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Effects of stick–slip motion on energy dissipation in small sliding solids

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Abstract. Friction is studied in a model consisting of a relatively short chain of particles (each one of which may be taken to represent a layer of atoms which is treated as rigid for simplicity) with anharmonic interparticle interactions, dragged at slow speeds over a potential which interacts with the particle on the end of the chain, with parameters chosen so that stick–slip motion takes place. A transition from dissipative to dissipationless sliding is found as a function of decreasing chain length, similar to that found for non-stick–slip motion. This could be a simplified model for a small lubricant particle anchored to a surface at one end, being dragged over a second surface at very slow speeds (about 1 cm s^{-1}).

1. Introduction

Recently, there has been a good deal of effort directed towards trying to understand the fundamental mechanisms responsible for kinetic friction. This is necessary in order to find ways to lubricate micron size mechanical devices [1] and disk drive heads which operate in extremely close proximity to the disk in order to store larger amounts of information in smaller spaces.

It was recently proposed by the present author that when two solids of sufficiently small (possibly molecular) size slide with respect to each other, they might be able to do so with almost no friction at sufficiently low temperatures [2], in the situation in which the bodies were only weakly coupled to the outside world. If we consider an insulator, for example, for which there are only vibrational excitations, each vibrational mode would act as an independent oscillator, and hence in the harmonic approximation the solids would not heat up (i.e. there would be no friction) because a driven undamped harmonic oscillator (more correctly, a weakly anharmonic oscillator) will not absorb energy from the driving field unless it is driven exactly at its resonant frequency, which does not usually occur. As either the temperature is raised or the solid is made larger (which results in the modes being closer together compared to their width), the anharmonicity of the oscillators becomes more important, eventually resulting in exchange of energy among the various vibrational modes, allowing the solids to heat up [3]. This contribution to the phonon mode width for an infinite solid, due to anharmonicity, is traditionally calculated by Fermi golden rule perturbation theory [4], which depends on the existence of a continuum of modes. Clearly, it does not apply to small solids, for which the modes are discrete.

A related phenomenon for which dissipationless behaviour might be possible is the dissipation that occurs in magnetic small particles in ferro- or ferrimagnetic resonance.

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It might be easier to study this phenomenon on nanometer size particles than to observe nanometer size particles sliding with respect to each other [5].

In slow speed sliding, there can be stick–slip motion, in which the system alternately becomes stuck and then slides forward suddenly. Stick–slip motion occurring at the points of contact of the two surfaces is likely to be responsible for 'dry friction' (i.e. a nonzero force of friction for slow speed sliding velocity) because it allows the rate of dissipation of energy to be nonzero even in the limit as the mean centre of mass velocity of a sliding solid approaches zero, due to the rapid motion that takes place [6, 7]. It is this motion at the points of contact which is believed to produce the energy dissipation due to kinetic friction in the very slow speed limit [6, 7]. (It should not to be confused with stick–slip motion of the sliding body as a whole, which is well known to result from an instability resulting from the fact that the kinetic friction is a decreasing function of velocity, if the sliding body is not too stiff [8].) In fact, in (6) and other work on friction in the slow speed limit, it is taken as an established fact that the kinetic energy generated in the slip part of the stick–slip motion occurring at very slow speeds is dissipated before the next slip takes place. A question that arises is whether this assumption is in fact always true. Specifically, the question considered here is whether frictionless behaviour in atomic level small (i.e. nanometre scale) solids will still occur for slow speed sliding when there is stick–slip motion because, in this case, we no longer have a situation in which each solid feels a steady time dependent force due to the second solid, but rather, there is abrupt motion which could excite many vibrational modes.

The connection of the present model to the usual picture of sliding friction between two bodies which are pressed together by a normal force is as follows: It is pretty well accepted that Amonton's law comes about because as the force pushing the surfaces together increases, the actual area of contact increases, either because the number of asperities in contact increases or because the area of contact at each pair of asperities that are in contact increases. The actual shear stress at any contact due to friction does not increase with increasing normal force. Since in the present study we will consider a model for what occurs at a single point of contact, we need not worry about the value of the normal force pushing the two surfaces in contact for the above reasons. The present study focuses on a single lubricant particle which undergoes stick–slip motion at slow speeds. It is found that if the particle has sufficiently few degrees of freedom, it can execute this motion with practically no energy dissipation. If this occurs at each contacting lubricant particle, the sliding of the solids can take place with practically no energy dissipation. In order for stick–slip motion of small lubricating particles to occur with practically no energy dissipation, as discussed here, these particles must be quite small (of the order of molecular dimensions). As we shall see, their coupling to the surface being lubricated must be sufficiently weak so that this coupling does not give the particle's phonon modes a width which is larger than their spacing.

2. Discussion of the model

In order to study the question of whether nearly frictionless behaviour is possible in small solids when stick–slip motion takes place, let us consider as a model a linear chain of interacting particles, one end of which is held fixed and the other end of which moves in a sinusoidal potential. (While the actual potential at the interface is not expected to be periodic, if the sliding velocity is sufficiently slow that the time between slips is long compared to the length of a slip, so that each slip is effectively independent, the use of a periodic potential should not affect the results in a qualitatively significant way.) The chain is not to be thought of literally as a chain, but rather each particle in the chain is taken to represent a layer of atoms, treated as rigid for simplicity, as illustrated in figure 1. For example, this could be a model for a layered solid lubricant, such as MoS_2, whose layers are quite rigid in contrast to the interlayer coupling. Damping of the vibrational modes of the chain resulting from the energy flow that must take place from the chain to the surface to which it is attached could prevent nearly frictionless sliding from occurring. This can be minimized, however, if the coupling between the chain and the surface (i.e. the force constant connecting the chain to surface atoms to which it is attached) is sufficiently weak compared to the force constant between the units making up the chain [2]. This is discussed in appendix A. The equation of motion for the chain studied is

$$m\ddot{x}_j = f(x_{j+1} - x_j) - f(x_j - x_{j-1}) + \delta_{j,N} f_0 \sin[Q(x_j - vt)] \tag{1}$$

where m is the mass of a single unit of the chain, x_j is the displacement of the jth unit (in units of the interparticle spacing in the chain), Q is the wavevector of the periodic potential which acts on the Nth unit in the chain, v is the velocity at which this potential is moving and f_0 is the amplitude of the force produced by this potential. We take x_0 to be constrained to be equal to zero at all times. The force between two neighbouring units was taken to be

$$f(x) = -\alpha[x - \beta(Ax^2 - Bx^3)] \tag{2}$$

where α is the force constant, a is the lattice constant, x is the displacement of a particle with respect to one of its neighbours in the chain, β is a parameter between zero and one which allows us to vary the strength of the anharmonic terms and A is taken to be equal to 9.354 4347 and B is taken to be equal to 49.077 139. The numerical values arbitrarily chosen for the coefficients of the x^2 and x^3 terms are the values obtained in the Taylor series expansion of the Lennard-Jones force up to this order. Not too much significance should be attached to this choice of coefficients, however, as our purpose here is only to illustrate qualitative effects of nonlinear interactions, rather than to model a particular experimental system. (It is necessary to include an x^3 in addition to an x^2 term because an x^2 term in the force results from an x^3 term in the expansion of the potential in x. A potential containing only x^3 anharmonic terms can lead to instabilities because its absolute minimum value is $-\infty$.) In most of the calculations reported here, the energy of the chain, defined as

$$E = \sum_j 0.5m\dot{x}_j^2 + \alpha\{0.5x_{j,j-1}^2 + \beta[-(A/3)x_{j,j-1}^3 + (B/4)x_{j,j-1}^4]\} \tag{3}$$

where $x_{j,j-1} = x_j - x_{j-1}$, is plotted as a function of the time.

(The model described by equations (1) and (2) reduces to the Tomlinson model [7], if a damping term $-m\gamma\dot{x}_j$ is included on the right hand side of equation (1) and β in equation (2) is set equal to zero. This is true because when x_j is expressed in terms of its normal modes, the resulting equations for these modes reduce to equations of motion for a collection of noninteracting driven harmonic oscillators [2, 9]. In order to study stick–slip motion in the Tomlinson model, α must be chosen to be sufficiently weak for stick–slip motion to occur and the damping term included in the equations of motion must be chosen to be sufficiently strong so that all of the kinetic energy produced in the slip part of the stick–slip motion is dissipated.)

The classical mechanical equations of motion for this model were solved using the Runge–Kutta method for various size systems and sinusoidal potential strengths. Unless a damping term proportional to the velocity of each unit is included in the problem, no energy is dissipated when we use the harmonic approximation (i.e. for β equal to zero), which is expected because in this case the model reduces to a collection of driven harmonic oscillators, the phonons, and it is well known that a driven harmonic oscillator does not absorb energy unless it is damped. (In contrast, an infinite system, which consists of a continuum of harmonic oscillators, will exhibit friction and dissipation [10].) Even without

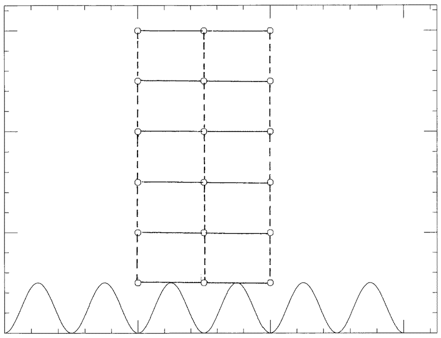

Figure 1. This figure illustrates the model studied in this article, which consists of a small solid interacting with a sinusoidal potential. For simplicity, the atoms in a single atomic layer are bound together rigidly (as denoted in this figure by the solid horizontal lines connecting the atoms), but shearing of the layers is allowed (as indicated by the dotted vertical lines connecting the atoms.) In the calculations performed in this article, the top layer is held in place while the sinusoidal potential is moved at speeds which are slow compared to the speeds that occur during the slip part of the stick–slip motion.

including a damping term in the model, the anharmonicity in the problem will in general produce friction [2].

Our goal here is to illustrate that it is possible to have a transition from dissipational to dissipationless stick–slip motion as a function of decreasing chain length. Therefore, in the calculations, whose results are reported in the next section, we chose the parameter $\alpha a/N$ sufficiently small compared to f_0 so that stick–slip motion occurs [7]. The parameter β was chosen to be sufficiently small so that dissipationless sliding would occur for a chain which is still long enough to exhibit stick–slip motion. For larger β but smaller N we would still be able to observe dissipationless behaviour [2], but not stick–slip motion. This is because for very small N, stick–slip motion will not occur unless the interparticle coupling is very weak. It is of course possible that small lubricant particles attached to a sliding surface might not be flexible enough to exhibit stick–slip motion at all. (There could still, however, be stick–slip motion due to flexibility of the larger body to which the lubricant particles are attached if this body is sufficiently thick.) Our choice of parameters is motivated by the fact that our purpose here is only to show that it is possible to have dissipationless sliding for very small solids in a situation in which stick–slip motion does occur.

3. Results of the calculations

Figures 2 and 3 show the results of calculations on anharmonic versions (i.e. $\beta \neq 0$ in equation (2)) of the model illustrated in figure 1. Figure 2 shows the displacement of the particle in contact with the sinusoidal potential for both a 30 and a 60 atom chain with $\beta = 0.2$ in order to show that the motion is indeed stick–slip in nature. In these calculations the sinusoidal potential moves at a speed of $v = 10^{-5}a/t_0$, where a is the interparticle spacing in the chain and $t_0 = 2\pi(m/\alpha)^{1/2}$ is the time scale in these calculations (or v is about 1 cm s^{-1}). In comparison, the Nth particle in the chain moves a distance of about $2a$ in a time of $3 \times 10^3 t_0$, implying a slip velocity which is a factor of about 10^2 faster than the velocity of the potential. Thus, we are justified in assuming that this calculation is being done in the limit of small average sliding velocity v. Figure 3 shows plots of

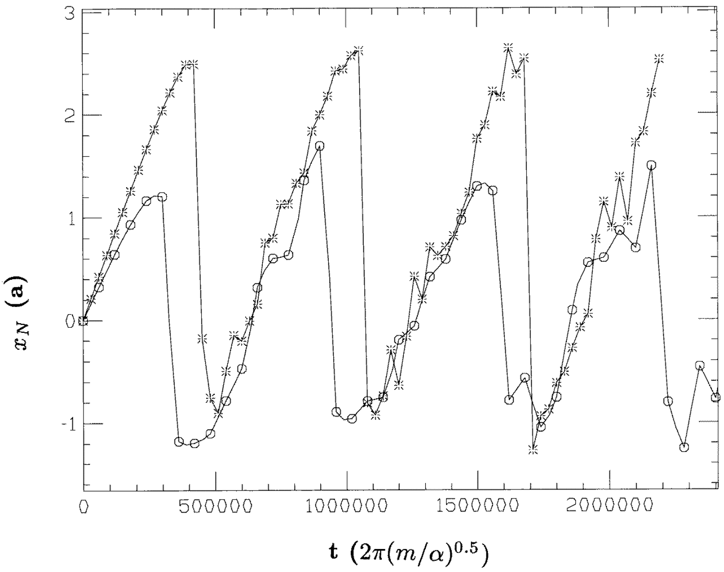

Figure 2. Results are presented of calculations of the x_N for a chain with an anharmonic interaction with $\beta = 0.2$ for $f_0 = 0.04\alpha a$ for a 30 (the circles) and a 60 atom chain (the asterisks), where α is the force constant for the harmonic part of the interparticle force, and the velocity of the sinusoidal potential is $10^{-5}a/t_0$, where $t_0 = (2\pi(m/\alpha)^{0.5})$.

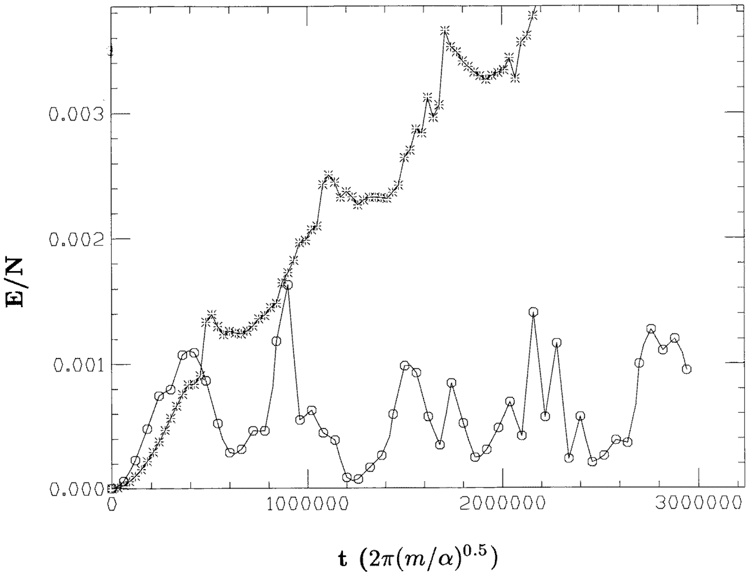

Figure 3. This figure shows the results of a calculation of the energy versus time for an anharmonic chain with the same parameters as in figure 2 for a 30 (the circles) and a 60 atom (the asterisks) chain.

the energy versus time for the same 30 and 60 atom anharmonic chains. The 60 atom chain shows behaviour reminiscent of the plot of the work done on the chain versus the time for the usual Tomlinson model [7] (i.e. a highly damped harmonic oscillator), which increases with increasing time, consistent with dissipative behaviour. While there exists no rigorous proof that the energy of the 60 atom chain will continue to increase forever as a function of time, it is quite clear that the behaviour of the energy of this chain is distinctly different from that of the 30 atom chain. This behaviour is consistent with a transition from nondissipative to dissipative behaviour as a function of increasing chain length for a chain exhibiting stick–slip motion, reminiscent of such a transition found in [2] for non-stick–slip motion.

In order to look experimentally for the phenomenon of nearly dissipationless sliding, one must construct a film of these small lubricant particles such that the phonon mode spacing is large compared to the damping constant γ, due to coupling of the chain to the outside world [9]. This quantity is likely to be dominated by the contribution from the flow of energy from the lubricant particles to the macroscopic surfaces that hold them. Estimates of the parameters in the problem for which the phonon mode spacing of the small lubricant particle is much larger than γ, and thus, nearly frictionless stick–slip motion is possible, are given in the appendix. Furthermore, for more concentrated films, coupling between the particles can make the film act like a macroscopic film to which the arguments presented in this paper do not apply, rather than a collection of individual particles. Calculations will be presented in a future publication, however, which support the possibility that this contribution to the friction can be minimized if the film is disordered so as to make the modes localized.

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Appendix A. Damping of the vibrational modes of a small solid due to coupling to a larger solid

While the vibrational modes of a small sample are discrete, when it is attached to a larger solid, it must be thought of as being part of the larger solid, whose modes are continuous. Nevertheless, if the coupling to the larger solid is weak, the discrete mode structure that the smaller solid would have if it were isolated must survive, but we would expect these modes to be broadened by their interaction with the modes of the larger solid. In order to study this damping more quantitatively, consider the model described by the following equations:

$$m\ddot{\boldsymbol{u}}_\ell = -\sum_{\ell'} \mathsf{D}(\boldsymbol{R}_\ell - \boldsymbol{R}_{\ell'}) \cdot \boldsymbol{u}_{\ell'} - \sum_{j'} \boldsymbol{\Gamma}(\boldsymbol{R}_\ell - \boldsymbol{R}_{j'}) \cdot \boldsymbol{U}_{j'} \tag{A1a}$$

$$M\ddot{\boldsymbol{U}}_j = -\sum_{j'} \mathsf{D}'(\boldsymbol{R}_j - \boldsymbol{R}_{j'}) \cdot \boldsymbol{U}_{j'} - \sum_{\ell'} \boldsymbol{\Gamma}(\boldsymbol{R}_j - \boldsymbol{R}_{\ell'}) \cdot \boldsymbol{u}_{\ell'} \tag{A1b}$$

where m, $\boldsymbol{u}_\ell$ and $\mathsf{D}(\boldsymbol{R}_\ell - \boldsymbol{R}_{\ell'})$ are the mass, displacement and dynamical matrix (denoted by a tensor) for an atom in the small solid and $\boldsymbol{R}_\ell$ is the location of the ℓth atom. Similarly, M, $\boldsymbol{U}_j$ and $\mathsf{D}'(\boldsymbol{R}_j - \boldsymbol{R}_{j'})$ are the mass, displacement and the dynamical matrix for an atom in the larger solid, and $\boldsymbol{R}_j$ is the location of the jth atom. The index ℓ runs only over atoms in the small solid and the index j runs only over atoms in the large solid. The tensor

$\boldsymbol{\Gamma}(\boldsymbol{R}_\ell - \boldsymbol{R}_j)$ gives the force constants acting between an atom in the small and an atom in the large solid. Equation (A1*b*) can be solved to yield

$$\boldsymbol{U}_j = -\sum_{j',\ell'} \mathbf{G}(\boldsymbol{R}_j - \boldsymbol{R}_{j'}) \cdot \boldsymbol{\Gamma}(\boldsymbol{R}_{j'} - \boldsymbol{R}_{\ell'}) \cdot \boldsymbol{u}_{\ell'} \tag{A2}$$

where $\mathbf{G}(\boldsymbol{R}_j - \boldsymbol{R}_{j'})$ is the Green function for equation (A1*b*). When this equation is used to substitute for $\boldsymbol{U}_{j'}$ in equation (A1*a*), we obtain

$$m\ddot{\boldsymbol{u}}_\ell = -\sum_{\ell'} \mathbf{D}(\boldsymbol{R}_\ell - \boldsymbol{R}_{\ell'}) \cdot \boldsymbol{u}_{\ell'} - \sum_{j',j'',\ell'} \boldsymbol{\Gamma}(\boldsymbol{R}_\ell - \boldsymbol{R}_{j'}) \cdot \mathbf{G}(\boldsymbol{R}_{j'} - \boldsymbol{R}_{j''}) \cdot \boldsymbol{\Gamma}(\boldsymbol{R}_{j''} - \boldsymbol{R}_{\ell'}) \cdot \boldsymbol{u}_{\ell'}. \tag{A3}$$

This equation will be used to estimate the damping of the discrete modes of the small solid due to its interaction with the large solid. Let us assume that $\boldsymbol{R}_\ell$, which gives the positions of the atoms in the small solid, only runs over a small distance in the direction transverse to the small particle and that $\boldsymbol{\Gamma}(\boldsymbol{R}_j - \boldsymbol{R}_\ell)$ is only nonzero when the atoms at positions $\boldsymbol{R}_j$ and $\boldsymbol{R}_\ell$ are on opposite sides of the interface. For simplicity, we will take $\boldsymbol{\Gamma}(\boldsymbol{R}_j - \boldsymbol{R}_\ell)$ to be diagonal in the coordinate indices. If we take the Fourier transform of equation (A1) on the index ℓ (which runs over the small solid) and express the Green function $\mathbf{G}$ in terms of its Fourier transform on the j index (which runs over the large solid), and we assume that only a single mode (i.e. only one value of $\boldsymbol{k}$) is excited in the small solid, the equation for that mode has the form

$$\ddot{\boldsymbol{q}}_{\boldsymbol{k}} = -\omega_0^2(\boldsymbol{k})\boldsymbol{q}_{\boldsymbol{k}} - \mathrm{i}\gamma\dot{\boldsymbol{q}}_{\boldsymbol{k}} \tag{A4}$$

where $\boldsymbol{q}_{\boldsymbol{k}}$ is the Fourier transform of $\boldsymbol{u}(\boldsymbol{R}_\ell)$, where γ is given by the imaginary part of the Fourier transform of

$$\gamma\omega = \sum_{j',j''} \boldsymbol{\Gamma}(\boldsymbol{R}_\ell - \boldsymbol{R}_{j'}) \cdot \mathbf{G}(\boldsymbol{R}_{j'} - \boldsymbol{R}_{j''}) \cdot \boldsymbol{\Gamma}(\boldsymbol{R}_{j''} - \boldsymbol{R}_{\ell'}). \tag{A5}$$

Then, because the arguments of $\boldsymbol{\Gamma}$ are essentially restricted to the interface and $\boldsymbol{R}_\ell$ is restricted to the width of the small particle, γ is of the order of

$$\Gamma_D^2 \,\mathrm{Im}\, G/\omega \tag{A6}$$

where Γ_D is a typical value of one of the diagonal elements of $\boldsymbol{\Gamma}$. Here $\mathrm{Im}\, G$ is equal to the phonon mode density of states, which is given by

$$3\Omega(2\pi)^{-3}\int \mathrm{d}^3k\,\delta(\omega^2 - \omega_0^2(\boldsymbol{k})) = 3\Omega(4\pi)(3)(2\pi)^{-3}\int_0^{k_D} k^2\,\mathrm{d}k\,\delta(\omega^2 - v_p^2k^2)$$

in the Debye approximation, where Ω is the unit cell volume, k_D is the Debye wave vector, $\omega_0(\boldsymbol{k})$ is the phonon dispersion relation and v_p is the phonon velocity. Thus we find that $\mathrm{Im}\, G = (9/2)(\omega/\omega_D)\omega_D^{-2}$. The Debye frequency $\omega_D = v_pk_D$ is of the order of 10^{13} rad s^{-1}. In this calculation, Γ_D is equal to the force constant acting across the interface divided by the square root of the product of the masses of an atom in the small solid and one in the large solid. In fact, for a very reasonable situation in which the coupling of the lubricant particle to the sliding solid is by van der Waal's forces, whereas the atoms within the large solid are bound to each other by covalent bonds, we might expect Γ_D to be considerably smaller than ω_D^2 (which is of the order of a typical force constant for the large solid divided by its mass). Thus, let us write Γ_D as $\sigma\omega_D^2$, where σ is a dimensionless quantity, which is much less than 1 if the intersolid force constants are much less than the intersolid force constants. Then $\gamma = (9/2)\sigma^2\omega_D$. Since each mode has an overlap with the displacement of the Nth layer of the order of N^{-1}, where N is the number of atomic layers in the small solid, the width of each vibrational mode of the small solid is approximately equal to γ/N [2]. Hence, this quantity will be much smaller than the mode spacing in the small solid, which is of the order of ω_D/N (assuming that the maximum phonon frequency of the small solid is comparable to the Debye frequency of the large solid) if $\sigma \ll 1$, which is true whenever the intersolid force constants are much smaller than the intrasolid force constants. If the lubricant particle's layers are coupled by van der Waal's forces, however, the minimum spacing of its modes will only be of the order of $\sigma^{1/2}\omega_D/N$. This is still large compared to γ/N, however, if $\sigma \ll 1$. Since the depth of typical wells of the Lennard-Jones potentials used to model interactions between molecules which interact with Lennard-Jones potentials are typically of the order of 10^{-2} eV, as compared to covalent bond strengths, which are typically of the order of several eV, it is not unreasonable to expect that it should be possible to find lubricating materials for which the conditions for observing nearly frictionless stick–slip motion of small lubricating particles will be satisfied.

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