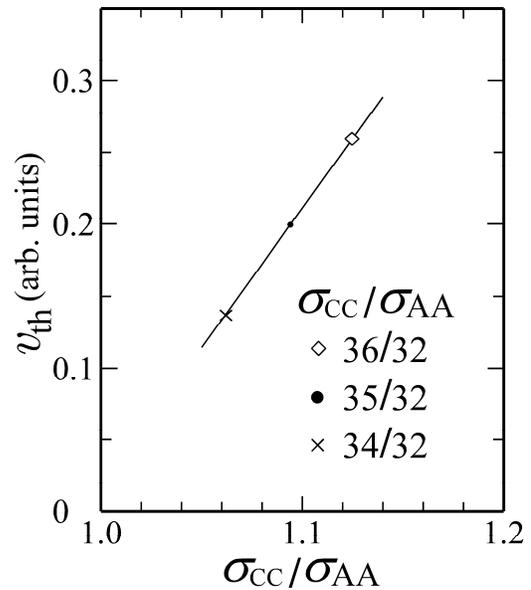


Fig.4. Relationship between the threshold sliding velocity  $v_{th}$  and the lattice-constant ratio  $\sigma_{CC} / \sigma_{AA}$ . The solid line is a least square fit to the data.

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