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O. Sahin, and A. Atalar

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Simulation of higher harmonics generation in tapping-mode atomic force microscopy

O. Sahin[a] and A. Atalar
Electrical and Electronics Engineering Department, Bilkent University, Bilkent, 06533 Ankara, Turkey

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In tapping-mode atomic force microscopy, nonlinear tip–sample interactions give rise to higher harmonics of the cantilever vibration. We present an electrical circuit to model the atomic force microscope cantilever with its first three flexural eigenmodes. An electrical circuit simulator is used to simulate the tapping-mode operation. Amplitude and phase responses of the third flexural eigenmode are obtained for different sample properties. It is found that amplitude and phase of higher harmonics depend highly on sample properties. © *2001 American Institute of Physics.*
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Tapping-mode atomic force microscopy has a great potential in mapping material properties at the nanometer scale. Phase images obtained while the tip is scanned across the sample shows significant material contrast.[1] Though not complete, a reasonably good understanding of the sources of relative phase shifts has been established. The relation between energy dissipation in tip–sample contact and phase difference between the driving force and the tip motion makes it possible to map energy dissipation,[2,3] which is a material dependent quantity. The mechanism of energy dissipation is not fully understood yet, however, several attempts have been made. These models relate phase contrast to wetting properties of different materials[4] or sample stiffness and tip–sample attractive forces.[5] All these models are quite complicated and we end up in a situation where we have more unknowns than equations to characterize the materials. For the purpose of imaging material properties, a different approach came from Stark and Heckl[6] suggesting the use of higher harmonics to probe the anharmonic tip–sample interaction. In this technique, a single or a group of higher harmonics of the cantilever motion is filtered and the resulting signal is utilized for imaging purposes. It is also shown that contact time can be estimated from these signals. The main advantage of using higher harmonics is the increased contrast and sensitivity to variations in properties of the sample.[7] A good understanding of higher harmonics generation is therefore crucial.

Here, we propose an equivalent electrical circuit in order to simulate higher harmonics generated in tapping mode with the help of a circuit simulator, HSPICE.[8] The electrical model we used in this work is similar to the previously described model.[5] We added two more resonators to represent two of the higher order modes. The complete model is depicted in Fig. 1. It is worth mentioning that the effects of the driving force on higher order modes are neglected, which is a reasonable assumption for high Q cantilevers. These modes are excited with the tip–sample interactions. In our electrical circuit, each loop on the left-hand side represents one of the eigenmodes of the cantilever–tip system and right-hand side loop represents the sample. Capacitances represent the effective spring constants (K) of the eigenmodes and the sample with the numerical equality $K=1/C$. Inductances represent the effective masses ($M=L$). Therefore, charges in each capacitance represent the displacement of that mode and their summation $C_1V_1+C_2V_2+C_3V_3$ represents the total displacement of the tip. Similarly, the sample surface level is represented with the charge in the capacitance of the right-hand side loop with the relation CV_C. The resistances represent the damping of the eigenmodes with the relation $Q=(L/C)^{1/2}/R$. Diamond-shaped symbols stand for voltage controlled voltage sources and $F(V_t-V_s)$ represents the force of interaction between the tip and sample. Note that the interaction force F depends on voltages instead of charges (charges represent the displacement). This is because HSPICE does not allow charge controlled voltage sources. To overcome this difficulty, we introduced two extra voltage controlled voltage sources V_t and V_s, whose voltages are numerically equal to the charges (see Fig. 1) and we defined the interaction force F with respect to V_t and V_s. Adjustable

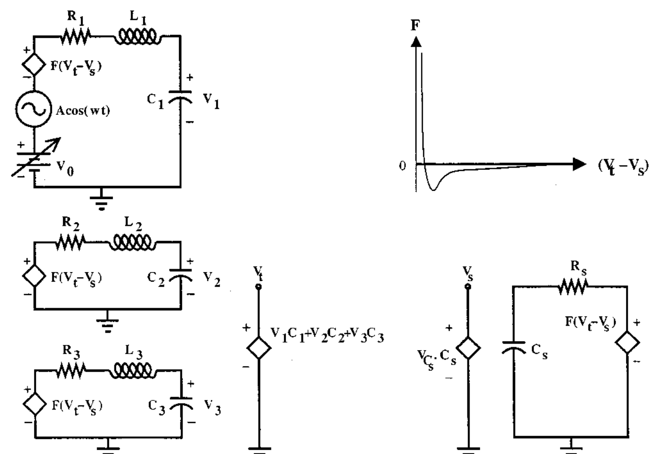

FIG. 1. Equivalent electrical circuit of the cantilever–tip system. Each loop on the left-hand side represents one of the eigenmodes of the cantilever–tip system and the right-hand side loop represents the sample. Diamond-shaped symbols stand for voltage controlled voltage sources and $F(V_t-V_s)$ represents the force of interaction between the tip and sample. Adjustable voltage source V_0 is used to adjust the rest position of the cantilever. V_t and V_s represent the positions of the tip and the sample, respectively.

[a]Electronic mail: osahin@ee.bilkent.edu.tr

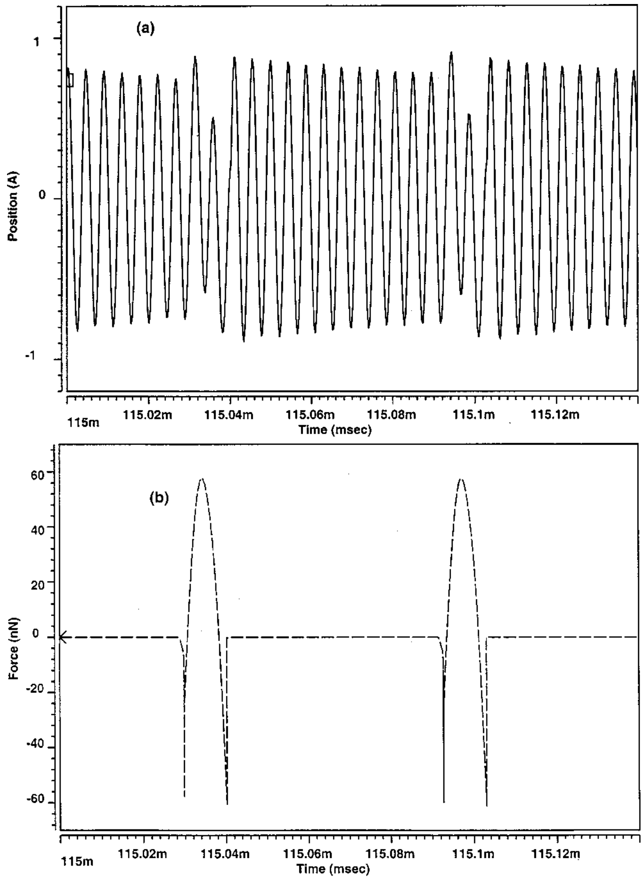

FIG. 2. (a) Response of the third eigenmode in tapping mode while the cantilever is driven at first-resonance frequency, (b) interaction force between the tip and the sample. Note that, response of the cantilever is slightly disturbed during the interactions.

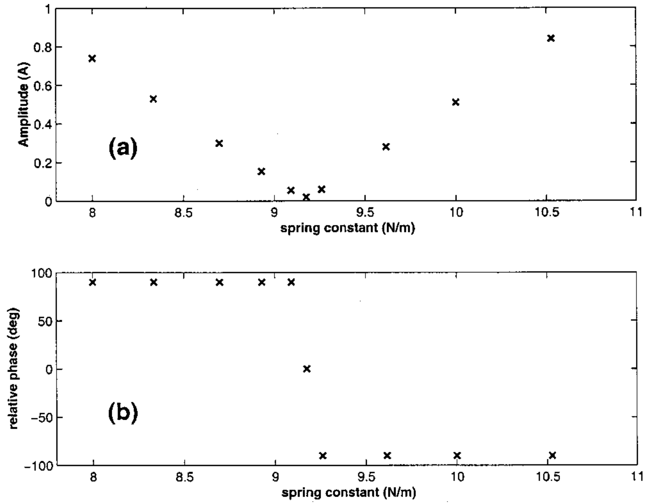

FIG. 3. Vibrations of the third eigenmode of the cantilever under low tip–sample energy dissipation condition: (a) amplitude and (b) phase of the vibrations with respect to equivalent spring constant of the sample. The phase at the amplitude minima is set to zero arbitrarily.

voltage source V_0 is used to adjust the rest position of the cantilever. The first resonance f_1 is at 15.92 kHz with a quality factor Q of 250, the second resonance f_2 is at $5.4f_1$ with a quality factor Q_2 of 450 and the third resonance f_3 is at $15.4f_1$ with a quality factor Q_3 of 450. We chose the resonant frequencies of the higher eigenmodes as a noninteger multiples of f_1, which is the general situation for most of the cantilevers used in experiments.[10] To complete the specifications of the cantilever, the equivalent spring constants of each mode must be given. These parameters are needed to determine the amplitude of the oscillations. In order to estimate the equivalent spring constants of the higher order modes, we use the formula for rectangular cantilevers[11]

$$\frac{K_n}{K_1}=\left(\frac{f_n}{f_1}\right)^2. \tag{1}$$

Here, K_n, f_n, K_1, and f_1 are the effective stiffness and resonance frequencies of the nth and fundamental modes, respectively. Together with these values and Eq. (1), we chose the values 10, 29, and 225 N/m for the effective spring constants of the first three flexural vibration modes. We construct the electrical equivalent circuit with these mechanical parameters and the relations between the electrical circuit and mechanical model parameters presented in our previous work.[5] In addition to the cantilever and tip, a feedback circuitry, which is not shown in Fig. 1, is used to fix the amplitude of the oscillations to the set-point amplitude of 80 nm. (The ratio of set-point amplitude to free amplitude is 0.64). This circuit adjusts the voltage V_0 of the dc source in Fig. 1 to ensure the constant swing of the oscillations of the tip.

A transient analysis of the circuit with HSPICE results in the position of the tip as a function of time. This function is band-pass filtered around the third resonance frequency to give the time wave form given in Fig. 2. In Fig. 2, the tip–sample interaction forces are also shown. These results show a good similarity with the experimental results of Hillenbrand *et al.*[7] Especially, during the tip–sample contacts, vibrations of the third eigenmode is highly affected and a deviation from sinusoidal motion occurs. There, this behavior was used to estimate the contact time.

Simulations are done for the same cantilever with a set-point amplitude of 80 nm and free amplitude of 125 nm and for various samples, which have different equivalent spring constants. Also, for each sample spring constant, three different interaction characteristics are used. These are high dissipation (75 eV per tap), medium dissipation (30 eV per tap), and very low dissipation in which, a purely repulsive interaction was assumed. We changed f_3 to be $15f_1$ to make it an integer multiple of f_1. Such a condition is preferable, since it increases the amplitude of the vibrations of that mode in addition to providing a natural band-pass filtering effect. It is important to note that in reality the eigenfrequencies are not equal to the harmonics of the fundamental frequency and hence the signals at the harmonics are significantly smaller. The amplitude and phase responses of the third flexural eigenmode in the very low dissipation case are given in Fig. 3. It is seen that the third-order vibrations completely disappear at a certain value of the spring constant of the sample. Note that this point is also the exact location of the phase jump of 180°. Since the amplitude varies around zero, amplitude measurements will be an efficient way to probe sample properties. A rough estimate gives that a stiffness variation of 15% results in 1 Å amplitude variation. It is reported that in some cases the quality factor of the third eigenmode can be as high as 900, which means a further gain of 2 in resolution.[9] Note that, if the cantilever position is

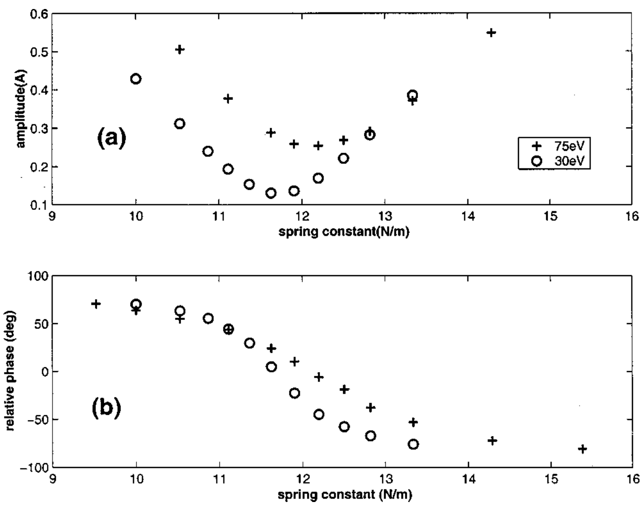

FIG. 4. Vibrations of the third eigenmode of the cantilever for medium and high dissipation cases: (a) amplitude and (b) phase of the vibrations with respect to equivalent spring constant of the sample. Phase references are set arbitrarily.

measured with the conventional optical detection method, the output signal depends on the slope of the cantilever which is higher in higher order vibration modes. Therefore, a good signal to noise ratio can be expected.

For the dissipative interactions, amplitude and phase responses are plotted in Fig. 4. It is seen that the third-order vibrations do not go to zero. As a consequence, the amplitude variations around the minimum are not sensitive to the sample stiffness variations. These time phase shift measurements become more useful to probe the sample variations. For the medium dissipation case about 6° of phase shift is expected for a stiffness change of 1%. The high sensitivity of the third flexural eigenmode is because the contact time and the period of the vibrations of the third flexural mode are nearly equal. We note that there is a relation between the contact time and the number of higher order modes that are efficiently excited. The smaller the contact time, the greater the number of higher order modes that are excited. In most materials, contact times are around 5%–10% of the main period, which corresponds to the periods of 10th to 20th harmonics. The third resonance is typically located at these frequencies. In very stiff or compliant samples, contact times can be as high as 12% or as low as 2% of the main period.[12] In those cases, other flexural modes can be more suitable for imaging.

To summarize, we have presented an equivalent electrical circuit to model and simulate the higher harmonics generation in tapping mode. The simulation results show that the third flexural vibration mode is highly sensitive to tip–sample interaction. Amplitude and relative phase shifts of these higher order vibrations could provide an opportunity to map material variations across the sample.

[1] R. Garcia, J. Tamayo, and A. S. Paulo, Surf. Interface Anal. **27**, 312 (1999).
[2] J. P. Cleveland, B. Anczykowski, A. E. Schmid, and V. B. Elings, Appl. Phys. Lett. **72**, 2613 (1998).
[3] J. Tamayo and R. Garcia, Appl. Phys. Lett. **73**, 2926 (1998).
[4] M. Luna, J. Colchero, and A. M. Baró, Appl. Phys. Lett. **72**, 3461 (1998).
[5] O. Sahin and A. Atalar, Appl. Phys. Lett. **78**, 2973 (2001).
[6] R. W. Stark and W. M. Heckl, Surf. Sci. **457**, 219 (2000).
[7] R. Hillenbrand, M. Stark, and R. Guckenberger, Appl. Phys. Lett. **76**, 3478 (2000).
[8] HSPICE: Avant! Corporation, 46871 Bayside Parkway, Fremont, CA 94538.
[9] U. Rabe, K. Janser, and W. Arnold, Rev. Sci. Instrum. **67**, 3281 (1996).
[10] K. Yamanaka and S. Nakano, Jpn. J. Appl. Phys., Part 1 **35**, 3787 (1996).
[11] Details of this equation and modeling of the higher order modes are unpublished.
[12] J. Tamayo and R. Garciao, Langmuir **12**, 4430 (1996).