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2009 J. Phys.: Condens. Matter 21 264008

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# Theoretical investigation of the anticorrugation effects on the tribological properties of the Xe/Cu interface

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Received 29 December 2008, in final form 23 February 2009

Published 11 June 2009

Online at [stacks.iop.org/JPhysCM/21/264008](http://stacks.iop.org/JPhysCM/21/264008)

## Abstract

We present a molecular dynamics study of the slip time and static friction for a slab of Xe deposited on a slab of Cu. To put in evidence the role played by the phonon field of the two blocks, we compare results obtained with a substrate formed by fixed atoms with one formed by mobile atoms. In the last case the scattering between Xe and Cu mobile atoms is inelastic and there is an exchange of momentum and energy between the two blocks which produces disorder in the interface plane. This disorder favors a decrease of the static friction and a consequent increase of the slip time. We describe the interaction between Xe and Cu with a phenomenological multi-ion potential which gives rise to an anticorrugation of the charge distribution and reproduces very well the *ab initio* density functional calculations. Our model potential is a linear superposition of a corrugating potential and an anticorrugating one. For this reason we can study the static friction by passing from an anticorrugated to a fully corrugated system. We also investigate the slip time and we compare our results with recent experimental data measured with the quartz crystal microbalance technique.

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

## 1. Introduction

Although tribology has been of technological interest since ancient times, the argument has returned in fashion today. The new interest in tribology is due to the progress and development of new experimental techniques that allow controlled measurements at atomic scales and to a new generation of computers that allow us to analyze the complex dynamics at an atomic scale of large systems. The major new atomic scale experimental methods developed in the last 20 years are the quartz crystal microbalance (QCM) [1–3], the atomic and friction force [4, 5] microscopies (AFM/FFM) and finally the surface force apparatus (SFA) [6]. The QCM technique is typically used to measure the tribological properties of solid monolayers of adsorbates atop a oscillating surface, the AFM/FFM techniques are used to study the interparticle contacts, adhesion, friction and load dependence in air, while the SFA, which is operating in a perfectly well-defined tribology configuration, is commonly used to measure

adsorption on and forces between molecularly smooth mica surfaces confining thin films of lubricants. The experiments with these new techniques have promoted new theoretical studies of friction, which have languished for the previous half-century. The difficulty in testing hypotheses was a major factor in the theoretical field. A tremendous amount of parameters affect the lateral force between two solids. The result obtained from macroscopic measurement is a single number: the friction coefficient. Thus the verification or the falsification of theories was basically impossible. The advent of controlled atomic scale measurements changed the situation and new computational techniques allowed theorists to study models that include most of the internal degrees of freedom of the contacting surfaces.

This paper addresses the study of the friction for a combined system of a slab of Xe atoms on a Cu(111) substrate with molecular dynamics simulations. This choice is dictated by the fact that for this system all the potentials involved are known. For the Cu substrate and for the

Xe–Cu interactions first-principles density functional calculations are available [7, 8]. The Xe–Xe interaction can be very well described by a Lennard-Jones potential [9]. Furthermore, this system has been studied experimentally by using the quartz crystal microbalance. In our analysis we will consider only the phonon contribution to friction because up to now there is no theory which can introduce on the same footing both electronic and phononic contributions.

This paper is organized as follows: in section 2 we will present and discuss the potentials that enter in the system, in particular the Xe–Cu interaction which has been determined from density functional calculations. These calculations have shown that at small distances this interaction between the closed shell of the adatom with the charge distribution of the surface metal atoms gives rise to the anticorrelation of the surface [7, 8]. The term ‘anticorrelation’ means that the electron corrugation is shifted away from the atomic positions and the equilibrium position of the Xe adatom is in the on-top position of the Cu atoms. If the Xe–Cu interaction would be generated by the usual sum of central two-body interactions the equilibrium position would be in a hollow site instead of being in a top site as indicated by the *ab initio* calculations. To reproduce the first-principles anticorrelation, in section 2 we use a multi-ion potential [10, 11] which is a superposition of a corrugating part and an anticorrelating part. Having an analytic form for the potential for this important part of the total interaction we can use a large number of particles in our dynamical calculations in order to study the tribological properties. With our multi-ion potential, by changing the mixing parameter we can describe both a purely corrugated surface and an anticorrelated one. Of course, for a particular value of this mixing parameter we can reproduce very well the *ab initio* results. The molecular dynamics sample is described in section 3. The effects of the corrugation or anticorrelation on friction are discussed in section 4: calculations are performed for the slip time as recently measured [12], as well as for the static friction. Finally, in the last section 5 we draw conclusions.

## 2. The potential

Rare gas atom adsorption on metal surfaces has been considered as a paradigm [13] of a simple physical adsorption system. The weak interaction between rare gases and metal surfaces has often been described using pair potentials like the Lennard-Jones potential (LJ). Because the Lennard-Jones potential favors close-packed structures, this led to the expectation that rare gas adatoms on metal surfaces preferentially bind in high corrugation hollow sites. This widely accepted apparent hollow site preference of adatoms on metals was first questioned by Rieder and Garcia [14]. Their measured corrugation for Ni(110) was in serious discrepancy with calculations based on two-body interactions. In recent years, quantitative LEED intensity analyses have confirmed that the on-top adsorption site for Xe on Cu(111) [7, 8] and other transition metal surfaces is preferred to the hollow site. Calculations based on density functional theory performed ten years ago by Petersen *et al* [15, 16] confirm for the Rh(111) that

the adatom is in a minimum of the potential energy surface on the on-top position. Now the recent energy calculations in the density functional theory (DFT) [7, 8] confirm that for the Xe on Cu(111) the on-top position is preferred. Calculations are performed in DFT in the local density approximation (DFT-LDA) by evaluating the perpendicular potential energy surface (PES) for Xe atoms in the on-top and hollow sites for different Xe heights, measured with respect to the topmost layer. These results indicated that the physisorption energy is lower in the on-top site than in the hollow site. The DFT-LDA results reproduce accurately only the values of the potential around the minimum of the PES where there is a strong overlap of the wavefunctions of the Xe and Cu atoms. At large distance they do not reproduce the van der Waals attraction. Several ways of introducing the correct van der Waals decay at large distances have been proposed [17]. In our approach we need an analytic form of the potential between the Xe atom and the Cu(111) surface. We use the most successful [13] function

$$V_{\text{tot}} = V_{\text{R}} + V_{\text{A}} \quad (1)$$

formed by a repulsive  $V_{\text{R}}$  and an attractive  $V_{\text{A}}$  part that we have used in the past to describe properly the scattering of He atoms from Cu and Rh surfaces. The repulsive short range part  $V_{\text{R}}$  is described by a multi-ion interaction which reproduces the anticorrelation around the minimum and the attractive  $V_{\text{A}}$  part by a van der Waals interaction with Tang–Toennies corrections [18] to avoid the divergence at the origin. The repulsive part is taken as a weighted linear combination of a central two-body interaction and a multi-ion interaction [10, 16]:

$$V_{\text{R}} = \sum_l \left\{ \alpha w(|\vec{r} - \vec{r}_l|) + 1/2(1 - \alpha)[w(|\vec{r} - \vec{r}_l - \vec{b}_1|) + w(|\vec{r} - \vec{r}_l - \vec{b}_2|)] \right\} \quad (2)$$

with

$$w(r) = V_0 \frac{e^{-\beta r}}{\beta r} \quad (3)$$

where the  $\vec{r}_l$  are covering the lattice points of the fcc(111) surface and the  $\vec{b}_l$  represent the positions of the hollow sites. The unit cell is drawn in figure 1. The  $\vec{b}_l$  introduce a basis in the hexagonal cell, shifting the charge profile with respect to the underlying atoms. The summation over the  $\vec{b}_l$  vectors is restricted only to the surface atoms.

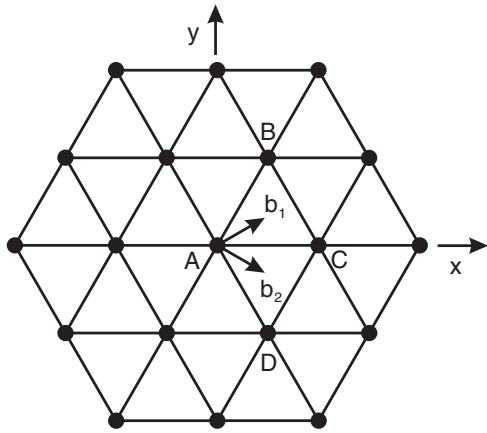
The attractive part is

$$V_{\text{A}} = \sum_l \frac{C_6}{|\vec{r} - \vec{r}_l|^6} f_6(|\vec{r} - \vec{r}_l|) \quad (4)$$

where the Tang–Toennies function [18] is

$$f_6 = 1 - e^{-\beta r} \sum_{k=0,6} \frac{(\beta r)^k}{k!}. \quad (5)$$

The parameters  $\alpha, \beta, V_0, C_6$  are fitted to the vertical PES around the minimum of the potential for Xe in the on-top and hollow sites. In this way the proper van der Waals behavior is preserved at large distances. The parameters obtained by the



**Figure 1.** The unit cell ABCD with the two basis vectors  $\vec{b}_1$  and  $\vec{b}_2$  relative to the two nonequivalent hollow sites, located at  $(\frac{a_0}{2\sqrt{2}}, \frac{a_0}{2\sqrt{6}})$  and  $(\frac{a_0}{2\sqrt{2}}, -\frac{a_0}{2\sqrt{6}})$ , respectively, where  $a_0$  is the lattice parameter.

fit are  $V_0 = 18\,000$  eV,  $C_6 = 91$  eV  $\text{\AA}^6$ ,  $\beta = 3.093$   $\text{\AA}^{-1}$  and  $\alpha = 0.06$ .

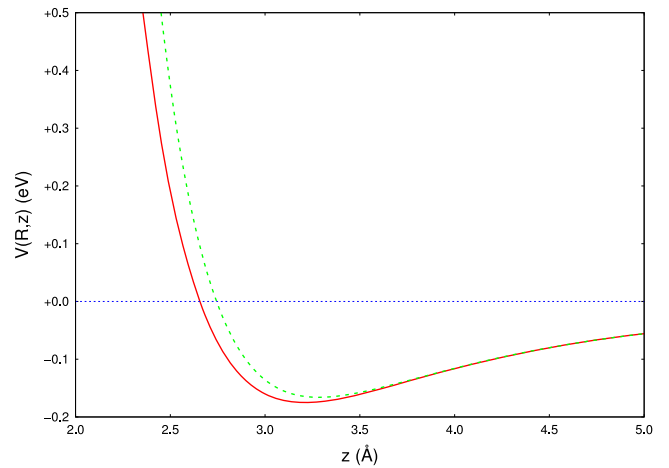
Note that for  $\alpha = 0$  we have a purely anticorrugated surface, whereas for  $\alpha = 1$  the surface is fully corrugated. The two interaction potentials, for on-top and hollow sites, are presented in figure 2.

In our model the adsorption energy  $E_{\text{ad}}$  of the Xe in the on-top position is  $E_{\text{ad}} = -176$  meV, while the experimental value is ranging from  $-183$  [19] to  $-190$  meV [20].

### 3. Construction of the slab Xe–Cu

The specimen used in our molecular dynamics calculations is formed by a top solid of 12 fcc(111) layers of Xe, while the bottom substrate is made by 24 (111) planes of Cu atoms. As mentioned before, the Xe–Xe interaction is described by an LJ potential [9] with  $\epsilon = 20.3$  meV and  $\sigma = 3.89$   $\text{\AA}$ . The interaction between the Xe and Cu atoms has been described in the previous section. For the Cu substrate we use a multi-ion potential whose parameters are fitted to *ab initio* calculations [21] for which we have an analytical expression. In the molecular dynamics method one has to impose periodic boundary conditions. In our geometry they are applied along the  $[11\bar{2}]$  and  $[1\bar{1}0]$  directions. For this reason, the two slabs need to have equal sizes in these two directions. To fulfill the requirement we build a simulation cell of the Xe top slab formed by  $9 \times 9$  surface cells in both directions for a total of 162 atoms. The Cu substrate slab is described by  $15 \times 15$  surface cells in each direction for a total of 450 atoms per plane. The mismatch between the two ideal cells is less than 2%. We then stretch the upper block to match the periodicity of the Cu substrate.

In this manner our simulation cell dimensions in the  $xy$  plane, where the periodic boundary conditions are applied, are the following: 38.25  $\text{\AA}$  in the  $x$  direction and 66.45  $\text{\AA}$  in the  $y$  direction. The equilibrium of the composed system is obtained by a Parrinello–Rahman simulation with a time step of 1.95 fs. To get the system in equilibrium at  $T = 0$  K and during the



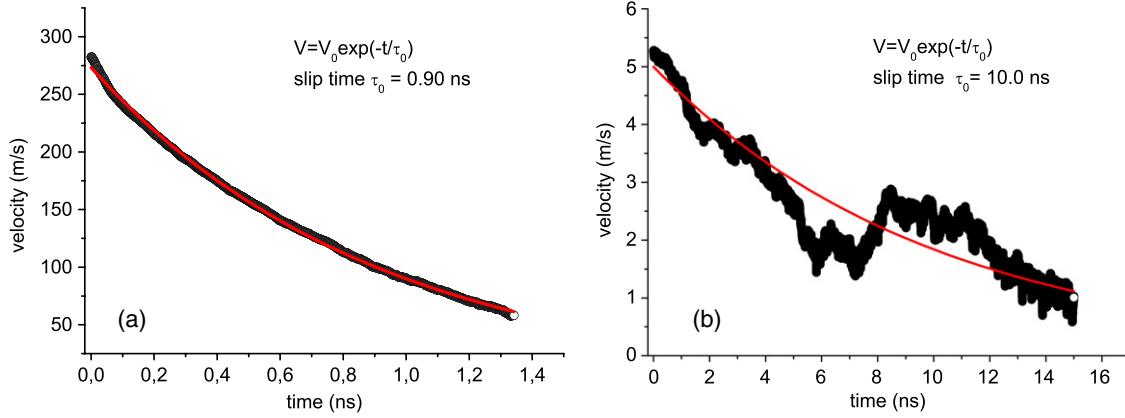
**Figure 2.** The interaction Xe–Cu potential  $V(\vec{R}, z)$  evaluated in the on-top site  $\vec{R}_{\text{top}}$  (continuous line) and in the hollow site  $\vec{R}_{\text{hollow}}$  (dashed line). The parameters used are those that fit the *ab initio* calculations.

successive cycles of simulation, we perform a quenching for a simulation time of 10.0 ns, reducing the kinetic energy of the particles very close to zero [22].

### 4. Calculations

In previous papers, concerning the  $\text{N}_2/\text{Pb}(111)$  system [22, 23], we have proved the importance of taking a thick substrate in studying the friction. Here we want to show that the same occurs for the case of Xe on Cu. In this case the Xe atoms of the top substrate have a heavier mass than those of the Cu atoms of the lower substrate. This is the opposite case of having  $\text{N}_2$  molecules on the Pb substrate. As in the previous case, the scattering of the Xe atoms with the Cu particles is inelastic and there is a transfer of momentum and energy which disorder the heavy atoms of Xe. The disorder mainly occurs in the top block because the Xe–Xe interaction is rather weak. If the substrate is taken, as usual, as formed by a few numbers of fixed atomic planes the scattering would be elastic and the geometry of the top layer would remain more ordered. In this case of ‘high commensurability’ [24] the static friction would be large. With mobile atoms, instead, the exchange of energy and momentum disorder the top block and several atoms of Xe can move in the valleys of the Cu substrate. This is the situation that we have found and we have discussed at some length in the previous paper on  $\text{N}_2$  on Pb [22]. The Xe atoms see a small effective energy barrier and the static friction becomes very small, as we will illustrate in the next paragraphs.

Experiments concerning the interaction of Xe with noble metals have been performed by Krim and co-workers [25, 26]. In particular, by using the quartz crystal microbalance method they have studied the slip time of Xe on metal surfaces, such as Xe on Ag(111), Xe on Ni(111) and Xe on Cu(111). They determine the slip time for increasing coverages. To compare our results with the experiments we apply an external force greater than the static friction force, parallel to the substrate, to all particles of the top slab for approximately 300 ps. The external force is then removed. This induces an initial center-of-mass velocity  $V_0$  in the block which decay at later times



**Figure 3.** PANEL (a) Slip time evaluated by considering the substrate formed by still atoms. The continuous curve is a best fit of the simulation data. PANEL (b) Slip time evaluated for mobile substrate. The full curve is the result of a best fit of the molecular dynamics data.

as  $V_0 e^{-t/\tau_0}$ , where  $\tau_0$  is the slip time. Experimentally the typical values of slip time for Xe on metal surfaces is of some nanoseconds: according to Daly and Krim [26] the slip time around 2 ML is about 2.4 ns for Xe on Ag(111) and according to Coffey and Krim [12] the slip time is 15.5 ns for one monolayer of Xe on Cu(111). Our calculations are performed both for a fixed Cu substrate and for the substrate with mobile atoms. The results are reported respectively in figures 3(a) and (b).

Again one notice a large difference in the value of the slip time in this two cases and a more complex behavior of the decay of the velocity due to the phonon–phonon interaction between the two systems, which is absent in the fixed case. It should be noted that for a fixed substrate the decay of the velocity is rather fast, because there is no exchange of energy and momentum between the upper and lower slab and after a long enough time period the upper film would stop and the friction would vanish. The rigid substrate approximation does not give rise to a realistic description of the sliding.

For a substrate with mobile atoms, because of the exchange of energy and momentum between the upper and lower slab, there is an increase of about a factor 10 with respect to the substrate with fixed atoms. For the mobile substrate we have  $\tau_0 = 10.0$  ns. The semiquantitative agreement with the data of Coffey and Krim could be related to the geometry of the system. In fact, they are evaporating the Xe and Cu on the quartz and then the sample is chilled to 77.4 K. For this reason there is no proof that Cu and Xe will form perfect crystals. Very probably both the Xe and the Cu films are disordered and a full quantitative comparison is not possible.

We now turn to discuss our results for the static friction. Before doing this we return to the Xe–Cu interaction potential. We define for the potential energy surface (PES) the function  $V(\vec{R}, z(\vec{R}))$ , with  $z(\vec{R})$  satisfying the equation

$$\left. \frac{\partial V}{\partial z} \right|_{z(\vec{R})} = 0 \quad (6)$$

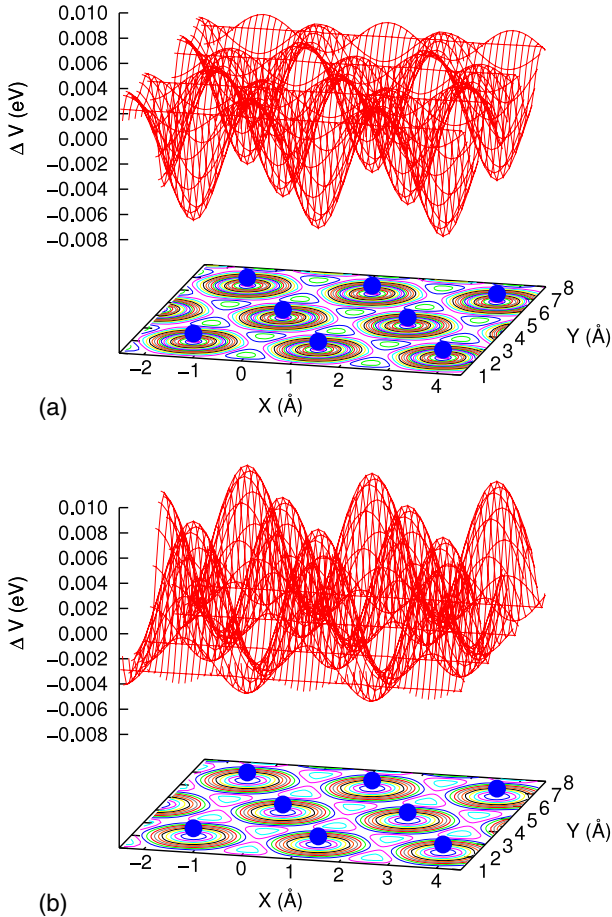
where  $z$  is measured with respect to the last plane of the Cu slab and the vector  $\vec{R}$  spans the 2D unit cell. The potential corrugation is defined as  $V(\vec{R}_{\text{top}}) - V(\vec{R}_{\text{hollow}})$ , where  $\vec{R}_{\text{top}}$  is the value of  $\vec{R}$  in the top position and  $\vec{R}_{\text{hollow}}$  is the value

in the hollow site. Note that this quantity is negative if the system is anticorrugated and positive for a corrugated system. In section 2 we have seen that our potential reproduces for the mixing parameter  $\alpha = 0$  a purely anticorrugated system and for  $\alpha = 1$  a corrugated one. The 3D plot of the PES at equilibrium for these two values of  $\alpha$  is presented in figures 4(a) and (b). One can see that in the anticorrugated case the minima of the PES are in the on-top position of the Cu atoms.

To study the static friction at  $T = 0$  K by using molecular dynamics calculations there are several operative ways [27, 28]. The search algorithm that we use is the following [22, 23]. We first guess the lower and the upper value for the static friction. The Xe upper block is considered to be stuck if the center of mass moves during the 1000 ps of the free simulation by less than our distance period of the Xe–Cu corrugation. The crystal is sliding if it moves more than three periods. We start by choosing a force  $F_{\text{rest}}$  for which the upper block is stuck and a force  $F_{\text{slid}}$  for which it slides. We take the average of these two forces and we perform a simulation of 1000 ps. If sliding occurs, this average force becomes the new guess of  $F_{\text{slid}}$ , while if the block is stuck it becomes the new guess of  $F_{\text{rest}}$ . We repeat this iterative procedure several times to obtain the difference between the two forces by less than 2%.

With the  $\alpha = 0.06$  value, which reproduces the DFT-LDA calculations, we obtain for the system with the Cu atoms held fixed in the official sites a static friction  $F_s = 177$  fN, while when the Cu atoms are allowed to move and phonons are excited on the lower block it becomes  $F_s = 3.00$  fN. Note that also in this case in which the heavy mass is the top layer, opposite to the case of N<sub>2</sub>/Pb, the result confirms our previous important conclusion that the substrate cannot be described by a flat undulated static surface as usually done in many calculations and the importance of the inelastic scattering between the particles of the two blocks. From now on we will only use a mobile substrate.

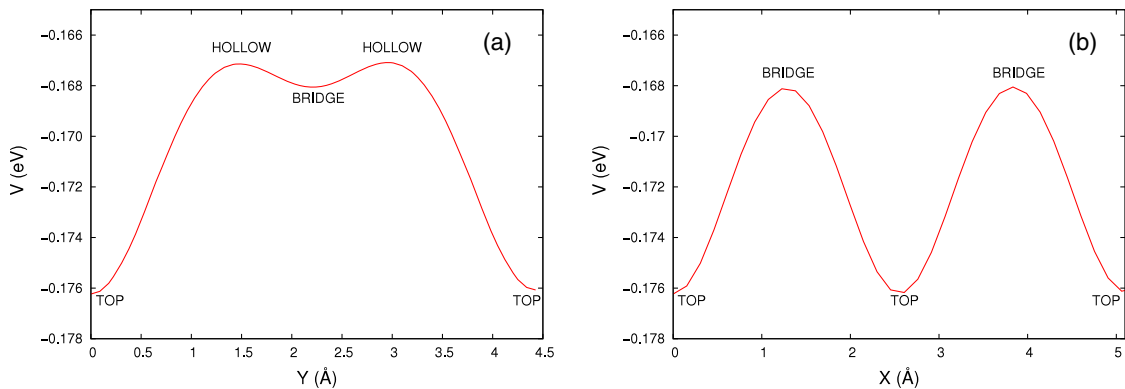
Since our model potential is a linear combination of a corrugated and an anticorrugated part, we can analyze different cases of the total corrugation. As an illustration, we draw the corrugation  $\Delta V$  at equilibrium along the  $y$  and  $x$  directions for



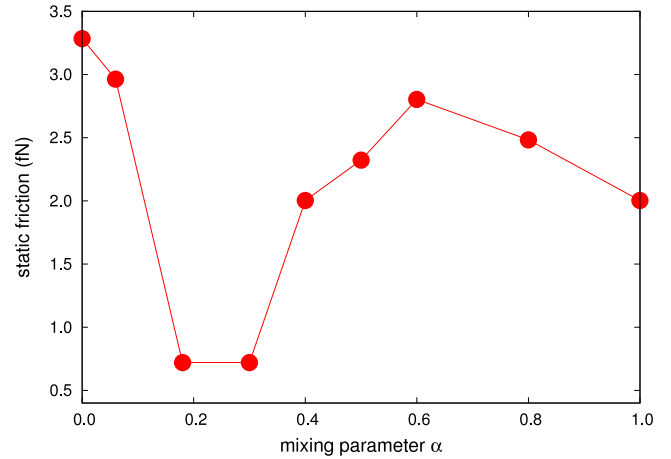
**Figure 4.** (a) 3D plot of the PES measured from its mean value for different values of  $\alpha$ , with contour plot projection on the surface. The full dots are the Cu atom sites. It refers to the  $\alpha = 0.0$  fully anticorrugated system. (b) As in (a) for the fully corrugated surface  $\alpha = 1.0$ .

$\alpha = 0.06$  in figures 5(b) and (a). Similar behavior is obtained for all the anticorrugated surfaces.

We present in figure 6 the calculations of the static friction for several values of the mixing parameter  $\alpha$ . Note that the static friction force  $F_s$  has a nonmonotonic behavior, showing a dip in the anticorrugating region and a local maximum in the corrugated zone. The static friction does not vanish for any



**Figure 5.** Potential  $V(\vec{R}, z(\vec{R}))$  for anticorrugated system with mixing parameter  $\alpha = 0.06$  evaluated for  $\vec{R}$  along the  $y$  direction (panel (a)) and along the  $x$  direction (panel (b)). Note that the potential corrugation amplitude  $V(\vec{R}_{\text{on-top}}) - V(\vec{R}_{\text{hollow}})$  along the  $y$  direction is negative.



**Figure 6.** The static friction force per atom as a function of the mixing parameter  $\alpha$ .

value of  $\alpha$ . This is due to the phonon inelastic scattering of Xe atoms with the vibrating Cu atoms of the substrate which give rise to an exchange of energy and momentum between the two systems. Only for a flat ideal layer, represented by the potential of equation (1), would the force  $F_s$  vanish, because in this case the interaction would be purely elastic.

## 5. Conclusions

In the present paper we have done calculations of the slip time and of the static friction by using the molecular dynamics simulation method for the system Xe/Cu(111). For this system there are recent calculations of the interaction potential between a Xe atom and a Cu(111) surface performed in the density functional theory approach. This potential is one of the most important ingredients in studying the frictional properties of this system. The *ab initio* calculations have proved that the interaction potential energy surface is anticorrugated and the Xe atoms are in equilibrium in the on-top position. To perform molecular dynamics simulations we have used a phenomenological multi-ion potential whose parameters have been fitted to reproduce the results of the *ab initio* calculations around the minimum of the interaction well. We have

chosen a two-body potential which at short distance is a linear combination of a corrugating and an anticorrugating potential, while at large distances it reproduces the van der Waals attractive interaction. The phenomenological potential is additive to reproduce the *ab initio* calculations and can be used to investigate the effects of the corrugation on the static friction, starting from an anticorrugated system to a fully corrugated one. We have found that for a mobile substrate the static friction decreases by a factor of 60 with respect to the fixed one. In this case the scattering is inelastic then there is an exchange of momentum and energy between the two systems and some disorder is produced in the interface plane of Xe atoms. The Xe atoms of a disordered layer can move easily in the valleys of the Cu substrate and there is a reduction of friction. This result is independent of having the top layer formed by heavier atoms with respect to the atoms of the substrate. The momentum and energy transfer occurring when we allow a phonon–phonon interaction between the two slabs is sufficient to disorder the interface layer. We have studied the slip time to compare our results with the experimental data of the system Xe/Cu(111) measured with QCM. The calculations with the mobile substrate are in reasonable agreement with the experimental values. This indicates that nowadays 3D molecular dynamics calculations can be used to interpret successfully the experimental data. With our model potential, by changing a parameter we can obtain either a corrugated system or an anticorrugated one. We performed calculations by varying this parameter from a fully corrugated to an anticorrugated system. One of the main results of our calculations with our model potential is to show that the smallest value of the static friction occurs for an anticorrugated surface. This minimum value is different from zero and is related to the phonon–phonon interaction between the two blocks. It would be identically zero if one would consider the Cu plane at the interface as a rigid flat surface. In this case there would be nonlateral interactions. We hope that the present paper will stimulate a theoretical and experimental analysis of the effects related to corrugated and anticorrugated potential energy surfaces. This in principle could be done by adding impurities on the surfaces by adding vertical forces to the top slab to reduce the interplanar spacing between the two slabs. For a sufficient high pressure for our system Xe/Cu(111) we expect that the system will acquire a corrugated surface energy.

### Acknowledgments

This research was partially supported by the MIUR Prin 2006023721. We would like to thank M C Righi for very useful discussions.

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