

CONTROL OF SCANNING PROBE MICROSCOPES USING QUARTZ TUNING FORKS

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Abstract

We present a simulated controller of a scanning probe microscope using tuning forks. In scanning probe microscopy, a new technology has been developed in the last years, exploiting a skew force which results from friction between the probe tip and the smooth surface of the sample. This force can be detected at a distance of several nm above the surface. It affects the parameters of oscillation of a vibrating optical fiber positioned above the surface with forcing frequency induced by quartz tuning forks. The distance from the surface sample can be determined by measuring the shift in resonance frequency and amplitude of the oscillation. This can therefore be used for precise positioning of the probe tip above the sample surface, and for reconstruction of the surface form. The simulation is based on an efficient and robust theoretically-based algorithm. The algorithm is devised to control the tip within a specified distance above the sample, at which a precise reconstruction of the form of the sample surface can be made. It was made for the purpose of developing a digital scanning probe controller which could substitute analogue controllers that are currently in use in scanning probe microscopy. This would enable improved precision, faster response and would reduce the cost of production of the controller.

Keywords: scanning probe microscopy, scanning probe control, resonance

Presenting Author's Biography

Neža Mramor Kosta is associate professor of mathematics at the Faculty of Computer and Information Science of the University of Ljubljana, and a researcher at the Institute of Mathematics, Physics and Mechanics in Ljubljana. Her research interests range from theoretical mathematics, in particular topology, to applications of mathematical methods in computer science.



1 Theoretical background

1.1 Introduction

The basic principle of torsion is that a force acts against friction between two bodies, and as a consequence, energy in the form of heat is released. Friction against liquids or solid layers, adsorbed on an ideally smooth surface, is opposed by a skew force which is the result of inter-atomic forces between atoms and molecules acting on the plane of contact. The physical nature of this force has not been sufficiently explained yet. In scanning probe microscopy a new technology has been developed in the last years which uses this skew force between the probe tip and the smooth surface of the sample to control a pointed optical fiber at a desired distance over the surface [1],[3], [5]. The tip, which vibrates in a direction parallel to the plane, detects at a distance smaller than 25 nm from the surface a damping effect which is the consequence of this skew force. The amplitude of the mechanical oscillations is proportional to the acting forces and can be measured through the piezoelectric effect which is a result of the skew friction force. Since a quartz tuning fork has a high goodness $Q \sim 10^3 - 10^5$, it is sensitive to very small forces (of the order of magnitude under pN). Because of this they are used in scanning probe microscopy for positioning the probe at a suitable distance over the surface[4],[2].

1.2 Parameters of oscillation in the vicinity of the surface

Oscillations of quartz tuning forks are described by the equation

$$M\ddot{u} + M\gamma\dot{u} + ku = F_D \exp i\omega t, \quad (1)$$

where u is the displacement, F_D is the amplitude, and ω is the forcing frequency. As the surface is approached, the parameters k and γ describing the damping and viscosity vary, and as a consequence the frequency at resonance changes. The dependency of k and γ on the distance z of the tip from the surface of the sample has been determined experimentally as

$$\gamma(z) = \gamma_\infty + \gamma_0 \exp\left(-\frac{z}{\delta_\gamma}\right) \quad (2)$$

$$k(z) = k_\infty + k_0 \exp\left(-\frac{z}{\delta_k}\right). \quad (3)$$

Figures 1 and 2 demonstrates experimental results which confirm these formulas.

For tuning forks used in scanning microscopy the values of parameters of oscillation far away from the sample (more than 22 nm) are $\gamma_\infty = 30.88 s^{-1}$, $K = k_\infty = 4220 N/m$, and $\omega_\infty = \sqrt{K/M} = 209040 s^{-1}$. The approximate values of other constants are $\gamma_0 = 72.0 s^{-1}$, $\delta_\gamma = 4.02 nm$, $k_0 = 93.9 N/m$ in $\delta_k = 2.90 nm$. The forcing amplitude is $F_D = 116 pN$, the effective mass (i.e. one fourth of the total mass of the forks) is $M = 0.966 \cdot 10^{-6} kg$.

A solution of equation (1) is of the form $A \exp i\omega t$

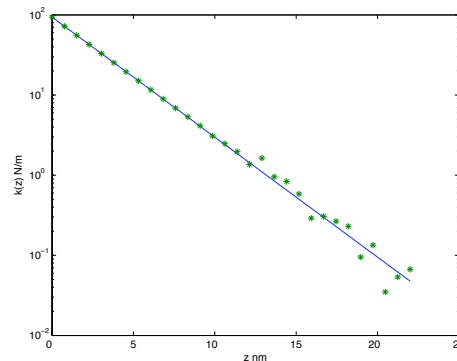


Fig. 1 The dependency of the oscillation parameters k on the distance of the tip from the sample n a logarithmic scale

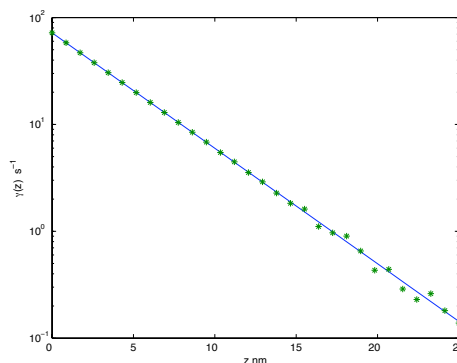


Fig. 2 The dependency of the oscillation parameters γ on the distance of the tip from the sample n a logarithmic scale

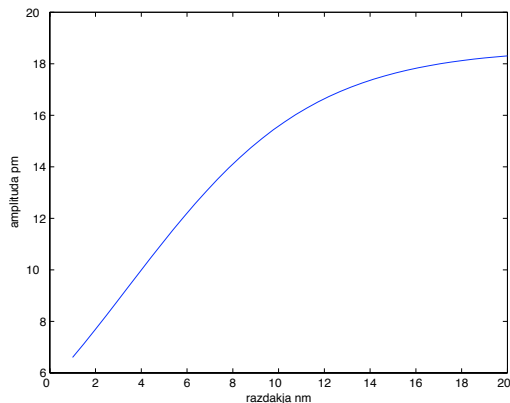


Fig. 3 Dependency of the resonance amplitude x on the distance from the sample z

where

$$A = \frac{F_D/M}{\omega_0^2 - \omega^2 + i\gamma\omega} \quad (4)$$

and $\omega_0 = \sqrt{k/M}$. The absolute value of the amplitude is thus

$$|A| = \frac{F_D/M}{\sqrt{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2}}, \quad (5)$$

and the phase is

$$\varphi = \arctan \frac{\gamma\omega}{\omega_0^2 - \omega^2}. \quad (6)$$

It follows that at resonance the phase equals $\pi/2$, it is smaller than $\pi/2$ if the forcing frequency is smaller than at resonance, and bigger than $\pi/2$ if the forcing frequency is bigger than at resonance.

The frequency at resonance is obtained from the homogeneous part of equation (1) and is equal to

$$\omega_{res}^2 = \omega_0^2 - \gamma^2/4 \approx \omega_0^2, \quad (7)$$

where γ^2 is much smaller than ω_0 , so the resonance frequency is approximately $\omega_0 = \sqrt{k/M}$. Far away from the sample it is equal to $\omega_\infty = \sqrt{K/M}$.

The approximate value of the amplitude of oscillation then

$$x = \frac{F_D/M}{\gamma\omega_0}. \quad (8)$$

Equation (2) now gives the theoretical solution of the problem, which is the basis of our algorithm:

Proposition. The dependency of the resonance amplitude x on the distance from the sample z is given by

$$x = \frac{x_\infty}{1 + \gamma_0/\gamma_\infty \exp(-z/\delta_\gamma)} \quad (9)$$

The resonance amplitude far away from the surface is

$$x_\infty = \frac{F_D/M}{\gamma_\infty\omega_\infty} = 18.6 \text{ pm} \quad (10)$$

The goodness Q , that is the quotient of the resonance frequency (i.e. the height of the resonance curve) and the width of the resonance curve at half of its height, is

$$Q = \frac{\omega_{res}}{\sqrt{3}\gamma} \approx \frac{\omega_0}{\sqrt{3}\gamma}$$

The goodness far away from the sample is thus

$$Q_\infty = \frac{\omega_\infty}{\sqrt{3}\gamma_\infty} = 3907.86,$$

and the amplitude is approximately proportional to the goodness:

$$x = \frac{F_D}{k\sqrt{3}} Q \approx \frac{F_D}{K\sqrt{3}} Q. \quad (11)$$

Equations (8) and (10) now give

$$\gamma = \gamma_\infty \frac{\omega_\infty x_\infty}{\omega_0 x} \quad (12)$$

and similarly

$$k = k_\infty \frac{\omega_0^2}{\omega_\infty^2} \quad (13)$$

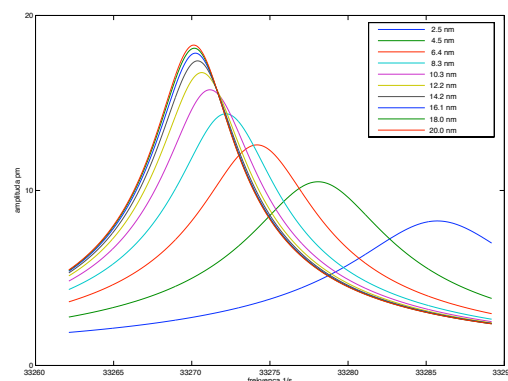


Fig. 4 The resonance curve at specific distances from the surface

2 The algorithm for controlling the probe

We describe an algorithm for digital control of a scanning probe, based on the principles described above. Such an algorithm would enable control with higher precision and lower costs than in the case of analog controllers [6].

The algorithm is devised to control the probe's position within the interval 8-12 nm from the surface, where the resonance amplitude is approximately 75 % do 85 % of the amplitude x_∞ .

We first choose a reference distance from the sample at the point where the resonance amplitude equals half the

value at ∞ . All distances are expressed as differences from this value, which we denote by z_0 .

Following is an overview of the algorithm.

2.1 Steps of the algorithm

1. Calibration. The initial step is to determine the value of the parameter δ_γ in (9). A detailed description is given below in 2.2.
2. One step of the algorithm consists of (possibly several) adjustments of the height of the probe after a horizontal move to the next point above the sample, and is decomposed into:
 - (a) determining the sign of the difference of the frequency from resonance
 - several values (four or five) of the displacement u_i of the oscillating probe tip are measured, from which the parameters in A and φ of oscillation are computed using least squares (compare 2.4)
 - the phase φ obtained in this way is compared to the value at resonance ($\pi/2$), the sign of the difference determines the sign of the frequency increment in step (b)
 - (b) several (in the implementation around five) points on the resonance curve are found in the following way:
 - the frequency is changed by an increment $\Delta\omega$ (of fixed sign determined above)
 - the amplitude of oscillation is computed from a few measured values u_i using least squares (as in step (a))
 - (c) the resonance curve is obtained from the computed values by a least squares fit, and the resonance amplitude (the height of the curve) is computed (computeresonanca)
 - (d) the computed resonance amplitude x is compared to the reference value $x_0 = x_\infty/2$, and the height adjustment dz is computed (compare 2.3)
 - (e) this step is repeated several times until the resonance amplitude is within the acceptable interval

In the following, details of some of the steps of the algorithm are given.

2.2 Calibration

The difference from the reference height z_0 is denoted by $\Delta z = z - z_0$.

The logarithmic decrement δ_γ of the viscosity $\gamma(z)$ is determined from a series of measurement at the initial point above the sample. Equation (2) now has the form

$$\gamma(z) = \gamma_\infty + \gamma_0 \exp(z_0/\delta_\gamma) \exp(-\Delta z/\delta_\gamma),$$

where $\Delta z = z - z_0$, so

$$\frac{x_\infty}{x} = 1 + \frac{\gamma_0}{\gamma_\infty} \exp\left(\frac{z_0}{\delta_\gamma}\right) \exp\left(-\frac{\Delta z}{\delta_\gamma}\right) \quad (14)$$

$$\frac{x_\infty}{x} - 1 = q \exp(-\Delta z/\delta_\gamma) \quad (15)$$

$$q = \frac{\gamma_0}{\gamma_\infty} \exp(z_0/\delta_\gamma) \quad (16)$$

for an estimate of the value δ_γ a series of moves $\Delta z = idz, i = 1, 2, \dots, n$ of the probe from the reference value z_0 is made and the changes in corresponding resonance amplitude x_i are measured.

By differentiating we obtain

$$dx \frac{x_\infty}{x^2} = \frac{q}{\delta_\gamma} \exp(\Delta z/\delta_\gamma) dz \quad (17)$$

$$\delta_\gamma = \frac{x(x_\infty - x)}{x_\infty} \frac{dz}{dx} \quad (18)$$

$$\approx \frac{x(x_\infty - x)}{x_\infty} \frac{dz}{\Delta x} \quad (19)$$

The value dz is constant. For each i we compute

$$\bar{\delta}_{\gamma,i} = \frac{x_{i+1}(x_\infty - x_{i+1})}{x_\infty} \frac{dz}{dx} \quad (20)$$

$$\underline{\delta}_{\gamma,i} = \frac{x_i(x_\infty - x_i)}{x_\infty} \frac{dz}{dx} \quad (21)$$

$$\hat{\delta}_{\gamma,i} = \frac{1}{2}(\bar{\delta}_{\gamma,i} + \underline{\delta}_{\gamma,i}) \quad (22)$$

As an estimate for δ_γ we use the average value of $\hat{\delta}_{\gamma,i}$ (up to two decimal places the obtained values coincide as long as dz is not bigger than 0.5 nm and we remain within the interval 8-12 nm).

2.3 Computation of the adjustment dz

The adjustment dz of the height of the probe tip above the sample is determined from the differential (19), rewritten as

$$dz = \delta_\gamma \frac{x_\infty}{x(x_\infty - x)} dx \quad (23)$$

Because of the convexity of the function $x = x(z)$ they are overestimated. Experiments will show if a relaxation might improve the results.

2.4 Computation the amplitude and phase

In order to compute the amplitude and phase of the oscillating tip several values u_i of the displacement, for example five or six, should be measure within one period of oscillation. The amplitude and phase is then computed from the equations

$$u_i = a \cos(\omega t_i) + b \sin(\omega t_i) \quad (24)$$

$$A = \sqrt{a^2 + b^2} \quad (25)$$

$$\varphi = \arctan \frac{b}{a} \quad (26)$$

using least squares.

2.5 Determining the resonance amplitude

As the forcing frequency is changed, the corresponding amplitude of oscillation A_i is computed for each value ω_i . Results are best if a few values above and a few values below the resonance are used. Assume that six values of the amplitude for different forcing frequencies have been obtained. For each i , we compute

$$S_i = \left(\frac{F_D}{|A_i M|} \right)^2, \quad (27)$$

quadratic function of ω_i , find the parabola which best fits the measured values (ω_i^2, S_i) , and determine ω_0 at the vertex (i.e. the lowest point) of this parabola.

The resonance amplitude should be computed within the time interval of a few (less than 10) oscillations, that is, in less than $< 1/3$ ms, which is more than realistic.

3 Simulation

The algorithm has been tested by computer simulations over different simulated surfaces.

3.1 The scenario

1. In the simulation, the average distance of the tip from the surface in three neighboring points was used.
2. The probe of a scanning probe microscope scans the underlying sample surface line by line so it suffices to generate a section of the simulated surface. The simulated surfaces used in the simulation were of two types. Figures 5, 6 and 7 demonstrate simulated control over surfaces which were generated as plots of functions (with Matlab). Figures 9 and 8 demonstrate simulation over a digitally rendered surface. The profile corresponds to the gray scale function of a digital image.
3. In the simulation, the probe tip was controlled within a region corresponding to 75 % do 85 % of the resonance amplitude far from the surface. Within this region, precise reconstruction of the underlying surface was achievable, with limited danger of collision of the tip with the sample.

3.2 Results

Results of some of the simulations are presented in figures 5, 6, 7, 8 and 9. On all graphs, the bottom curve represents the simulated surface, the middle curve represents the reconstructed surface, positioned at 10 Å above the simulated surface for better clarity. The top curve represents the path of the probe tip.

Figure 5 shows that the reconstruction of a smooth artificial surface (in this case modeled by $f(x) = a(1 - bx^2) \sin x^2$) is very precise. In areas where the slope of the surface is relatively steep, the tip movements are delayed. In areas where the surface is almost flat the tip there are no unnecessary movements of the tip which remains at a constant height within the given bounds.

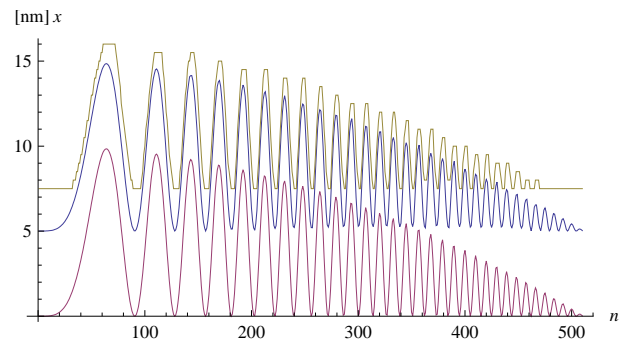


Fig. 5 Simulated control over a Matlab generated surface

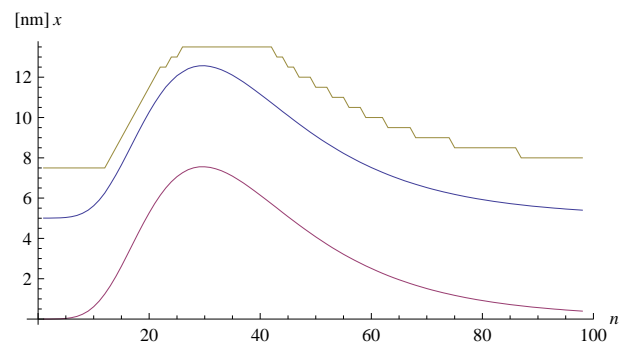


Fig. 6 Control over a smooth obstacle

Control over a smooth obstacle which is shown on figure 6 gave similar results. The errors of the reconstruction in both cases are of far smaller order than the surface features.

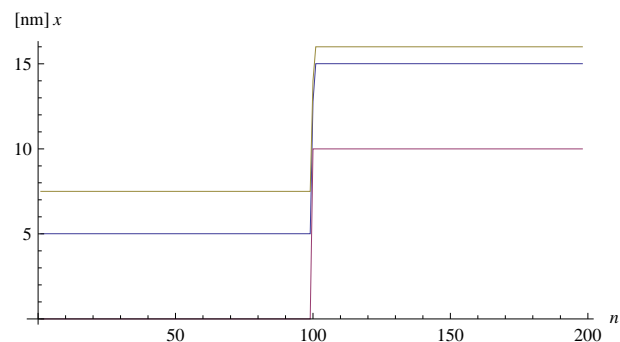


Fig. 7 Control over a sharp obstacle

Perhaps the most interesting simulation is shown on figure 7 which demonstrates the results of control over a simulated sharp obstacle on the surface. The reconstruction in this case is not precise, and the obstacles appears smoothed in the reconstruction. This is due to the fact that the force magnitude was simulated using the average distance from three neighboring points which seems reasonable. Nevertheless, since the physical nature of the friction force between the surface and the probe tip in reality is not completely understood yet, this effect should be verified experimentally.

Figure 8 demonstrate the results of control over a simulated surface of a completely different type. The surface profile corresponds to the gray scale function of a digital image. the resulting surface is highly non-smooth, with many perturbations and irregularities. As the top curve shows, the movements, required to keep the probe tip within the required bounds are relatively few, and the tip typically does not follow the profile of the surface closely. Nevertheless, the reconstructions are very precise.

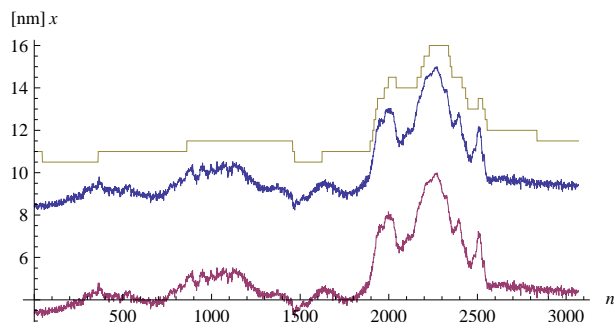


Fig. 8 Control over a digitally simulated surface

A similar simulation on a different surface of the same type is shown in figure 9

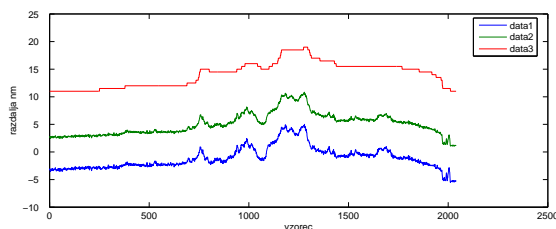


Fig. 9 Control over a slightly different digitally simulated surface

The simulations indicate that the algorithm reconstructs surfaces of very different type successfully. It is also sufficiently efficient to enable real-time control of the actual probe of a scanning probe microscope, assuming that relatively fast processor and implementation are used. Nevertheless, actual testing on samples will be necessary for a realistic evaluation of its performance.

4 References

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