

Analysis of tip-sample interaction in tapping-mode atomic force microscope using an electrical circuit simulator

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We present a mechanical model for the atomic force microscope tip tapping on a sample. The model treats the tip as a forced oscillator and the sample as an elastic material with adhesive properties. It is possible to transform the model into an electrical circuit, which offers a way of simulating the problem with an electrical circuit simulator. Also, the model predicts the energy dissipation during the tip-sample interaction. We briefly discuss the model and give some simulation results to promote an understanding of energy dissipation in a tapping mode. © 2001 American Institute of Physics. [DOI: 10.1063/1.1369614]

There have been many attempts to model the tapping-mode operation of atomic force microscope.^{1–7} Some authors tried to solve the problem analytically^{2,6} and others attempted to solve it with computer simulations,^{3–5,7} both adding to a better insight in understanding and treating the data collected. It is now possible to map local energy dissipation profiles. We hope that a better modeling of the problem will lead to better imaging ability.

Early models neglected attractive forces and treated the tip as a forced oscillator hitting a damped elastic surface.² By using boundary conditions on the surface, the differential equation resulting from this model was solved. More involved models take attractive forces into account as well. This was hard to solve analytically, but numerical approaches succeeded in explaining many experimentally observable effects like attractive and repulsive regimes,⁴ hysteresis in the frequency sweep,³ and bistability.⁵ However, these models did not take hysteresis in the adhesive forces into account, which was later shown by Tamayo and Garcia⁸ that this is the main source of energy dissipation in a tapping mode. Some recent works treat the interaction forces as a double valued function and solve the resulting differential equation numerically.⁷ The results of this simulation showed the asymmetry of the necks formed by the sample surface during approach and retraction.

In this letter we present a model, which takes all the previously discussed effects as well as hysteresis. The model treats the tip as a forced oscillator, as usual. The sample is modeled with an equivalent spring constant¹ (contact stiffness) and a damping effect, which is due to the internal viscosity of the sample. There is a negligible equivalent mass of the sample that we will totally neglect in this work. Interaction forces due to adhesion, surface charges, and some other sources are defined as a single valued function of the distance between the tip and sample surface ($x_t - x_s$). The schematic of the model is sketched in Fig. 1. It is important to note that, although the interaction force is defined as a single valued function of the distance between tip and sample, the resulting force-distance relation exhibits hysteresis. Since

the attractive forces between tip and sample are proportional to $1/(x_t - x_s)^n$, there may be more than one stable solution⁵ for the sample position x_s . When the tip approaches the sample, the level of the sample surface increases because of the attractive forces. After a certain point, the system becomes unstable and the sample surface jumps to contact with the tip. However, during retraction, the contact is lost at a higher sample surface level. This results in different force-distance relations during approach and retraction.

In order to estimate the spring constant k_s of the sample, we used the Hertz model applied to deformable bodies.^{1,2,7} When the model is applied to the tip-sample interaction, the equivalent spring constant is given by the formula

$$k_s = \frac{3}{2} E^* \sqrt{R \times z_{\text{def}}} \quad (1)$$

Here R is the effective radius of the tip, E^* is the effective elastic modulus of the system, and z_{def} is the deformation of the sample. This value changes with force applied to the sample. Therefore, a nominal value of force is needed to estimate the spring constant of the sample. The best choice of this value is the adhesion force, since it is observed when no external force is applied to the tip and reflects the equi-

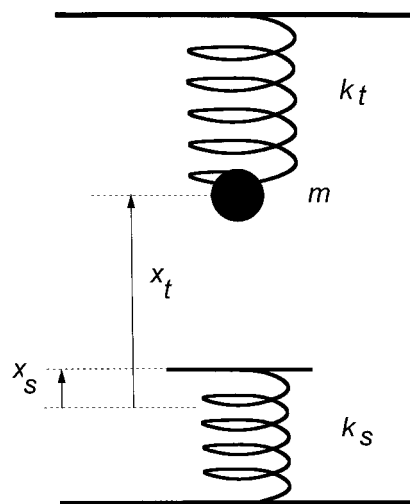


FIG. 1. Mechanical model of the tip-sample system. Upper spring represents the cantilever and the lower spring represents the sample. Damping of the cantilever and sample are not shown.

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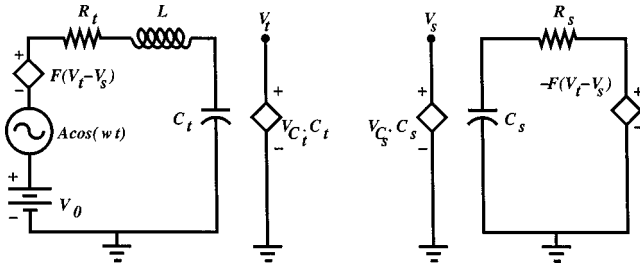


FIG. 2. Equivalent electrical circuit of the mechanical model presented in Fig. 1. Left-hand side loop represents the cantilever-tip system and the right-hand side loop represents the sample. Diamond shaped symbols stand for voltage-controlled voltage sources. $F(V_t - V_s)$ represents the force of interaction between tip and sample. Constant voltage source, V_0 is used to adjust the set point.

librium position.¹ Also, the forces observed in tapping modes are around this value. The equivalent spring constant can be written in terms of this force as

$$k_s = \sqrt[3]{6E^*2RF_{adh}}. \quad (2)$$

This parameter has a wide range, since elastic modulus varies by several orders of magnitude. The most important approximation we have done up to now is to assume that this spring constant would be applicable also when the surface is pulled up. That is mainly because the forces of adhesion are effective at very short distances and, therefore, the surface is pulled up from a small volume in the vicinity of the tip. This is similar to the repulsion where the force is applied from a

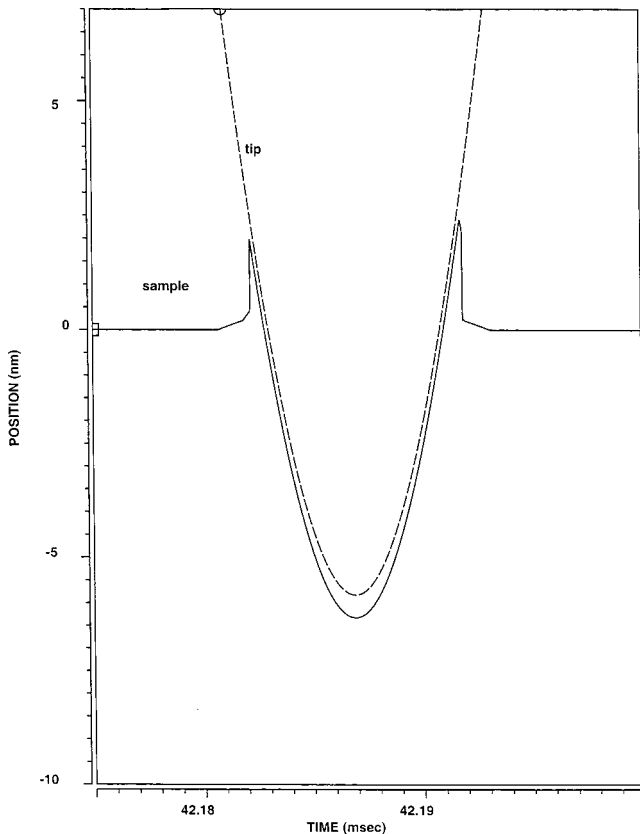


FIG. 3. Simulated tip-sample positions with respect to time. The solid line shows the position of the sample and the dashed line shows the position of the tip. The height difference of the sample right before and after the contact results in an energy dissipation.

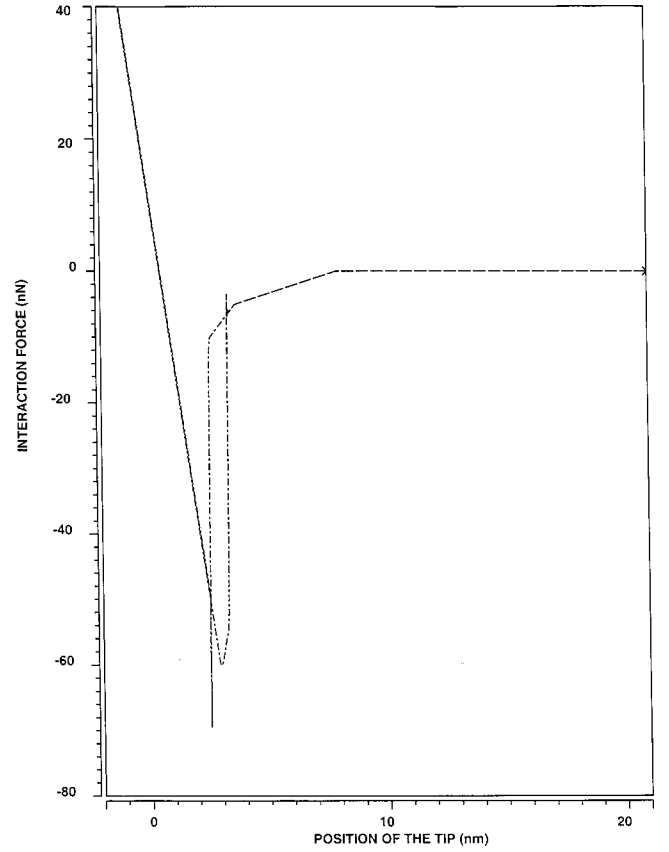


FIG. 4. Simulated force-distance curve of the tip. Although the tip-sample interaction forces are defined single valued, the resulting force curve shows a hysteresis. The glitches are due to convergence problems and they decrease with smaller time steps.

small contact area but to the opposite direction. By making this assumption, we can then write the resulting coupled differential equations of motion as

$$m \frac{d^2 x_t}{dt^2} + \frac{m \omega_0}{Q} \frac{dx_t}{dt} + k_t [x_t - a_{sp}] - F(x_t - x_s) = A \cos(\omega t), \quad (3)$$

$$\gamma_s \frac{dx_s}{dt} + k_s x_s + F(x_t - x_s) = 0, \quad (4)$$

where m , k , ω_0 , ω , Q , a_{sp} , and A are the mass, spring constant, free resonance frequency, excitation frequency, quality factor, set point, and driving amplitude of the tip, respec-

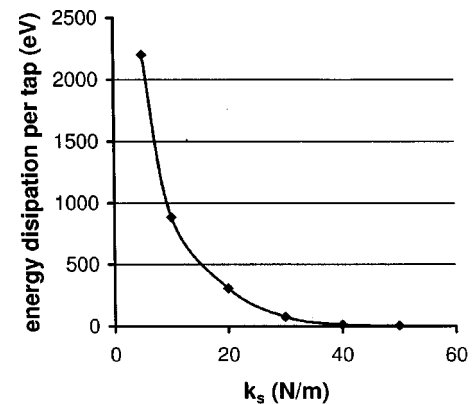


FIG. 5. Calculated energy dissipation with respect to contact stiffness k_s .

TABLE I. Correspondence between the mechanical model parameters and electrical circuit parameters. The values given are the ones used in our simulations.

Circuit parameter	Mechanical equivalent	Value
R_t	$1000 m \omega_0 / Q$	$400 \mu \Omega$
L	$1000 k_t / \omega_0^2$	$1 \mu H$
C_t	$1/(1000 k_t)$	$100 \mu F$
R_s	$1000 \gamma_s$	$100 \mu \Omega$
C_s	$1/(1000 k_s)$	$40 \mu F$
$F(q_t - q_s)$	$1000 F(x_t - x_s)$...
V_0	$1000 k_t a_{sp}$	$0.6 mV$

tively, and γ_s and k_s are the internal damping coefficient and contact stiffness of the sample. x_t and x_s represent the positions of the tip and sample surface, respectively, as measured from the equilibrium point of the sample.

Since we are dealing with masses and springs to model the problem, we can easily convert them to electrical circuit components. We replace masses with inductors, springs with capacitors, damping with resistors, and forces with voltages. The interaction force is represented by a nonlinear controlled source. The resulting electrical circuit is depicted in Fig. 2. We can then write the coupled differential equations for the charges q_t and q_s , of the capacitors as

$$L \frac{d^2 q_t}{dt^2} + R_t \frac{dq_t}{dt} + \frac{q_t}{C_t} - F(q_t - q_s) = A \cos(\omega t) + V_0, \quad (5)$$

$$R_s \frac{dq_s}{dt} + \frac{q_s}{C_s} + F(q_t - q_s) = 0. \quad (6)$$

The complete analogy between the mechanical and electrical system makes it possible to simulate the mechanical problem with an electrical circuit simulator such as SPICE.⁹ This program can make a transient analysis of nonlinear circuits to predict the node voltages and branch currents. We preferred to use HSPICE,¹⁰ a commercial version of SPICE, which incorporates very efficient algorithms for fast solution of nonlinear circuits. Since HSPICE does not allow charge controlled voltage sources, we added two extra nodes (V_t and V_s) whose voltages are numerically equal to the charges q_t and q_s in capacitors ($q_t = C_t V_{Ct}$, $q_s = C_s V_{Cs}$). The multiplications are achieved by two voltage-controlled voltage sources gains of which are numerically equal to the respective capacitor values. We give the correspondence between the mechanical model parameters and the electrical circuit parameters in Table I.

HSPICE allows us to define nonlinear voltage-controlled voltage sources as piecewise linear functions. For the function $F(q_t - q_s)$, we use values similar to those measured by Tamayo and Garcia.⁸ We made transient analysis on this circuit for typical values of set point (60 nm), force constant

of tip (10 N/m) and surface (25 N/m), quality factor for the cantilever (250) and center frequency (15.9 kHz). For the sample viscosity, we have found that its value does not affect the results and therefore we have chosen something smaller than the damping of the cantilever. The extra factor of 1000 in Table I is there simply to scale the element values into an appropriate range as required by HSPICE.¹¹ In Fig. 3 we give the positions of tip and sample during interaction and in Fig. 4, the forces of interaction with respect to the position of the tip.

The neck formed during retraction is longer than the one formed during the approach. This is due to the hysteresis in the forces. After the tip is totally separated, the energy stored in the neck is completely lost. Since this energy is smaller than the energy gained right before contact, there is net dissipation. This dissipation is equal to the area inside the force–distance curve shown in Fig. 4. The value is approximately a few hundred eV, which is similar to those experimentally measured values by Tamayo and Garcia.⁸ In Fig. 5 we plotted the energy dissipation per tap with respect to the equivalent spring constant of the sample. These results show that energy dissipation in tip–sample interactions, which is a measurable quantity,^{8,12} depends on elastic properties of the sample. Especially for compliant surfaces, energy dissipation can easily be related to local mechanical properties.

We have proposed a model to interpret the mechanism of energy dissipation in the tip–sample interaction in tapping mode. This will be useful in predicting energy dissipation profiles and mapping of local mechanical properties of samples. Furthermore, it is now possible to simulate the tapping mode operation much easier and faster with a circuit simulator.

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- ¹U. Rabe, K. Janser, and W. Arnold, Rev. Sci. Instrum. **67**, 3281 (1996).
- ²R. G. Winkler, J. P. Spatz, S. Sheiko, M. Moeller, P. Reineker, and O. Marti, Phys. Rev. B **54**, 8908 (1996).
- ³A. Kuehle, A. H. Soerensen, and J. Bohr, J. Appl. Phys. **81**, 6562 (1997).
- ⁴Ricardo Garcia and Alvaro San Paulo, Phys. Rev. B **60**, 4961 (1999).
- ⁵M. Marth, D. Maier, J. Honerkamp, R. Brandsch, and G. Bar, J. Appl. Phys. **85**, 7030 (1999).
- ⁶L. Wang, Appl. Phys. Lett. **73**, 3781 (1998).
- ⁷D. Sarid, J. P. Hunt, R. K. Workman, X. Yao, and C. A. Peterson, Appl. Phys. A: Mater. Sci. Process. **66**, S283 (1998).
- ⁸J. Tamayo and R. Garcia, Appl. Phys. Lett. **73**, 2926 (1998).
- ⁹L. W. Nagel, SPICE2: A Computer Program to Simulate Semiconductor Circuits, University of California, Berkeley, Tech. Rep. Memo ERL-M520 (1975). A public domain version can be downloaded from www.repairfaq.org/ELE/F_Free_Spice.html
- ¹⁰HSPICE: Avant! Corporation, 46871 Bayside Parkway, Fremont, CA 94538.
- ¹¹HSPICE, version 99.2 does not accept resistor values less than $10 \mu \Omega$.
- ¹²J. P. Cleveland, B. Anczykowski, A. E. Schmid, and V. B. Elings, Appl. Phys. Lett. **72**, 2613 (1998).