Possible Nearly Frictionless Sliding for Mesoscopic Solids

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A linear chain of atoms, interacting with anharmonic forces, one of whose end atoms is forced to vibrate harmonically, is studied as a simple model for kinetic friction between ideal crystalline solids. It is found that there is a transition, as a function of chain length and driving frequency between a regime in which there is dissipation (i.e., the internal energy increases as a function of time on the average) and one in which there is practically no dissipation. This suggests that there can be dissipationless sliding for sufficiently small solids.

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It was shown in previous work on atomic level friction [1,2] that whereas energy dissipation (which is generally understood to mean the conversion of organized translational into vibrational energy) will occur when two infinite solids slide in contact with each other, for a finite harmonic solid, significant energy dissipation will only occur if the inverse phonon lifetime is larger than the spacing between the modes [2]. Since the mode spacing increases as the size of the solid decreases, the question arises as to whether there exists a critical size for real solids, which are anharmonic, below which energy is not dissipated when they slide relative to each other. This question is addressed in this Letter.

The main source of phonon damping is the anharmonicity of the lattice, which causes the vibrational energy of a phonon to be transferred to other phonon modes [3]. It is well known that a harmonic oscillator anharmonically coupled to other oscillators will only exchange significant energy with them if its frequency is equal to a linear combination of the frequencies of those oscillators [3]. For a finite system, this rarely occurs because unlike an infinite solid in which the modes form a continuum, in a finite solid the modes are discrete, and hence it is rare to find a linear combination of modes of frequency equal to that of a given mode. Therefore, we might expect that the phonons will not be damped by anharmonicity in a finite solid. Although interaction of the surface atoms with the environment does lead to some damping of the phonons because the motion of these atoms is damped by their interaction with the surrounding atmosphere and by radiation, it was found to be much smaller than the mode spacing [2], even for samples with linear dimensions as large as 1 cm. The contribution to the damping due to the surrounding atmosphere was estimated in Ref. [2] by determining the damping constant (for damping assumed linear in the velocity) of surface atoms which will give the experimentally observed rate of cooling of a typical solid sitting on a solid surface and in contact with the atmosphere. Similar arguments could also be applied to damping due to contact of the body with a macroscopic solid if the coupling is relatively weak. The question of whether anharmonicity can lead to damping of the phonons in a finite sample was addressed in work by Fermi, Pasta, and Ulam [4]. In this work, energy was initially given to a single vibrational mode of a model solid with a small amount of anharmonicity. Contrary to the usual hypotheses of statistical mechanics the energy did not spread to the other modes of the system in time (the equipartition principle). Later, it was argued by Ford, Chirikov, and others [5,6] that the systems studied in Ref. [4] have anharmonicity which is weak enough so that they will be nonchaotic, and hence nonergodic, by the Kolmogorov, Arnold, and Moser (KAM) theorem [7]. If the anharmonic terms were stronger, however, the atoms in the solid would no longer follow periodic orbits in phase space characteristic of harmonic oscillators but would instead execute chaotic trajectories, resulting in ergodic behavior (i.e., the spread of the energy among all the phonon modes of the solid). This point was discussed by Chirikov using his overlap of resonance criterion [5]. Chirikov's work shows that, since as the system size increases the phonon mode spacing decreases, there will be a greater tendency of the phonon mode resonances of the solid to overlap as the number of atoms in the solid increases, leading to a transition to ergodic behavior at a critical size.

The problem considered here deals with a model like that considered by Fermi, Pasta, and Ulam driven by an external force. In line with the above discussion, we would expect that there should also be a transition from nearly frictionless to frictional behavior as the size of the solid increases. This opens up the possibility that for such small solids, since the phonon modes are practically undamped, there will be practically no dissipation of energy when such small solids slide relative to solids of similar size (i.e., there will be no friction in solids of sufficiently small size). Such a phenomenon could find application in micromechanical machines (for example, a nanometer size wheel turning on an equally small axel).

In order to study the possibility of dissipationless behavior in small solids, I have studied the following model for friction in a small solid: Consider a chain of atoms in which the atom at one end of the chain is held fixed and the atom on the other end is forced to move harmonically.

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The equation of motion is

$$m\ddot{x}_j = -\alpha(2x_j - x_{j-1} - x_{j+1}) + \beta[(x_j - x_{j-1} - a)^2 - (x_{j+1} - x_j - i)^2] - \beta'[(x_j - x_{j-1} - a)^3 - (x_{j+1} - x_j - a)^3], \quad (1)$$

where x_j is the location of the jth atom in the chain, a is the equilibrium lattice spacing, α,β,β' are parameters, m is the atomic mass, and $x_0=0$ and $x_N=A\cos(\omega t)$ where N is the number of atoms in the chain and A and ω are the amplitude and frequency of the motion that the end atom in the chain is forced to undergo. The parameters α, β, and β' were chosen to have the values corresponding to the coefficients in the expansion of the force calculated from the Lennard-Jones potential out to third order in the displacement from equilibrium. (This choice avoids the problem that one would encounter if one used only the second order expansion, namely, that the assumed equilibrium state of such a model in which the atoms are equally spaced is not the ground state, leading to a possible instability if the system is driven hard enough.) This equation of motion was integrated by a fourth order Runge-Kutta method and the vibrational energy was calculated as a function of time. This model is a simplified version of the friction models studied in Refs. [1] and [2]. The atoms can be taken to represent individual atomic planes and the forced motion of the end atom can be thought of as being due to atomic level height variations of the surface of a second solid on which it is sliding. Then, ω is the "washboard" frequency $2\pi v/a$, where v is the velocity of relative sliding and a is the lattice constant of the second solid with which this one is in contact along the sliding direction. The results for several system sizes are shown in Fig. 1. The value of A used in these calculations was $0.001a$. As can be seen, there is a transition from nondissipative to dissipative behavior as the size of the system increases beyond a critical value [in the sense that the internal energy of the 100 atom system of frequency $0.3\omega_1$, where $\omega_1=(\alpha/m)^{0.5}$, shown in Fig. 1 does not increase on the average as a function of time, whereas the energy of the 200 atom system of the same frequency does]. The critical size also appears to depend strongly on the driving frequency. For example, the 100 atom system when driven at a frequency of $0.6\omega_1$ was ergotic, whereas when driven at $0.3\omega_1$ it was not. The critical driving frequency for a 64 atom chain was found to fall between $0.8\omega_1$ and $1.2\omega_1$. This apparent inverse proportionality of the critical value of N with ω implies that for lower values of ω, which are more realistic, the critical size will be considerably larger. For example, if the sliding velocity at an interface is 1 cm/sec and the relevant length scale of the potential fluctuations at the interface is approximately 10^{-8} cm (this is the lower limit), ω would be about 6×10^8 rad/sec. Since the frequency scale in the present calculations ω_1 is of the order of 10^{13} rad/sec, we would expect on the basis of the apparent inverse proportionality of N with ω that the critical N would be about 10^6, which is a reasonable size for a mesoscopic system. This behavior can be understood qualitatively on the basis of Chirikov's overlap of resonances criterion because as the system size increases, the spacing of the vibrational modes decreases. The present calculations give a dependence which is an inverse proportionality of the critical N to ω, whereas a calculation based on Chirikov's overlap of resonance criterion gives a much stronger frequency dependence [5], but Chirikov's method does predict the general result that the critical N decreases with increasing ω. The calculations presented here were done at zero initial temperature. At higher initial temperature, the transition from nondissipative to dissipative behavior occurs for smaller solids and smaller values of A and ω, as expected [8].

The one-dimensional chain differs in a qualitatively important way from higher dimensional models in that whereas the modes in this model are all nondegenerate, in a higher dimensional solid the vibrational modes are in general degenerate. The existence of degeneracy of the resonances is believed to make it more likely that a system will be chaotic [6]. Therefore, an anharmonic version of the two-dimensional square lattice considered in Ref. [2] was studied. The equation of motion for this model is

$$m\ddot{u}_{jl} = -f_{\mathrm{LJ}}(\mathbf{r}_{j+1,l} - \mathbf{r}_{j,l}) + f_{\mathrm{LJ}}(\mathbf{r}_{j,l} - \mathbf{r}_{j-1,l}) - f_{\mathrm{LJ}}(\mathbf{r}_{j,l+1} - \mathbf{r}_{j,l}) + f_{\mathrm{LJ}}(\mathbf{r}_{j,l} - \mathbf{r}_{j,l-1}) + \delta_{l,N}\lambda_0\sin(\omega t + \pi j), \quad (2)$$

where $\mathbf{r}_{j,l}=(ja+u_{j,l},la)$ and $f_{\mathrm{LJ}}(\mathbf{r})$ is the force due to the Lennard-Jones potential between atoms a distance $\mathbf{r}$ apart and λ_0 is the strength of a harmonic force acting on the atoms at one edge of the solid (at $l=N$) to simulate approximately the force of a second solid of lattice constant $2a$ which is sliding relative to this solid. In this model the atoms are only allowed to move in the direction parallel to the edge at $l=N$ for simplicity. (The contribution to the dissipation from motion in the y direction is of the same order of magnitude.) Results for this model (with $\lambda_0=0.09425\alpha a$) shown in Figs. 1(e) and 1(f) indicate that a transition from dissipational to dissipationless sliding occurs in this model similar to that found for the one-dimensional chains studied.

In order to give further insight into the nature of the transition to dissipative behavior, the time Fourier transform of the velocity-velocity correlation function for one of the systems which shows ergodicity is shown in Fig. 2. As can be seen, when the system is ergotic many modes become excited, as expected, whereas when the motion is not ergotic the motion remains concentrated mainly in one or two modes. These calculations were performed by

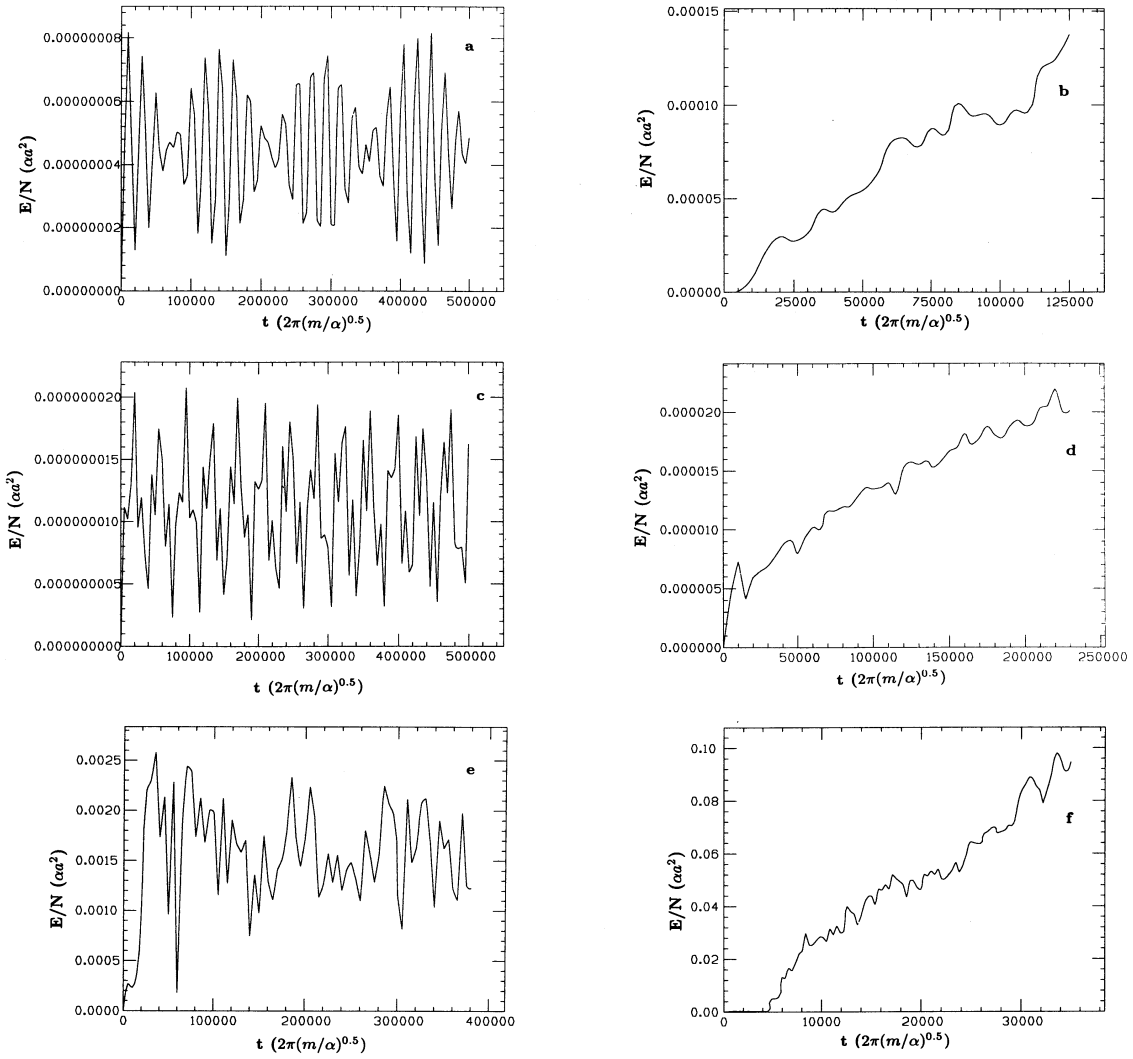

FIG. 1. The energy per atom (measured in units of αa^2) as a function of time [in units of $2\pi(m/\alpha)^{0.5}$]: (a) for a 100 atom chain with $\omega=0.3(\alpha/m)^{0.5}$, (b) for a 100 atom chain with $\omega=0.6(\alpha/m)^{0.5}$, (c) for a 200 atom chain with $\omega=0.15\times(\alpha/m)^{0.5}$, (d) for a 200 atom chain with $\omega=0.3(\alpha/m)^{0.5}$, (e) for a 3×3 atom square lattice with $\omega=1.6(\alpha/m)^{0.5}$, and (f) for an 8×8 atom square lattice with $\omega=1.6(\alpha/m)^{0.5}$. In (e) and (f), α is the compressional force constant of the lattice.

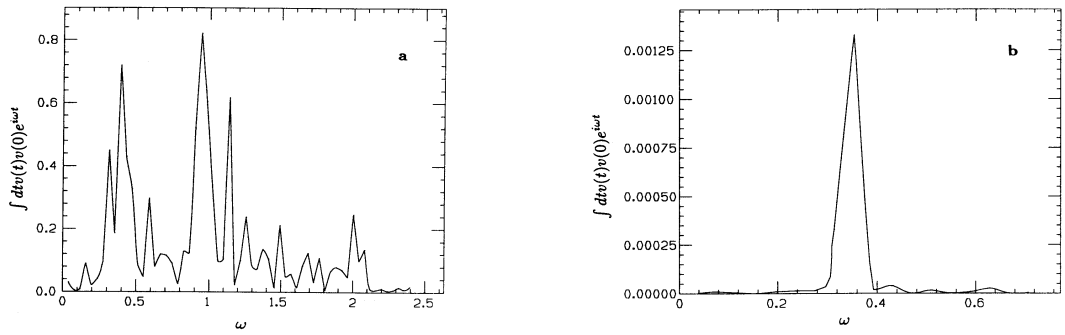

FIG. 2. Time Fourier transform of the velocity-velocity correlation function for the 50th atom in a 100 atom chain; (a) with $\omega=0.6(\alpha/m)^{0.5}$ and (b) with $\omega=0.3(\alpha/m)^{0.5}$.

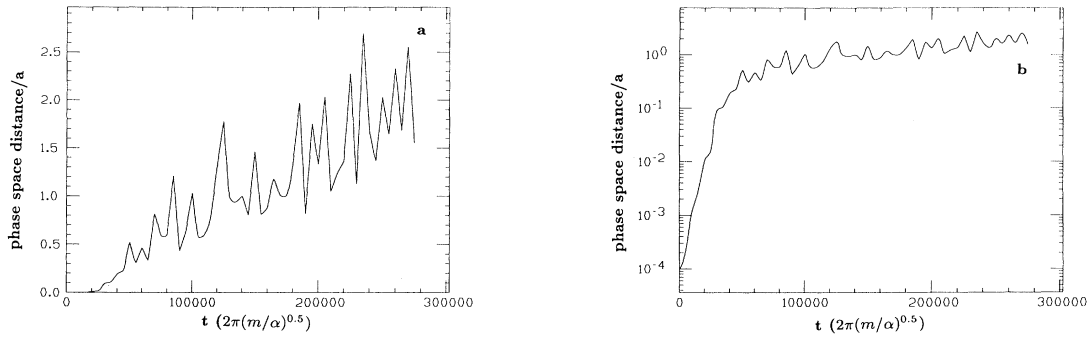

FIG. 3. The distance in phase space between two 64 atom systems with $\omega = 1.2(a/m)^{0.5}$ as a function of time, in which the initial configurations of the two systems differed only in the fact that the position of the 32nd atom differed by $0.001a$; (a) shown on a linear scale and (b) shown on a semilogarithmic scale.

first integrating the equations of motion for 1.25×10^5 time units. The equations were then integrated for another 200 time units and the velocity-velocity correlation function was calculated for one of the atoms in the system and Fourier transformed using a standard fast Fourier transform routine. (This procedure was repeated for other atoms, giving results which were qualitatively similar to those shown in Fig. 2.) As can be seen, the Fourier transformed correlation function for a dissipative system, shown in Fig. 2(a), exhibits many peaks, whereas the same quantity for a nondissipative system, shown in Fig. 2(b), exhibits only one peak. This supports our hypothesis that energy gets distributed among many phonon modes in the dissipative case, whereas it remains concentrated mainly in one mode in the nondissipative case. In Fig. 3, the difference in the distance in the $2N$-dimensional phase space between the point describing the system at two different close lying initial points in phase space is shown for a system that is dissipative. The behavior is characteristic of a bounded chaotic system in the sense that the distance in phase space grows with time, its initial growth being exponential [9]. This is the standard method for identifying a transition to chaotic behavior in many-body systems, where it is not practical to study in detail the behavior of the KAM surfaces because they have high dimensionality [6,10].

The calculations presented in this Letter were done on a model for friction between small solids sliding relative to each other, but calculations on the present model could also describe the damping of an atom excited by ferromagnetic resonance. In this case, the driving force is produced by the interaction of the magnetic modes of the ion with the vibrational modes of the solid. Thus, a similar lack of dissipation in small solids excited by ferromagnetic resonance should also be a possibility. Furthermore, the possibility exists that these results might also hold if the dissipation is caused by the excitation of other types of excitations, such as spin waves, which can also be approximated by harmonic oscillators in the small amplitude limit, and which are believed to be damped by spin-wave–spin-wave scattering caused by nonlinearity, which is neglected in the approximation in which the modes can be treated as noninteracting harmonic oscillators. It is not clear at this point whether the ease with which small atomic clusters diffuse on a surface, which has been observed in the past [11], is due to the phenomenon discussed in this Letter (i.e., the occurrence of low dissipation in small solids) or to the occurrence of low activation energies.

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