Force measurement with a scanning tunneling microscope

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We present a scheme to measure forces with a scanning tunneling microscope. During atomic manipulation experiments with a scanning tunneling microscope the tip height curve is recorded. It is shown here that the amplitude of the manipulation curve is a measure of the interaction force between the microscopes tip and a single atom adsorbed on a surface. A simple formula is derived and tested.

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The scanning tunneling microscope (STM) has proven its unique abilities in imaging surfaces up to atomic resolution. Soon after its invention by Binnig and Rohrer it was realized that, due to its close proximity to the surface atoms the STM tip often influences and modifies the surface. This disadvantage however was used positively by modifying substrate surfaces in a controlled way. Eigler et al. showed that even single atoms can be positioned on selected adsorption sites proving the startling possibilities to build up man-designed functional nanostructures atom by atom. The manipulation process itself is a subject of fundamental experiments with single atoms. The data recorded during the positioning with the microscopes tip yields information whether the interaction is attractive or repulsive and about the atoms path on the surface.3,4 The nature of the tip-atom interaction for metal atoms was determined recently as a chemical force, dependant only on the tip-atom distance.5 Recent insights into single atom processes on crystal surfaces include friction measurements with atomically sharp cantilever and the dynamics of single atom switching.7 The force required to move a single atom across a crystal surface however has not been measured yet and we show here a simple way to measure forces with a STM. A formula is presented and tested with simulated manipulation curves.

Atomic manipulation can be described within a simple model where the surface is assumed to have a continuous sinusoidal potential with the amplitude of the diffusion barrier.3 We describe here the tip with a Morse potential and let the atom reside in the local minimum of the combined tip and surface potential. The scheme used here is not dependant on the used potential, other potentials or results from first-principle calculations can be used too. The atom moves on a two dimensional surface and the tip is assumed to be spherical. With these assumptions one can realistically describe atomic movements and tip height curves once the tip-atom force and the diffusion barrier are known. A simulation starts by placing the tip above the atom and the height is adjusted with closed feedback loop until the current set point is reached. The local potential minimum of the combined potentials is determined and the atom is shifted to it. Again the tip height is adjusted to reach the set point value of the current. These feedback loop cycles are repeated until the atom stabilizes only then the tip is shifted laterally. Figure 1 shows a description of the potential model where the atom always resides in a local potential minimum of the combined potentials of tip and surface.3 In this equilibrium position the tip-atom force is counterbalanced by the surface forces expressed by the migration barrier \(U_0\). With this description topography curves or manipulation curves at constant current can be calculated. The reverse, namely the tip-atom interaction forces can be determined too. They require experimental manipulation curves. In such case first the atoms position is determined and then the tip-atom interaction force can be calculated. Hereby one uses that the projected lateral force component \(F_{\text{lat}} = F_{\text{tip}} \cos \varphi\) needs to be equal to the surfaces force \(F_{\text{surface}}\). By using an approximate potential for the surface one can follow a simpler way and the force can be determined from a single formula shown in the following.

Figure 2 shows simulated tip height or manipulation curves for a quasi-one-dimensional periodic surface potential. Experimental values for the height are typically \(\pm 0.1 \text{ Å}\) and the amplitudes range is \(\approx 0.1 \text{ Å}\). The tip moves over the atom and changes thereby the lateral force component which is pulling the atom across the surface plane. Once the lateral force component exceeds the counterforces from the surface the atom will jump to the next local potential minimum. The recorded tip height shows a characteristic shape which can

![Graph showing the potential model to describe the atomic manipulation.](image)
We derive in Fig. 3 a formula which expresses the tip-atom force through the amplitude and height of the manipulation curve. If one approximates the atoms potential with a δ-like potential then the atom does not move until a force threshold is reached. In such a case the segments of the tip-height profile become circular shaped. We denote this radius with \( h \) as shown in Fig. 3(a). In Fig. 3(b) the lateral force component \( F_L \) is the projection of the radial force \( F_R \). Both, geometrical and force quantities are related through the angle \( \varphi \). From the amplitude \( a \), the height \( z \), and the tip-atom distance \( h \) the tip-atom interaction force can be calculated straight forward. The result is shown in Fig. 3(c), here \( F_L \) needs to be expressed through the migration barrier \( U_0 \) and amounts to

\[
F_L = 2 \pi a_0 U_0 \quad \text{with} \quad a_0 \quad \text{the lattice constant.}
\]

In good approximation one can use

\[
z = \sqrt{h^2 - \left(\sqrt{h^2 - (h-a)^2} - a_0\right)^2} \approx h
\]

and then only two entities are needed to calculate the force. We stress that this formula is derived independent of the tip-atom interaction potential and can be used to measure any potential forms.

We have tested this formula against simulated manipulation curves. For a quasi-one-dimensional potential surface a range of initial tip heights were chosen and manipulation curves simulated. From the resulting amplitudes and heights the tip-atom interaction forces were calculated and displayed in Fig. 4. The solid line denotes the Morse potential used for the tip-atom interaction. The parameters of the Morse potential correspond to a binding energy of 1.0 eV and a potential minimum at a distance of 3.0 Å, resembling the density functional theory calculation results for single Ag atoms on a Ag(111) surface. Taking into account an adatom diffusion barrier \( U_0 = 0.1 \) eV, the theoretical values are well reproduced. At larger tip-atom separation the calculated values are larger than the used potential. Here the shape of the manipulation segments is no longer circular because the atoms are pulled away from their equilibrium positions where they would stay without the presence of the tip. Such a movement around their equilibrium positions results in false values for the height as compared to the static situation and causes the shown deviation from the given force values. The direction of the movement depends upon the specific shape of the tip-atom interaction potential.

We conclude that the used tip-atom interaction force can be recovered with good agreement. The evaluation of experimental data requires additionally a calibration of the tip-height with I-Z spectroscopy. The resulting error in the height values scales nonlinear with \( 1/h \). On the open fcc(111) surfaces which are often used for manipulation ex-
The tip path runs parallel to a closed-packed height and FR analytically. Here the tip atom interaction force amounts to with a mechanically controlled break junction. Following in the measured tip-atom distance range exponential profile is expected with values in the order of a few distances typically used in manipulation experiments an exponential shape of the manipulation segments is the reason for the deviation.

The tip-atom interaction force for a single adatom adsorbed on a surface (●) is shown together with the theoretical curve for a Morse potential (−) with a binding energy of 1.0 eV at 3.0 Å. Taking into account an adatom diffusion barrier $U_i=0.1$ eV, the theoretical values are well reproduced. The deviation from a circular shape of the manipulation segments is the reason for the deviation.

According to the literature, the tip-atom interaction forces measured in this way can be described by the interaction of a Morse potential $V(r)=D_0(e^{-αr}−1)^2$ with a binding energy of 1.0 eV at 3.0 Å. For tip-adatom distances of 2 Å the surface is still 2 Å further away from the local potential minimum. Nevertheless with typical tip-atom distances of 2 Å the surface is still 2 Å further away making this surface contribution negligible and the simplified tunneling junction a good approximation. The vertical force component can reduce the migration barrier or even desorb the atom but was neglected here since the binding energy is much larger than the migration barrier. We consider elastic tip and surface deformation as the dominant experimental uncertainty in the measurement of the tip height curves.

We note that the quantity which is measured within this scheme is the force required to pull a single atom across the surface. By pulling the atom energy is transferred to the atom. The transferred energy dissipates during the jumps into the new local potential minimum by electron-hole excitation and phonon creation. The dissipating energy is transferred from the tip to the atom by lifting the local potential minimum up until the next jump occurs. The dissipation is not expected to show up in the manipulation curves at low temperature and small currents.

In conclusion we have measured tip-atom interaction forces with a scanning tunneling microscope by analyzing the amplitude of tip height data recorded in lateral manipulation experiments. The presented single atom experiment scheme opens up new possibilities for future research on single particle interaction present in van der Waals, ionic or covalent bonds.

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References:


See EPAPS Document No. E-PRBMDO-75-012703 for a sequence of images showing the calculated manipulation curve in constant current mode. The potential and the tip height are shown. For more information on EPAPS, see http://www.aip.org/pubservs/epaps.html.


