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Theory of static friction: temperature and corrugation effects

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Abstract

We present a study of the static friction, as a function of temperature, between two thick solid slabs. The upper one is formed of light particles and the substrate of heavy particles. We focus our attention on the interaction between the phonon fields of the two blocks and on the interface corrugation, among the various mechanisms responsible for the friction. To give evidence of the role played by the dynamical interaction of the substrate with the upper block, we consider both a substrate formed by fixed atoms and a substrate formed by mobile atoms. To study the effect of the corrugation, we model it by changing the range parameter σ in the Lennard-Jones interaction potential. We found that in the case of the mobile substrate there is a large momentum transfer from the substrate to the upper block. This momentum transfer increases on increasing the temperature and produces a large disorder in the upper block favouring a decrease of the static friction with respect to the case for a rigid substrate. Reducing the corrugation, we found that with a rigid substrate the upper block becomes nearly commensurate, producing an enhancement of the static friction with respect to that with a mobile substrate.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The recent developments of experimental techniques and of fast computers allow us to study the frictional properties of two sliding surfaces at a microscopic level [1–10]. Recent experimental studies tried to exclude many of the unknown factors by preparing well defined surfaces. For this reason molecular dynamics simulations for controlled surfaces can be used to try to interpret the experiments performed in a controlled way. Even for well prepared surfaces, the interactions that give rise to friction between two sliding blocks involve many physical phenomena. The interaction between the upper block and the lower block gives rise to static corrugation between the two surfaces and to adhesion [11]. The adhesive force between them acts as an effective load resulting in a finite friction force. At fixed temperature T the motion of the atoms of the upper block and also of the substrate contributes significantly to the friction force. We recall that in one-dimensional models, as well as in many simulations, the substrate is generally described as a rigid slab, neglecting the phonon field of the lower block. Also the commensurability or the incommensurability of the interface strongly affects the static force of friction F_s.

In a previous paper [12] (hereafter referred to as paper I) we have studied the static friction between two blocks with a very high static corrugation. The top block was made of a slab of N_2 molecules and the lower block, the substrate, of a slab of Pb atoms. This system has been studied experimentally extensively in the past [13, 14]. We considered mobile atoms in both slabs. Our main result was that on increasing the temperature there is a transfer of momentum from the heavy atoms of the substrate to the top block. This effect induces a disorder in the top block, noticeable already at 20 K, opening several channels for the N_2 molecules. This produces a very rapid drop in the static friction. These results confirm the experimental data on static friction obtained in a controlled way on the same physics system [15].

The aim of this paper is to study in detail the interactions of the substrate with the upper block. To give evidence of this effect we evaluate the static friction for a rigid substrate and we compare the results with those previously found for a substrate with mobile atoms. In this way we can highlight the importance of the lattice dynamics of the two subsystems.

The other important parameter which governs the friction is the corrugation. We will modify the value of the corrugation,

enlarging the distance between the two blocks. We can then study the change, at fixed temperature, of the momentum transfer [16] from the heavy particles of the substrate to the light particles of the top system. In addition, we can study the role of the interface corrugation and of the surface roughness. We will compare the results obtained with the mobile substrate with those obtained with the rigid one. In this way give evidence of the effect of the change of corrugation between the two sliding blocks.

Section 2 describes the preparation of the sample formed of 12 (111) planes of N_2 and 24 (111) planes of Pb. The boundary conditions imposed on the combined system are presented together with the molecular dynamics simulation procedure needed to obtain the equilibrium configuration. The potentials used are also discussed.

In section 3 we briefly outline the molecular dynamics procedure used to obtain the static friction at fixed temperature. In this section we also present the calculation of the static friction for the upper block sliding on the substrate with rigid atoms. The comparison of the results with those obtained in paper I with a mobile substrate is also discussed.

In section 4 we arbitrarily reduce the interactions between the N_2 and Pb blocks, changing the interface corrugation. We discuss the preparation of the new sample and we present results for the static friction at different temperatures. Calculations are performed both for the mobile substrate and for the rigid substrate. In the final section 5 we summarize the results of the present work and we draw conclusions.

2. The system

The system considered is 'made' of a substrate formed by a stacking of hexagonal Pb(111) planes with fixed atoms. A substrate of Pb describes properly the static properties of a semi-infinite crystal. The interaction potential is determined by the embedded atom method with parameters fixed to *ab initio* calculations [17, 18]. The upper N_2 slab is formed of 12 layers. The molecules are taken with spherical symmetry and are interacting with a Lennard-Jones potential. The interactions between the two blocks are also described by a Lennard-Jones form as discussed in paper I. Since periodic boundary conditions are applied along the $[11\bar{2}]$ and $[1\bar{1}0]$ directions the sizes of the two slabs need to be equal along these two directions. The simulation cell of Pb is made by taking 10 cells in the $[11\bar{2}]$ direction and 10 cells in the $[1\bar{1}0]$ and contains 200 atoms per plane. The simulation cell of N_2 has 8 cells in both directions, for a total of 128 atoms per plane. In this way there is a small mismatch between the Pb and N_2 planes. We then stretch the upper slab by 1% to match the periodicity with the lower slab.

3. Static friction as a function of the temperature for the rigid substrate and high corrugation

The system is equilibrated by using a Parrinello–Rahman simulation with a time step of 1.47 fs. The detailed procedure for getting the system in equilibrium at a given temperature is given in paper I. At $T = 0$ K the Pb atoms form an ideal fcc structure. The projections of the N_2 particles on the (111) interface plane are slightly distorted from the ideal geometry. In the direction normal to the surface, the N_2 molecules are spread over the range of 0.8 Å, as shown by our calculations depicted in figure 1. This result is a consequence of the high corrugation, which in energy is about 80 meV (see paper I).

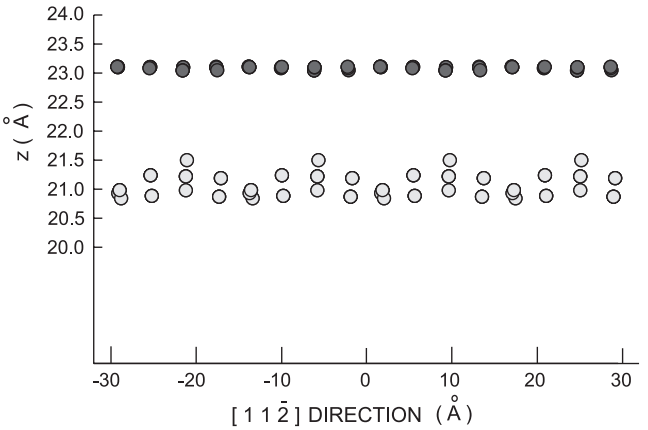

Figure 1. Distribution of the N_2 particles in the z direction, normal to the surface, at $T = 0$ K. The open circles refer to the highly corrugated system, discussed in section 3. The full circles refer to the low corrugation system and will be discussed in section 4. The positions have been drawn for the equilibrated system. The atoms are drawn along the $[11\bar{2}]$ direction.

To evaluate the static friction at a given temperature we proceed as in paper I. We start from the sample that we have constructed at $T = 0$ K, setting the velocities of the particles at very small random values. Then we heat the sample at the desired temperature by rescaling the velocities of the particles at each time step to adjust the kinetic energy at the given temperature. A second run for a total time of 3 ns is performed without temperature control to stabilize the system. Finally we collect statistics by taking an average over a simulation time of 500 ps. Having got the system to a given temperature, we apply a force to each of the N_2 molecules of the upper block along the direction $[1\bar{1}0]$ which has the highest atom packing.

To determine the static friction F_s we apply the iterative procedure described in paper I. The results of the calculations at different temperatures are presented in figure 2, where we have also drawn for comparison the static friction previously obtained in the case of a Pb substrate with atoms not held at rest.

The key result is that at low temperature with a rigid corrugated slab the static friction is two orders of magnitude larger than that obtained with a vibrating slab. For this reason we have used a logarithmic scale to present both curves. With the mobile substrate F_s is slowly decaying up to 25 K. This result can be simply explained by noticing that in the case of the vibrating slab there is a large momentum transfer from the Pb atoms to the N_2 slab. This transfer of momentum, as discussed in paper I, introduces a strong disorder in the N_2 slab, with the formation of stacking faults producing a misplacing of planes in the sequence ABC. This disorder opens many channels to the N_2 molecules when the external force is applied, independently of the high corrugation of the interface.

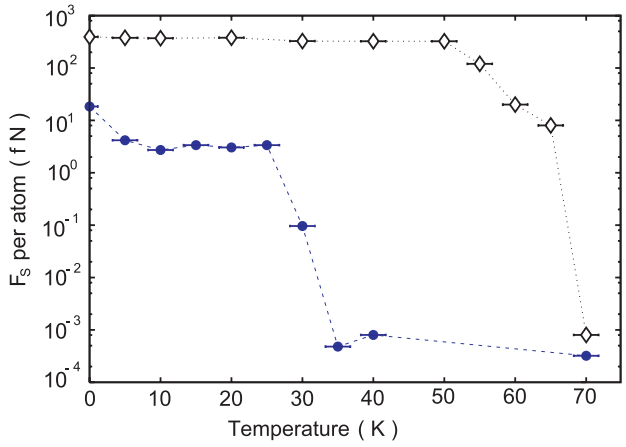

Figure 2. The evaluated static friction per atom F_s, as a function of the temperature. The open diamonds refer to the system with fixed substrate, while the full circles are relative to the previous calculations for the mobile substrate [12], drawn for comparison.

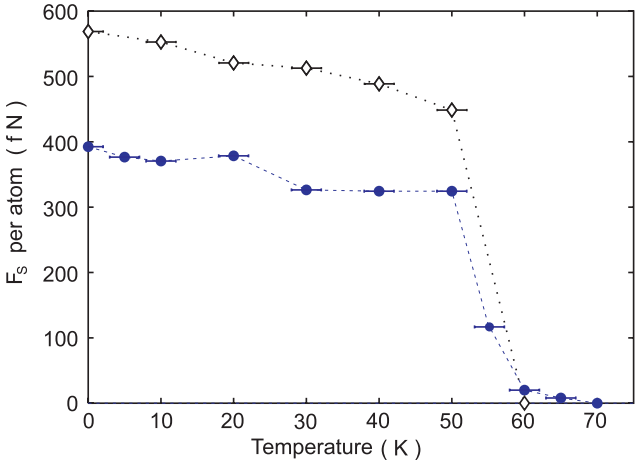

Figure 3. Static friction per atom F_s for the fixed substrate on an enlarged scale. The full circles refer to the strongly corrugated interface, while the open diamonds refer to the low corrugation system, discussed in section 4.

Table 1. Mean square displacements normal to the interface of the N_2 molecules. Columns A and B refer to mobile and fixed substrates for high corrugation; columns C and D relate to mobile and fixed substrates for low potential corrugation.

	A	B	C	D
Temperature (K)	u_z^2 (Å^2)	u_z^2 (Å^2)	u_z^2 (Å^2)	u_z^2 (Å^2)
10	0.036	0.004	0.006	0.001
20	0.040	0.007	0.011	0.002
30	0.046	0.011	0.016	0.003
40	—	0.014	0.021	0.005

In the present calculations, with a rigid substrate, the transfer of energy from the bottom slab to the upper slab is strongly reduced. This is illustrated in table 1, where we have written out the normal component of the mean values of the displacements $\langle u_z^2 \rangle$. Column A refers to the substrate with mobile atoms, and column B refers to the fixed substrate. One notices a reduction of a factor of the order of 5 of the $\langle u_z^2 \rangle$ for the fixed substrate with respect to the mobile one. This strong reduction in the vibrational amplitude of the N_2 particles at the same temperature T indicates that also the transverse momentum transfer from the Pb atoms to the N_2 molecules is strongly reduced. The high corrugation and the small kinetic energy of the N_2 molecules is responsible for the very high values of the static friction F_s, which is the minimum force needed to overcome the potential barrier.

On the log scale of figure 2 the F_s relative to that of the fixed substrate seems to be constant up to 50 K. To bring out its behaviour we have plotted it on an enlarged scale in figure 3. In the same figure we have plotted the F_s relative to that of the 2σ model which will be discussed later on.

On this scale one notices a non-linear decay. To interpret this fact, we plot in figures 4 and 5 the side views of the N_2 slab normal to the $[11\bar{2}]$ direction, respectively for $T = 20$ K and $T = 30$ K. We observe the presence of a few stacking faults, due to temperature effects. They are introducing some disorder in the slab, which is reflected in the change of F_s. For this highly corrugated system the disorder due to the temperature

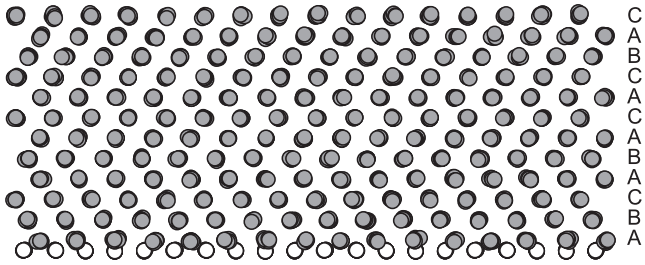

Figure 4. Side view of the N_2 slab at $T = 20$ K with particles in the $[11\bar{2}]$ direction. The open circles are the Pb atoms of the fixed substrate. Some stacking faults are visible in the region between the fifth plane and eighth plane, starting from the bottom interface layer.

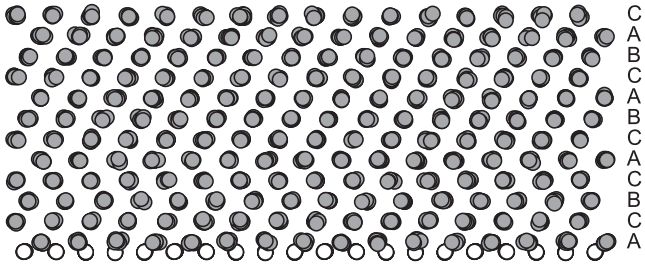

Figure 5. Same as figure 4, but for $T = 30$ K. The stacking faults are now closest to the interface, between the third and the fifth layer, starting from the bottom.

is evident in figure 6. Here we have drawn the structure factor of the N_2 slab, for several temperatures, as a function of the layer index. In the range of the fourth to sixth layers, at $T = 20$ and 30 K, one notices a change in the structure factor in correspondence with the position of the stacking faults observed in figures 4 and 5.

The disorder has its maximum value for the interface layer at all temperatures, below the melting of the slab. At $T = 0$ K, because of the strong interaction, the interface plane is corrugated and this causes the disorder of the interface N_2

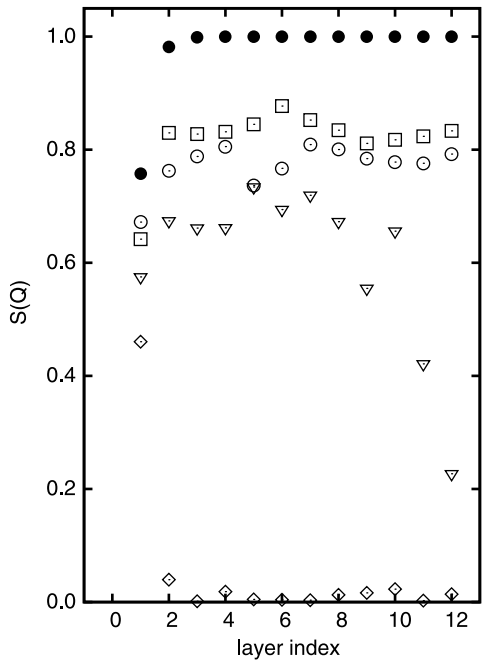

Figure 6. Structure factor $S(\vec{Q})$ as a function of the index L of the layers of the N_2 slab, evaluated for $\vec{Q} = \frac{2\pi}{a}(0, \frac{4\sqrt{6}}{3}, 0)$ for different temperatures for the high corrugation system with fixed Pb substrate. Full circles ● refer to $T = 0$ K, open squares □ to $T = 20$ K, open circles ○ to $T = 30$ K, down triangles ▽ to $T = 50$ K and finally open diamonds ◇ to $T = 70$ K.

molecules, while all the other planes have the ideal structure of the fcc configuration. Only a few channels are open and F_s remains very high. Above 50 K the N_2 slab starts to melt. The system is highly disordered, as shown by the decaying of the structure factor in figure 6, and there is a very rapid drop in the static friction. At 70 K we are close to the bulk melting of N_2.

What we can learn from these calculations is that for the high corrugation system the temperature effects produce a disorder in the N_2 block which is very large when we allow the N_2 molecules to vibrate in their own potential. On the other hand the large momentum transfer produces a drop of the static friction of two orders of magnitude when we move from the fixed to the mobile substrate.

4. Static friction for low corrugation

We now consider the case of low corrugation. As a test case, the low corrugation is obtained simply by doubling the parameter σ in the Pb–N_2 Lennard-Jones potential. All the other N_2–N_2 and Pb–Pb interactions are kept as in paper I.

The interaction potential evaluated with 2σ is represented in figure 7. We have drawn the interaction potential Pb–N_2 at the equilibrium distance $z(R)$ where the z-component of the gradient of the potential is equal to zero. The resulting low corrugation is equal to 14 meV.

In order to bring the new system to equilibrium at a given temperature we perform a Parrinello–Rahman simulation for 3 ns with the same time step as before. We are forced to increase the length of the simulation because the interaction between the two blocks is now very weak.

At $T = 0$ K the Pb atoms remain in the ideal interface hexagonal structure. The projections of the N_2 molecules in the (111) interface plane form a hexagonal structure very close to the ideal one. Because of the low corrugation the spreading in the z direction is now less than 0.1 Å; see figure 1. Therefore the N_2 interface layer geometry is very close to an ideal plane.

In order to evaluate F_s some care should be taken because of the weak interaction between the two slabs. In order to get stable results we use a simulation time of 1 ns. With the procedure already outlined we evaluate F_s versus temperature. The results are plotted in figure 8 both for the mobile and for the fixed substrate.

We start by discussing the system with the mobile substrate. At $T = 0$ K the value of F_s is around 4 fN (see figure 8), comparable with the value obtained with the mobile substrate and high corrugation (see figure 2), even if the mean interlayer Pb–N_2 distance is larger than 4.3 Å. The F_s decays

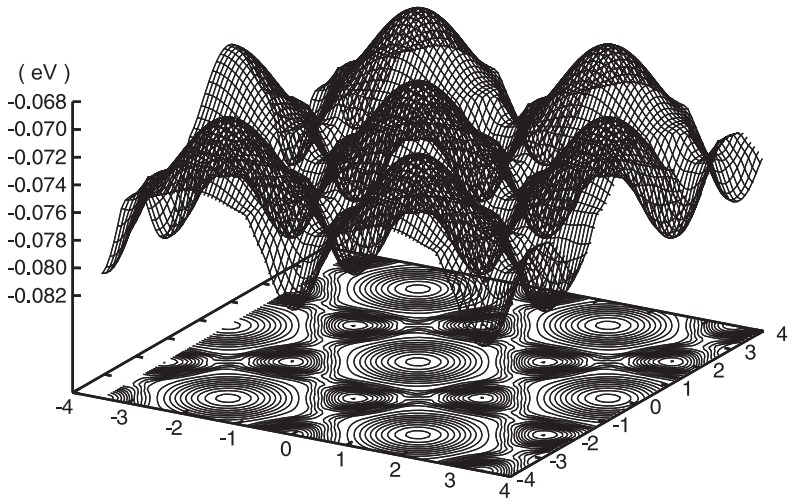

Figure 7. The N_2/Pb interaction potential evaluated at the interface for the equilibrium distance of Pb and N_2 molecules in the case of low corrugation. The vertical axis potential is in eV. The in plane axes refer to the $[1\bar{1}0]$ and the $[11\bar{2}]$ directions respectively. The distances are in Å.

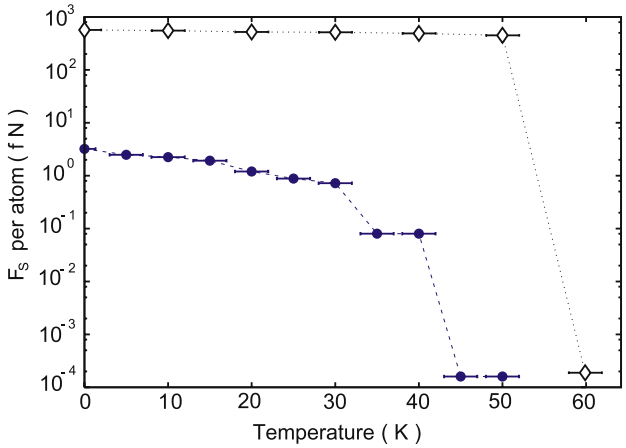

Figure 8. The static friction per atom F_s for the low corrugation interface. The full circles refer to the mobile substrate case, while the open diamonds refer to the fixed substrate calculations.

linearly in the region of low temperature, below the melting point. This behaviour has been explained [19] by considering a one-dimensional model with thermally activated transition described by a Kramers rate [20].

There is an appreciable momentum transfer from the Pb to the N_2 particles. This momentum transfer can be estimated by taking the difference between the $\langle u_z^2 \rangle$ of column C of table 1 and column D relative, respectively, to the reference systems with mobile and fixed Pb atoms. However this momentum transfer does not produce the formation of stacking faults, contrary to the situation for the high corrugation case, discussed in paper I.

In spite of that, the structure factor of figure 9 reveals the presence of atomic disorder. At $T = 0$ K the structure factor is close to 1, in agreement with the small spreading in the z direction shown in figure 1. Increasing the temperature the structure factor goes down with small oscillations inside the N_2 crystal. At $T = 40$ K the slab starts to melt, while at $T = 50$ K all the planes up to the surface are melted.

We now turn to discussing the case of the fixed substrate. At $T = 0$ K the structure factor of figure 10 is near to 1 for all the layers. This indicates that also the interface N_2 layer is close to an ideal lattice plane. Therefore this is the system configuration, among the ones considered here, with highest commensurability [9, 21]. Therefore, the resulting F_s, presented in figure 8, is increasing and is even larger than that obtained for the 1σ potential, discussed in section 3. Since there is no momentum transfer from the rigid substrate to the N_2 molecules, the F_s decays very slowly up to 50 K and the melting of the surface occurs over $T = 60$ K. The melting temperature of the whole N_2 slab is consistent with the experimental one.

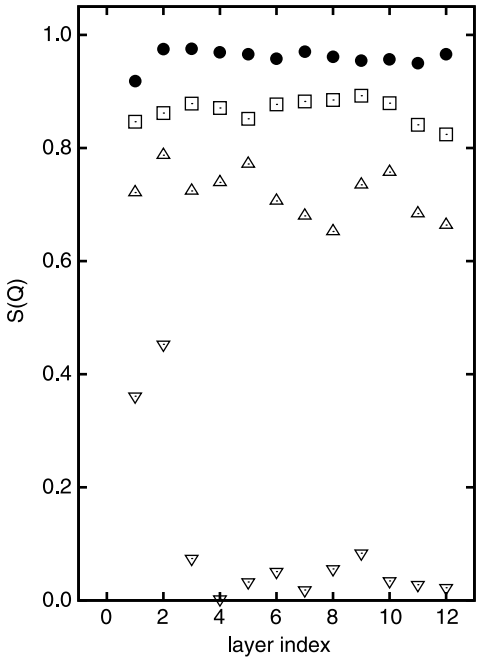

Figure 9. Structure factor, as in figure 6, for the low corrugation interface with mobile substrate. Full circles ● refer to $T = 5$ K, open squares □ to $T = 20$ K, open triangles up △ to $T = 40$ K and finally open down triangles ▽ to $T = 50$ K.

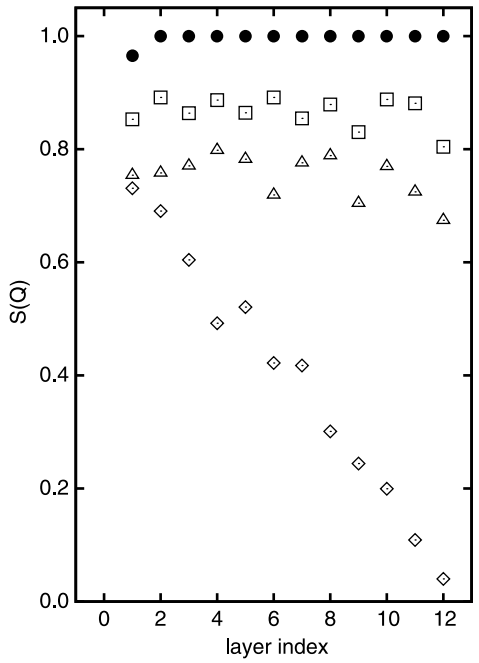

Figure 10. Structure factor, as in figure 6, for the low corrugation interface with fixed substrate. Full circles ● refer to $T = 0$ K, open squares □ to $T = 20$ K, open triangles up △ to $T = 40$ K and finally open diamonds ◇ to $T = 60$ K.

5. Conclusions

In this paper we have investigated the effect of the vibrations and of the interface corrugation on the static friction F_s. In the case of high corrugation we have compared the system formed with a mobile substrate with the one with a rigid substrate. The results indicate the existence of a very large momentum transfer if both the upper block and the lower block are formed by mobile atoms. This large momentum transfer produces a disorder of the top block which is reflected in the low value of F_s. In contrast, for the case of a rigid substrate, the interface

plane retains a disordered geometry, while the other planes present only a small temperature dependent disorder. So F_s attains a large value. For the small corrugation case, we have found for the mobile substrate a reduced disorder, which combined with the small potential barriers to be overcome gives a static friction comparable with that obtained in the case of high corrugation and mobile substrate. Finally, for the fixed substrate, the interface is very close to being fully commensurate and the F_s is the highest.

Acknowledgments

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