# Frictional Force between a Sharp Asperity and a Surface Step

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We report a detailed study of the frictional force between the tip of a scanning force microscope and a step on a crystalline surface. Experiments on surfaces of freshly cleaved graphite reveal different contributions to the lateral force at steps with distinctly different dependencies on normal load and scan direction. The different contributions can be attributed to topography-induced tip twisting and an increased dissipative force due to the Schwoebel barrier at the steps. The latter contribution is strongly reduced when near-surface step dislocations are imaged. [S0031-9007(97)04871-0]

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Friction between the surfaces of two sliding bodies is of utmost technological relevance, as it widely determines the lifetime of literally all mechanical machinery. The search for a quantitative understanding of the microscopic processes involved when two rigid bodies slide against each other has been the subject of scientific studies for almost 300 years and still drives a vivid field of science [1]. With the advents of the surface forces apparatus (SFA) [2] and the scanning force and friction microscope (SFFM) [3,4], highly sensitive experimental techniques became available, which can complement macroscopic friction measurements and allow one to test microscopic models on the atomic scale [5–7]. In their pioneering SFFM work, Mate *et al.* [4] found that the friction coefficient between a sharpened tungsten tip and freshly cleaved graphite surface was about an order of magnitude smaller than a typical macroscopic friction coefficient of graphite. Ruan and Bhushan studied the same system and observed an increased lateral force in certain line-shaped areas of the cleaved surface [8]. However, since both experimental studies were performed under ambient atmosphere, contaminant adsorption could not be excluded which may well have influenced the observed frictional forces. In a more quantitative study, Meyer *et al.* recently investigated the frictional force at stepped NaCl(100) surfaces [9] cleaved under ultrahigh vacuum (UHV) conditions. The authors observed an increased lateral force at steps.

In this paper, we aim at a better understanding of the basic phenomena involved when a sharp asperity slides over an atomic step on an otherwise flat and homogeneous crystal surface. To ensure that we are working with a very simple and reproducible model system, we study monatomic and multiatomic steps on the surface of freshly cleaved highly oriented pyrolytic graphite (HOPG). To avoid complications due to adsorption of water or other contaminants, both sample preparation and friction measurements were performed under UHV conditions. A step represents a surface inhomogeneity in two ways. On the one hand, it can be considered merely as a topographic step of well-defined height. On the other hand, because of differences in the local atomic structure near the step, it should be characterized by different electronic states as compared to the flat terrace. Both topographic and electronic effects are expected to contribute to a change in the lateral force when the asperity slides over the step. We shall show that the lateral force is indeed composed of at least two contributions behaving differently with respect to the applied normal force and to the scan direction. Under certain experimental conditions, only one of the contributions is observed, which helps to identify their physical origins.

For our experiments, we used a home-built UHV-SFFM based on the beam deflection technique [10]. Both the HOPG samples and the SFFM tips could be changed without breaking the vacuum. For the present experiments, we used commercial $Si_3N_4$ tips with spring constants of 0.05 and 140 N/m for normal bending and torsional bending, respectively. Surfaces of freshly cleaved HOPG were prepared in UHV immediately before SFFM investigation. Together with a topography image, lateral force images were taken in both the forward and backward scan directions.

Figure 1 shows a typical topography image of a stepped HOPG surface. The height of the steps shown in Fig. 1 ranges from one to three graphite layers. As can be seen in the cross sections shown on the right-hand side of the figure, the lateral force is increased when the tip slides across a step, no matter whether the steps are scanned upwards or downwards. However, the increase in lateral force is always larger when a step is scanned upwards as compared to scanning the same step in downward direction. An important detail is revealed when comparing the position of the lateral force peaks with the position of the steps in the topography image. It turns out that the maximum of the lateral force appears at the base of the step, i.e., before the step is actually imaged in the normal force mode. The lateral force starts decreasing as the tip moves up onto the step. This behavior is generally observed for upwards scans. It suggests that the tip sticks at the base of the steps and is twisted until the torque is large enough to overcome the sticking. Then, as the tip moves on, the torque decreases. A similar although less

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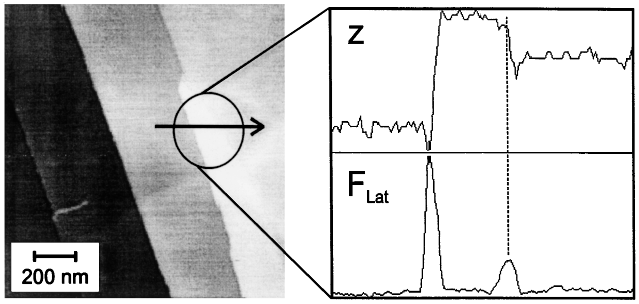


FIG. 1. Topography image (left) of an HOPG surface after UHV cleavage. The image was taken at an external load of 2 nN. The right-hand side shows cross sections through the topography ("$z$," top) and the lateral force ("$F_{\mathrm{lat}}$," bottom) images taken at the line indicated in the topography image (left). The step heights correspond to one and two graphite layers, respectively. The amplitudes of the lateral force peaks amount to about 6 nN (two atomic step) and about 1.3 nN (monatomic step), respectively.

pronounced effect is observed when scanning down the step. Again, the lateral force increases before the step is imaged in the topography mode.

A noticeable difference between scanning a step upwards and downwards appears, if one determines the lateral force as a function of the applied normal load. As can be seen in Fig. 2, we find a monotonous increase in the lateral force with increasing normal load for upward scans. The rate of increase is found to grow with increasing step height. Over a wide range of normal forces the data are well described by a linear relation between the normal and lateral forces. Only in the limit of very small normal forces a deviation from the linear behavior is observed [11]. For downward scan on the other hand, the lateral force is barely affected by a variation of the normal load. For increasing step heights, only a slight increase of the lateral force is observed.

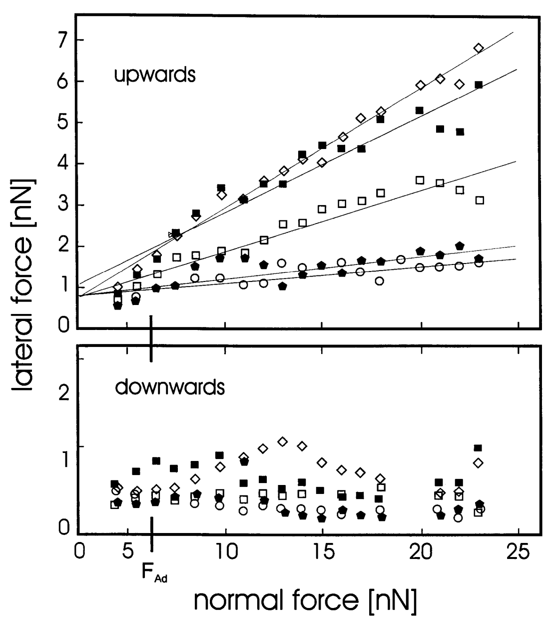


FIG. 2. Lateral force versus normal force for steps of different step heights: 2 atomic layers (circles and solid pentagons), 4 atomic layers (open squares), and 10 atomic layers (solid squares and diamonds). The solid lines are linear least squares fits to the data merely meant as guides to the eye. Note that the vertical scale has been blown up for the data from downward scans (bottom). The value of the adhesive force was determined from force-distance curves.

To gain deeper insights into the physical processes underlying the above observations, we take a closer look at the actual shape of the lateral force signal as a step is imaged. It turns out that the single peak in the lateral force (Fig. 1) reveals a far more complex structure if imaged with increased spatial resolution. This effect is most pronounced when steps are scanned downwards, so we will concentrate on this case first. Figure 3 shows a lateral force image [Fig. 3(a)] together with cross sections through normal [Fig. 3(b)] and lateral force taken during a downward scan over a monatomic step at two different values of the normal load [Figs. 3(c) and 3(d)]. It turns out that while a single peak in the lateral force is observed at a normal load of 6 nN [Fig. 3(c)], the lateral force peak exhibits a sharp dip in its center when the normal load is increased to 20 nN [Fig. 3(d)]. The latter effect is clearly revealed in the lateral force image [Fig. 3(a)], which was taken at a normal load of 20 nN.

We note that the normal load $F_N$ acting on the tip is the sum of the adhesive force $F_{\mathrm{ad}}$ and the external load $F_{\mathrm{ex}}$, which is applied to the cantilever. We generally find that a second, narrow peak of opposite sign is superimposed on the lateral force signal as soon as the normal load is larger than the adhesive force, i.e., for *positive* external load. The amplitude of the narrow peak grows as the normal load is further increased. The width of the narrow contribution quantitatively relates to the width of the step as revealed from the topography image. We conclude

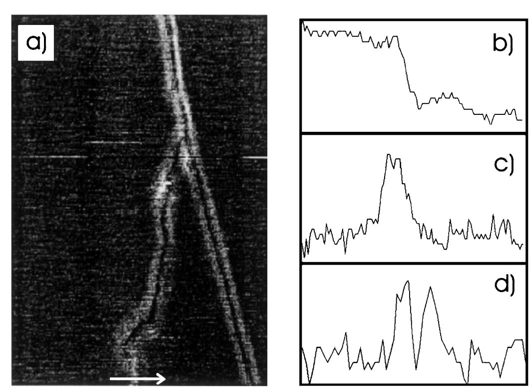


FIG. 3. (a) Lateral force image of two steps on a HOPG surface taken at a normal load of 20 nN [size: $340 \times 500\ \mathrm{nm}^2$]. The right-hand part of the figure shows a cross section through the monatomic step of the corresponding topography image (white arrow) (b) and two cross sections through lateral force images taken at a normal load of 6 nN (c) and 20 nN (d), respectively. The amplitudes of the measured lateral force peaks are in both cases about 0.5 nN.

at this point that a repulsion between tip and surface is necessary for the narrow peak to appear.

So far we have concentrated on steps being scanned in the downward direction. When scanning in the upward direction, a similar scenario is observed. However, in contrast to the downward scans described above, for upward scans the narrow peak *adds* to the overall lateral force. Consequently, the deconvolution of the measured lateral force signal into the two components is much easier for steps being scanned downwards as compared to upward scans.

The experimental results presented so far can be summarized as follows: The lateral force observed when scanning across a HOPG step consists of at least two different contributions. One (the "broad peak") leads to an increase of the lateral force no matter whether the step is scanned upwards or downwards. The other (the "narrow peak") appears only in the repulsive regime. It increases the lateral force when a step is scanned upwards, while it decreases the lateral force, when a step is scanned downwards.

We start our discussion with the broad peaks observed in the lateral force signal. As they change sign with changing scan direction, they represent a truly dispersive force, which is always acting in the direction opposite to the moving tip. We assume that this frictional force is due to the particular electronic environment in the vicinity of a step. When scanning a step downwards, the tip atoms experience a potential barrier before reaching the step edge. This barrier (often referred to as the "Schwoebel barrier" [13]) has to be overcome, before the tip can slide down the step [7]. Given a typical torsion spring constant of some 200 N/m and a barrier height of some $0.1, \ldots, 0.2$ eV [14], the torsion of the cantilever induced by the barrier should be easily detectable. As the barrier height is not affected by an increase in the normal load, this contribution should be rather independent of the normal force applied to the cantilever. This is in agreement with the experimental data presented in Fig. 2. The situation is more complex when a step is scanned upwards. Following the notion of a Schwoebel barrier, the tip atoms are expected to be "trapped" in a potential minimum located at the base of the step, and they have to overcome a significantly larger energy barrier as compared to the downward scan. One can think of the trapping as a formation of temporary bonds between the tip atoms and the unsaturated $sp^2$ electrons at the step edge [15,16]. On increasing normal load, the tip will be pressed into the topmost graphite layers and an increased number of contact points between tip and step will be established. This notion is in agreement with the finding that the lateral force observed during upward scans is generally larger as compared to downward scans and that it increases with increasing normal load. In addition, it explains the fact that the maximum lateral force is observed before the step is actually imaged, i.e., before the tip moves across the step.

In contrast to the broad peaks, the narrow peaks do not change sign when the scan direction is reversed. In addition, they only appear in the repulsive regime, i.e., when the tip is pressed against the step by an external force. Both characteristics indicate that the torsion of the cantilever is geometrically induced. The step edge constitutes a contact point, which is not necessarily located underneath the center of the cantilever, thereby creating an additional torque as soon as the tip is pressed against the surface. The resulting torsion of the cantilever is characteristic for the tip/step geometry and should not depend on the scan direction. Obviously, the torque will increase with increasing normal load as observed in the experiment. The notion of a topography-induced tip torsion is corroborated by the experimental finding that the resulting contribution to the lateral force is highly localized at the step. One is tempted to calculate the topography-induced torsion of the cantilever in a simple mechanical model. It turns out, however, that the problem is rather complex as the cantilever can bend not only perpendicular but also parallel to the sample surface. The latter bending imposes a serious problem for a model calculation, as the axis of torsion is no longer fixed in space but moves as the tip is pressed against the step. So far, we were not able to come up with a reasonably simple mechanical model which could account for the observed lateral forces. Numerical calculations, taking into account all degrees of freedom of the cantilever, will probably be needed to further confirm the proposed model.

Although model calculations are lacking at present, the suggested assignment of the lateral force contributions are strongly confirmed by further experimental evidence. Consider a step dislocation which is localized a few graphite layers underneath the surface of the sample. It can be thought of as a monatomic step which is covered by a set of homogeneous graphite layers. As the top graphite layers will smoothly follow the underlying step topography, the step dislocation will appear similar to a regular step in the surface topography. However, in terms of the electronic states at the surface, it shall resemble a flat terrace rather than a real surface step as no unsaturated $sp^2$ electrons are present at the surface. According to the above model, we shall therefore expect to find a lateral force signal which is dominated by the topographic contribution, i.e., a narrow peak. The broad peak, on the other hand, is expected to be significantly reduced. This is indeed the case. Figure 4(a) shows a typical topographic image of a HOPG surface after cleavage. We concentrate on the step highlighted by the white box in the lower left part of Fig. 4(a). Figures 4(c) and 4(d) show a blowup of the corresponding lateral force for two different scan directions. The lateral force at the lower part of the step reveals the typical behavior; i.e., it changes sign as the scan direction is reversed. The lateral force at the upper portion of the step, however, behaves quite differently. A much smaller lateral force is observed, which does not change sign with changing scan direction. The effect becomes most pronounced in Fig. 4(b), where the difference between the lateral forces for both scan directions is shown in a three dimensional

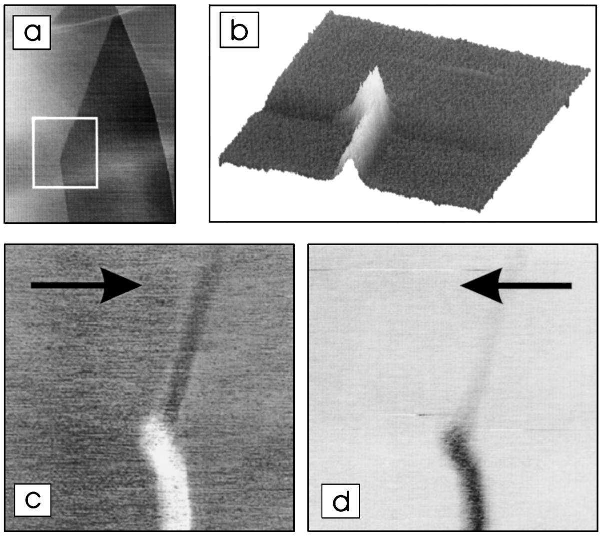


FIG. 4. Topography image of an HOPG surface (a) [size: 3 × 2.3 $\mu m^2$]. In the bottom part, a blowup of the corresponding lateral force image is shown for the two different scan directions indicated by the arrows (c) and (d) [size: 1 × 1 $\mu m^2$]. The upper right part of (b) shows the difference between the images (c) and (d) in a three dimensional presentation and therefore represents the true friction force at both steps.

plot. This difference relates to the total energy which is dissipated when the tip slides across the step and back in a closed loop. It becomes clear that for the upper part of the step, no dissipative contribution to the lateral force can be observed. Similar effects are observed, whenever a real surface step is covered by a flake of HOPG torn out and moved over the surface during the imaging process. We therefore conclude that the upper part of the "step" shown in Fig. 4 is actually a near-surface step dislocation covered by a few homogeneous HOPG layers.

In conclusion, we have investigated the lateral force acting on an SFFM tip which is scanned across monatomic and multiatomic steps on freshly cleaved HOPG surfaces. Two different contributions to the lateral force could be identified and their origin could be attributed to topographic and electronic effects, respectively. Additional experiments on near-surface step dislocations corroborate the model. The results of this work show that even for a simple surface inhomogeneity the frictional force is quite complex. In addition, the results indicate that scanning force and friction microscopy can in principle be used to image surface energy barriers related to particular defects on a surface.

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