

## Computation Time Effective Simulation of Non-Contact Atomic Force Microscope

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Recent NC-AFM simulations include the cantilever motion, the automatic gain control loop, and the phase locked loop based frequency tracking system [1,2]. Due to the complexity of the NC-AFM, successful simulation requires either long time steps, or extremely long computation time. NC-AFM simulations use the following the tip's equation of motion:

$$m\ddot{d}(t) = -kd(t) - \frac{m\omega_0}{Q}\dot{d}(t) + F_{ts}(d-z) + g(A) \cdot d(t - \Delta t) \quad (1)$$

Here,  $m$ ,  $d$ ,  $k$ ,  $Q$  represent the effective mass of the cantilever, cantilever bending, spring constant and quality factor, respectively. Meanwhile, the variable gain and the  $\frac{\pi}{2}$  phase shift of the feedback loop is modeled by  $g(A)$  and time shifting term  $d(t - \Delta t)$ , respectively.

Q controlled tapping mode atomic force microscope uses similar feedback loop, but in this case the gain of the feedback loop is constant. Recent result showed that the solution of the force equation of the Q controlled tapping mode system is identical with the well known solution of the damped harmonic oscillator provided its effective quality factor is chosen properly [3]. It has been also shown that simulation of the damped harmonic oscillator requires significantly less computation time [3]. To spare computation time, Eq. 1 can be rewritten as follows:

$$m\ddot{d}(t) = -kd(t) - \left( \frac{m\omega_0}{Q} + \hat{g}(A) \right) \dot{d}(t) + F_{ts}(d-z) \quad (2)$$

Based on Eq. 2 we modeled the whole NC-AFM operation including phase locked loop and control system. In present contribution, we give further details about the simulation program. In addition, we studied the dynamical properties of the NC-AFM probe by simulation of surface step imaging.

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[2] J. Polesel-Marais, S. J. Gauthier Appl. Phys. **97** (4) art. num: 044902 (2005)

[3] J. Kokavecz, Z. L. Horváth, Á. Mechler, Appl. Phys. Lett. **85**(15), 3232 (2004)