Stick–slip motion in the atomic force microscope

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Measurements of atomic friction in the atomic force microscope frequently show periodic variations at the lattice spacing of the surface being scanned, which have the saw-tooth wave form characteristic of “stick–slip” motion. Simple models of this behaviour have been proposed, in which the “dynamic element” of the system is provided by the elastic stiffness and inertia of the cantilever which supports the tip of the microscope, in its lateral, i.e., torsional mode of vibration. These models have been successful in predicting the observed motion, but only by assuming that the cantilever is heavily damped. However, the source of this damping in a highly elastic cantilever is not explained. To resolve the paradox, it is shown in this note that it is necessary to introduce the elastic stiffness of the contact into the model. The relationship between the contact stiffness, the cantilever stiffness and the amplitude of the periodic friction force is derived in order for stick–slip motion at lattice spacing to be achieved.

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Measurements of atomic friction in the atomic force microscope frequently, but not universally, show periodic variations at the lattice spacing of the surface being scanned, which have the saw-tooth wave form characteristic of “stick–slip” motion, e.g., Erlandsson et al. [1], Fujisawa et al. [2]. This process has been modelled in a simple way for a one-dimensional scan by Tomanek et al. [3] and for a two-dimensional scan by Holscher et al. [4], with considerable success in reproducing the observed variations in friction force, notably in the two-dimensional case where the microscope tip responds to motion and forces in both longitudinal and lateral directions.

Despite this success, these models incorporate idealisations which raise questions on physical grounds:

(1) Friction is measured by the torsional deflexion of the elastic cantilever which supports the contacting tip. The above models recognise that the compliance and inertia of the cantilever comprise a dynamical system which responds to the fluctuation in friction force. Following an unstable jump (“slip”), the cantilever carrying the tip oscillates in its torsional mode. If the models referred to above it has been assumed that such vibrations are heavily damped. In the absence of this assumption the models do not predict regular stick–slip motion at lattice spacing as generally observed; instead “multiple jumps” and irregular motion are predicted. However, the cantilever is highly elastic and so would be expected to have low inherent damping. This paradox will be examined.

(2) More recently, however, it has been recognised that an additional compliance is provided between the end of the cantilever and the specimen by the contact of the tip and specimen. This is the tangential analogue of the normal compliance of a Hertz contact (see Johnson [5, pp. 216–220]). It has been measured by Lantz et al. [6] and by Carpick et al. [7]. The effect of this additional compliance on the dynamics of the system will be considered in this note.

(3) The contact area of a typical AFM tip in a friction test has a radius of around 4 nm, which corresponds to around 100 atoms. The models mentioned above assume a sinusoidal interaction potential varying at the lattice spacing of the specimen. This is an obvious concept with a tip comprising a single atom, but how the atoms actually move during sliding of a tip of finite contact size and their influence on the interaction potential is an open question which will not be pursued here.

Since the limited aim of this investigation was to examine the influence of the contact compliance on the dynamics of the system and, if possible, to resolve the paradox concerning damping, it was decided to adopt the idealisations in the earlier models in all other respects. Further, since these issues apply equally to one- and two-dimensional motion, a one-dimensional line scan was considered for simplicity.

The cantilever and tip in its lateral (torsional) mode is shown in figure 1(a); the equivalent spring-mass system is shown in figure 1(b). The lateral displacement of the tip due to twist θ is denoted by x and that due to tangential compliance of the contact by z. The cantilever lateral stiffness is $k_t = T_t / x$ and the combined stiffness of the tip and contact is $k_c = T_c / z$, where $T_t$ and $T_c$ are the tensions in the two springs shown in figure 1(b). The mass $m$ is the equivalent mass of the cantilever associated with its fundamental torsional frequency $\omega_t = \sqrt{k_t / m}$. Motion in the higher modes is likely to be small and will be neglected.
The total static compliance \( c \) of the system is then given by

\[
c = 1/k_c = 1/k_l + 1/k_c. \tag{1}
\]

Following Tomaee et al. [3] a force potential is assumed which gives rise to a sinusoidal variation of tangential force at the lattice spacing \( \lambda \) of the specimen surface, expressed by

\[
T_c(s) = T^* \sin(2\pi s/\lambda), \tag{2}
\]

where \( s \) is the tangential displacement (slip) of the specimen relative to the tip. Assuming that the cantilever is damped by a viscous force \( b \), its motion is given by

\[
m \left( \frac{d^2x}{dt^2} \right) + b \left( \frac{dx}{dt} \right) = T_c - T_l = T^* \sin(2\pi s/\lambda) - k_l x. \tag{3}
\]

During a scan the surface is displaced by \( y(t) = V t \), where \( V \) is the scan velocity. The slip may then be expressed by

\[
s = y - x - z = y - x - (1/k_c)T^* \sin(2\pi s/\lambda). \tag{4}
\]

Under quasi-static conditions \( (d^2x/dt^2) = 0 \), so that

\[
s = V t - T_c (1/k_c + 1/k_l) = V t - T_c/k_c. \tag{5}
\]

We now introduce the non-dimensional notation:

\[
S = s/\lambda, \quad X = x/\lambda, \quad Y = y/\lambda, \quad Z = z/\lambda,
\]

\[
F_c = T_c/T^*, \quad F_l = T_l/T^*, \quad K_c = \lambda k_c/T^*, \quad K_l = \lambda k_l/T^*,
\]

\[
q = \omega_l t, \quad \delta = b \omega_l/2k_l,
\]

\[
S = Y - X - (1/k_c) \sin(2\pi S), \tag{7}
\]

and under quasi-static conditions

\[
S = Y - F_c/K_c = Y - (1/k_c) \sin(2\pi S). \tag{8}
\]

The simultaneous solution of equations (6) and (7) must be obtained numerically. An efficient algorithm for this process is given in appendix A. As an illustrative example, the solution for \( K_l = 4, K_c = 3, \delta = 0.1 \) and \( 2\pi V/\omega_l = 15 \) is presented in figure 2.

In the absence of dynamic effects, equation (8) applies. Its solution is given in figure 2(a) by the intersection of \( F_c(S) \) by a line of slope \(-K_c\) which, during a scan, traverses to the right with the scan velocity \( V \).

Starting from an intersection point at \( O \), where \( F_c = F_l = S = X = Z = V t/\lambda = 0 \), intersection points in the
segment OE are stable and quasi-static. The tangent point E
locates the onset of instability at which the cantilever starts to
move according to equation (6) at a rate governed by
the combined stiffness \( K_e \). At point A, at which the slope
of \( F_c(S) \) is \(-K_e\), the contact “spring” becomes unstable
and snaps through to point B. Since the contact spring has
negligible mass, it will relax in a time of the order of that
for a stress wave to traverse the contact diameter, of order
\(10^{-12}\) s, which is short compared with the natural period
of the cantilever. Thus, at B, \( X_B = X_A \) and \( \frac{dX}{dt}_B = \left[ \frac{dX}{dt} \right]_A \approx 0 \). The strain energy released in this relaxation
will be entirely dissipated in phonons. Subsequently the
extension of the contact spring \( Z \) will be quasi-static and
given by \( F_c(S)/K_e \). The dynamical behaviour of such an
elastic contact is discussed in [5, pp. 342–349].

The subsequent motion is one of damped oscillation of
the cantilever at its natural frequency \( \omega_n \). In figure 2(a)
the friction force \( F_c \) fluctuates in the segment BM until it
damps out and a second cycle begins. In figure 2(b) the
friction force is plotted against the scanning displacement
\( Y \), showing the snap-through from A to B, followed by the
cantilever oscillation. For the purpose of illustration of
the motion, an untypically low value of the cantilever
frequency \( \omega_n \) and high value of the damping factor \( \delta \) have been
used in the calculation of figure 2. In reality, the period of
the oscillation will be much shorter than shown. Even if
the damping factor is much less than 0.1, the oscillation
will have died out before the next point of instability \( E' \)
is reached. In any case, the recording equipment of the AFM
is unlikely to resolve the oscillatory motion, whereupon the
familiar saw-tooth wave form associated with stick-slip will
be observed. We note that the overshoot \( [(F_{cM} - (F_c)_B)]\)
is approximately equal to \( [(F_{cB} - (F_c)_B)] \).

In the example shown in figure 2 the stick-slip motion
takes place at the lattice spacing \( \lambda \) of the specimen. A can-
tilever of lower stiffness, however, would reduce the com-
bined stiffness \( K_e \), which would raise the point \( N \) in the
figure and hence the height of the first overshoot \( M \). If the
overshoot reaches the instability point \( E' \) in the next cycle,
the cantilever will jump (slip) two or possibly more cycles
before sticking. In the numerical solution of equations (6)
and (7), \( M \) is located by the first occasion when \( \delta S/dq = 0 \).
Denoting the maximum value of \( S \) in the first overshoot by
\( S_M \), multiple jumps will be avoided if \( S_M < S_0 \). In
this calculation the “worst case” is obtained by taking the damped
\( \delta \) in the cantilever to be zero. Also, since the frequency
of the cantilever is much higher than the lattice scan fre-
quency, the scanning displacement \( (Y_M - Y_2) \) during the
slip from E to M is neglected. The results of these calcula-
tions are shown in figure 3, which specifies the threshold
of multiple jumps.

Energy is dissipated in the snap-through from A to B.
However, if the contact stiffness \( k_e \) exceeds the maximum
gradient of \( T_c(s) \), i.e., if \( K_e > 2\pi \), the contact “spring”
will be continuously stable and no snap through will occur.
In these circumstances, neglecting cantilever damping, en-
ergy of the system will be conserved between E and E'. It

![Figure 3. Map of cantilever and contact stifferesses, \( K_1 \) and \( K_e \), showing the threshold of multiple jumps: (a) neglecting cantilever damping (\( \delta = 0 \)); (b) \( \delta = 0.1 \).](image)

is shown in appendix B that, at the threshold of multiple
jumps, the cantilever and contact stiffnesses \( K_1 \) and \( K_e \)
are related by the equation

\[(K_1/2)^2 + (K_e/2\pi)^2 = 1.0, \quad (9)\]

where \( K_e \) can be expressed in terms of \( K_1 \) and \( K_e \) by
equation (1). When the contact stiffness is small (< 2\pi),
multiple jumps will not occur if \( K_1 > 0.75K_e \).

The effect of damping in the cantilever is to reduce the
height of the overshoot and hence to reduce the likelihood
of multiple jumps. Some individual computed points us-
ing a cantilever damping factor \( \delta = 0.1 \) are shown in fig-
ure 3.

To illustrate the occurrence of multiple jumps two cases
have been computed, one on each side of the threshold
(\( \delta = 0.1 \)) in figure 3. In the first (figure 4(a)) \( K_e = 3 \) and
\( K_1 = 1.4 \), which lies just above the threshold, so that a
slip occurs at each lattice spacing \( (V_t/\lambda = 1) \). The first
overshoot very nearly reaches the limit before decaying. In
the second example (figure 4(b)) \( K_e = 3 \) and \( K_1 = 1.3 \),
which lies just below the threshold. The first overshoot
(which can be just detected in the figure) carries the slip
into the next lattice spacing before decaying into the stick
phase, which occupies a period \( V_t/\lambda = 2 \). If the cantilever
stiffness is further reduced it is possible to slip three or more
 spacings before sticking.

Finally we note that the motion is steady, without stick-
slip, if the combined stiffness \( k_e \) exceeds the maximum
gradient of \( T_c(s) \), i.e., if \( K_e = K_cK_l/(K_e + K_l) > 2\pi \).
Even so the graph of force \( F_c \) against displacement \( Y \)
may still be very unsymmetrical. We note that this condi-
tion of steady motion may be realised, even with compliant
springs, if the amplitude \( T^* \) of the periodic force is suffi-
ciently small.

Energy dissipated by phonons in the snap-through of the
contact and in the damping of oscillations of the cantilever
contribute to sliding friction. The mean friction force may
be calculated from the stable part of the force-displacement curve, thus

\[ T = \frac{1}{\lambda} \int_{S_n}^{S_k} T \, dy, \]

i.e.,

\[ \overline{F}_c = \int_{S_n}^{S_k} F_c \, dY = \int_{S_n}^{S_k} \sin(2\pi S) \left[ 1 + \frac{2\pi}{K_e} \cos(2\pi S) \right] dS \]

\[ = -\frac{1}{2\pi} \cos(2\pi S) \bigg|_{S_n}^{S_k} \frac{S_k}{4K_e} \cos(4\pi S) \bigg|_{S_n}. \quad (10) \]

Computations of \( \overline{F}_c \) are shown as a function of \( K_e \) in figure 5(a). The mean friction varies from zero when the entire cycle is stable (\( K_e > 2\pi \)), and approaches \( 1.0 \) (i.e., \( T \to T^* \)) when \( K_e \to 0 \). Similar calculations have been made by Colchero et al. [8]. The results in figure 5(a) have been used, together with the data of figure 3, to produce the map in figure 5(b), which shows contours of non-dimensional friction \( \overline{F}_c = \overline{T}_c/T^* \) in terms of the compliances \( 1/K_e \) and \( 1/K_t \).

Conclusions

1. It is generally realised that the existence of stick–slip motion in the atomic friction microscope depends upon the lateral compliance of the measuring system (cantilever and tip) in relation to the amplitude of the lateral force potential. In this note the compliance of the tip and contact region has been separated from that of the force-measuring cantilever in a simplified study of the dynamic response of the system. A significant feature of the behaviour lies in their very different frequencies of response. The lattice traverse frequency: \( \approx 10^5 \) Hz; the cantilever frequency: \( \approx 10^3 \) Hz; the tip and contact frequency: \( \approx 10^{13} \) Hz.

2. The instability inherent in stick–slip motion excites vibrations of the cantilever at its natural frequency which, for a sufficiently compliant cantilever, could cause a jump of more than one lattice spacing in each "slip".
It is shown in this note that the slip of the tip and contact spring is purely dissipative, which helps to damp the motion of the cantilever and to reduce the likelihood of multiple jumps. It is shown that multiple jumps are avoided: when the non-dimensional contact stiffness $K_c > 2\pi$, if the cantilever stiffness $K_t > 1.9$, and under all circumstances if $K_t > 0.75K_c$.

In the experiments of Carpick et al. [7] the cantilever stiffness $k_t$ was estimated to be 190 N/m, while the combined stiffness of tip and contact $k_c$ varied with load from 9.5 to 66 N/m. In the experiments of Lantz et al. [6], the cantilever stiffness $k_t = 110$ N/m. The stiffnesses of the tip itself and the contact deformation were separated to vary from 84 to 108 N/m and 60 to 100 N/m respectively, giving the variation of the combined tip and contact stiffness $k_c = 35–52$ N/m. We note that throughout the range of both sets of experiments $k_t > k_c$, whereby $K_t > K_c$, so that multiple jumps would not be expected. Carpick et al. observed stick-slip at single lattice spacing as predicted. Lantz et al. did not record any stick-slip motion, which would imply that the amplitude of the periodic tangential force was too small in relation to the equivalent stiffness $k_e$, i.e., $T^* < \lambda k_e/2\pi$.

It would appear from this limited data that the relative cantilever and contact stiffnesses in typical AFM applications are such as to eliminate multiple slips. It would be instructive, however, to carry out an experiment with a very compliant cantilever to see whether the multiple slips predicted by this model actually occur.

(3) Stick-slip motion implies frictional energy dissipation, such that the mean level of the friction trace, as shown in figure 2(b), lies above zero. As the effective stiffness $k_e$ is reduced, the mean friction increases and the drop at slip decreases. However, the mean friction observed in the experiments of Erlandsson et al. and Carpick et al., for example, show a mean friction which is higher than would be expected by this mechanism alone. It would appear that the tangential force has a steady component in addition to the sinusoidally fluctuating component considered in this note. As mentioned above, the combination of steady and fluctuating components presumably arises from the finite size of the contact area and the probable irregularity of the atomic structure of the tip. This aspect of the problem presents a challenge for atomic modelling.

(4) It is recognised that a sinusoidal potential provides only the simplest representation of a periodic friction force, and that the threshold of multiple slips presented in figure 3 is likely to be influenced to some extent by the form of the potential. Work is in progress to examine the behaviour of a contact consisting of many atoms and its influence on the frictional potential.

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Appendix A

To produce the numerical simulations shown in figures 2(b) and 4, an efficient algorithm was employed which has been used in the past for simulation of nonlinear oscillations of musical instruments (including real-time simulation for musical synthesis): see McIntyre et al. [9]. Writing the solution of equation (6) in terms of its Green’s function, the problem is to solve simultaneously

$$K_c Z = \sin 2\pi (V t / \lambda - X - Z) \quad (A1)$$

and

$$X(t) = \frac{K_c \omega}{K_t} \int_0^t \sin \omega (t - \tau) \exp [-\delta (t - \tau)] Z(\tau) d\tau$$

$$= \text{Im} \left\{ \frac{K_c \omega}{K_t} \int_0^t \exp[i\omega (t - \tau)] \tau Z(\tau) d\tau \right\}. \quad (A2)$$

For a short time step $h$, (A2) can readily be shown to imply

$$X(t + h) \approx \frac{K_c \omega}{K_t} Z(t) h + e^{i\omega h} \frac{K_c \omega}{K_t} \int_0^h \exp[i\omega (t - \tau)] Z(\tau) d\tau,$$

where

$$X(t) = \text{Im} \{X(t)\}.$$

Thus for each time step, the apparently time consuming convolution integral can be evaluated with a single complex multiplication and addition to yield the new value of $X(t)$. The new value of $Z(t)$ is then found from (A1), by linear extrapolation from the previous value, improved if necessary by a few Newton–Raphson iterations. If jumps are present, these must be detected and implemented at this stage.

Appendix B

In this appendix the threshold of multiple jumps is investigated for the case in which the contact spring is stable throughout, i.e., when $K_c > 2\pi$. Thus no energy is dissipated at the contact and, in the “worst case”, damping in the cantilever is taken to be zero, so that total energy is conserved throughout the motion. At the threshold the velocity of the cantilever will fall to zero at the instability points $E$ and $E'$ etc. in figure 2(a). In a complete cycle from $E$ to $E'$ the work done by the sinusoidal friction force $F_c$ is zero, so that the elastic strain energy in the cantilever is conserved as it swings from maximum tension at $E$ to maximum compression at $E'$, through a total displacement:

$$X_{E'} - X_E = S_{E'} - S_E = 1.0$$
and
\[(F rituals}_V = -(F rituals}_E = -(F rituals}_E = - \sin(2\pi S_E),\]
hence
\[
(2/K_i) \sin(2\pi S_E) = 1.0. \quad (A4)
\]
Now \(E\) is the point where the gradient of \(T_C(S)\) equals the combined stiffness, i.e.,
\[
2\pi \cos(2\pi S_E) = -K_e. \quad (A5)
\]
which give
\[
(K_i/2)^2 + (K_e/2\pi)^2 = \sin^2(2\pi S_E) + \cos^2(2\pi S_E) = 1.0. \quad (A6)
\]
Recalling that \(K_e = K_i K_e / (K_i + K_e)\), this equation relates the cantilever and contact stiffnesses \(K_i\) and \(K_e\) at the threshold of multiple jumps when \(K_e > 2\pi\).

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