1/f Performance Limits of Scanning Tunneling Microscopes

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Abstract. The feedback loop of the Scanning Tunneling Microscope (STM) maintains a constant current throughout the circuit and utilizes a piezoelectric crystal to control the tip-sample separation distance. The piezoelectric crystal is a source of quantum 1/f noise which can reduce detection limits. Both the fluctuations in the tunneling current and the spatial fluctuations of the piezoelectric crystal result in deviations in tip-sample separation distance. Here, for the first time, using the quantum 1/f theory, the fluctuations in the tip-sample separation distance due to the fluctuating relaxation rate, τ, of the piezoelectric crystal are calculated.

Keywords: Quantum 1/f noise, piezoelectric, Scanning Tunneling Microscopes, resolution limits.

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QUANTUM 1/F NOISE IN PIEZOELECTRICS

The phonon emission within the piezoelectric quartz crystal can be caused by scattering events with higher frequency phonons or by scattering events on defects or impurities occurring in the crystal. The phonon emission rate Γ is equal to 1/τ , where τ is the relaxation rate of the quartz. Fluctuations in the relaxation rate, τ, produce fluctuations in the Young's modulus of the crystal, E_0 , which ultimately give rise to fluctuations in tip position.

First, we define the velocity change of a phonon in the crystal due to dissipation as

$$\frac{s-s_0}{s_0}=\frac{CT\left\langle \gamma_{eff}^2\right\rangle}{2\rho s_0}\frac{\Omega_0^2\tau^2}{1+\Omega_0^2\tau^2} \tag{1}$$

where C is the specific heat, T is the temperature, γ is the Grüneisen constant, s_0 is the speed of sound in the absence of dissipation, Ω_0 is the resonance frequency of the crystal, ρ is the crystal density, and τ is the relaxation time [1]. To simplify, we let $\Delta E = CT \langle\gamma^2\rangle$ = constant and also use the low frequency Young modulus $E_0 = \rho\, s_0^2$ = constant. Now after letting $x = \Omega_0^2\, \tau^2$, Eq. (1) can be written

$$\sqrt{\frac{E}{E_0}} = \frac{DE}{2E_0}\frac{x}{1+x} + 1 \qquad (2)$$

Differentiating, and assuming $E - E_0 << 1$, we obtain an expression for the variation in the Young modulus δE, which is proportional to the change in the relaxation time $\delta\tau$

$$\delta E = \Delta E \frac{2x}{(1+x)^2}\frac{\delta\tau}{\tau} \qquad (3)$$

Applying a force to the crystal, or applying a voltage across the crystal, causes spatial displacement, X, in the vertical direction, which we take to be the direction of crystal length. Fluctuations in the Young modulus, E_0, produce tip-sample distance fluctuations $\delta X/X = -\delta E_0/E_0$, which gives the spectral density of fractional fluctuations as

$$S_{\frac{\delta X}{X}} = S_{\frac{\delta E_0}{E_0}} = \frac{1}{E_0^2} S_{\delta E_0} \qquad (4)$$

The relation between quartz quality (Q-factor), relaxation time and frequency given by [1], is $Ex/\Delta E \approx Q^2$, which allows for the spectral density of fractional spatial fluctuations to be written as

$$S_{\frac{\delta X}{X}} = 4\left(\frac{\Delta E}{E}\right)^2 \frac{x^2}{(1+x)^4} S_{\frac{\delta\tau}{\tau}} \approx \frac{4}{Q^4} S_{\frac{\delta\tau}{\tau}} \qquad (5)$$

Recall that the phonon emission, or interaction, rate Γ is equal to $1/\tau$, where τ is the relaxation rate of the quartz. Therefore, the fractional fluctuations in phonon emission rate are equal to the fractional fluctuations in relaxation rate: $S_{\delta\tau/\tau} = S_{\delta\Gamma/\Gamma}$. According to the general quantum 1/f formula, $\Gamma^{-2} S_{\Gamma}(f) = 2\alpha A/f$, where $\alpha = e^2/\hbar c$ is the fine structure constant and $A = 2(\Delta \mathbf{J}/ec)^2/3\pi$ is the quantum 1/f effect in any physical process rate Γ [2], [3]. The current discontinuity $\Delta\mathbf{J}$ in the Ampere-Maxwell equation equals the discontinuity $\Delta d\mathbf{P}/dt$ in the rate of the crystal dipole moment change $d\mathbf{P}/dt$. The spectral density of fluctuations in the rate Γ of phonon emission /removal from the main resonant oscillation mode of the crystal can be written

$$S_{\Gamma}(f) = \Gamma^2 4\alpha \left(\Delta\dot{P}\right)^2 / 3\pi e^2 c^2 f \qquad (6)$$

where $(\Delta\dot{\mathbf{P}})^2$ is the square of the discontinuity in the dipole moment change rate, in the process causing the removal of a phonon from the main oscillator mode. To calculate this change, we write the energy W of the interacting resonator mode $<\omega>$ in terms of d**P**/dt

$$W=n\hbar<\omega> =2(Nm/2)(dx/dt)^2 =(Nm/e)^2(edx/dt)^2 = (m/Ne^2)(dP/dt)^2 .$$

The factor 2 includes the potential energy contribution. Here m is the reduced mass of the elementary oscillating dipoles, e their charge, and N their number in the crystal. Considering $\Delta n=1$ for 1 phonon, we obtain the fractional energy variation

$$\Delta n/n =2|\Delta dP/dt| /(dP/dt), \quad \text{or } \Delta dP/dt =(1/2n)\, dP/dt$$

Taking $\Delta dP/dt$ fro the expression of W, substituting it into the last expression here, we obtain an expression for the jump in the rate of change $|\Delta \dot{\mathbf{P}}| = (N\hbar<\omega>/n)^{1/2}(e/2)$. Substituting $\Delta\dot{\mathbf{P}}$ into Eq. (6), the expression for the spectral density is then

$$\Gamma^{-2}S_\Gamma(f) = N\alpha\hbar\left\langle\omega_{eff}\right\rangle/3\pi nMc^2 f \qquad (7)$$

where N is the number of oscillating dipoles in the crystal, n is the number of thermal phonons at the resonant frequency of the quartz (which we set to unity), M is the reduced mass of the elementary oscillating dipoles, and c is the speed of light. $<\omega_{eff}>$ replaces the crystal resonator mode frequency, which is usually much smaller. The frequency $<\omega_{eff}>$ is the frequency that gives the average of the quantum 1/f contributions. Indeed, the quantum 1/f effect calculated from Eq. (7) includes contributions from all 3 phonons involved in the process in which a phonon from the main resonator mode combines with a thermal phonon of much higher frequency, yielding another thermal phonon of similar high frequency. The largest contribution will not come from the main resonator 1/n factor, but from the 1/n factor corresponding to the high-frequency thermal modes that have n close to 1. Furthermore, n is the number of thermal phonons at the frequency $<\omega_{eff}>$ of the quartz, which we set equal to unity [2], [3].

Each coherence volume ε^3 of the quartz crystal has independent dissipation fluctuation, with ε being the phonon coherence length. Their variances add, and cause a (ε^3/V) factor to be present in the spectral density of the fractional legth fluctuations for the whole crystal.

Using eq. (7), the fractional spatial fluctuations of equation (5) can be written in terms of the fractional fluctuations of the phonon emission rate Γ

$$S_{\frac{\delta X}{X}} \approx \frac{4}{Q^4}\frac{\varepsilon^6}{V^2}\left[\frac{N\alpha\hbar\left\langle\omega_{eff}\right\rangle}{3\pi nMc^2 f}\right] = \frac{4}{Q^4}\frac{\varepsilon^6}{V}\left[\frac{\left(\frac{N}{V}\right)\alpha\hbar\left\langle\omega_{eff}\right\rangle}{3\pi nMc^2 f}\right] \equiv \frac{4\beta'\varepsilon^6}{fVQ^4} \quad (8)$$

Here V is the quartz crystal volume, (N/V) is the number of SiO_2 molecules in the volume of one unit cell of the quartz crystal, ε^6 is the squared phonon coherence volume. In this final form, we can make an approximation to the spatial fluctuations in the STM due to the phonon emission rate Γ of the piezoelectric quartz crystal which controls the feedback loop.

DISCUSSION

As a first approximation, assume the piezoelectric element is a cylinder with diameter and length of 1 cm, giving a crystal volume of 7.85×10^{-7} m^3. Solving kT = ħ < ω_{eff} > , we obtain < ω_{eff} > = 6.3×10^{12} /s. A phonon coherence length of 0.1mm is assumed, along with a quartz lattice constant of 4.9 Å. If there is only one SiO_2 molecule in the volume of the quartz unit cell, then (N/V) = 8.5×10^{27} m^{-3} . The reduced mass of the oscillating dipoles was taken to be 10^{-23} kg, at room temperature, where kT = 4×10^{-21} J. Substituting n = kT/ħ < ω_{eff} > for thermal phonons, and these assumed values into Eq. (8), we obtain fractional spatial fluctuations of $S_{\delta X/X} = 3.6 \times 10^{-21}$ / Hz for Q = 1000 and $S_{\delta X/X} = 3.6 \times 10^{-17}$ / Hz for Q = 100.

Finally, to calculate the rms spatial fluctuations along the length of the piezoelectric crystal, δX, we use the following relation, in the case of Q = 1000,

$$\frac{\delta X}{X} = \sqrt{S_{\frac{\delta X}{X}}} = \sqrt{\frac{3.6x10^{-21}}{Hz}} = \frac{6x10^{-11}}{\sqrt{Hz}} \tag{9}$$

The rms spatial fluctuations are obtained by multiplying by the crystal length, X, which in this case is 1 cm,

$$\left(\delta X\right)_{rms} = \frac{6x10^{-11}}{\sqrt{Hz}} X = \frac{6x10^{-11}(1cm)}{\sqrt{Hz}} = \frac{0.6x10^{-10}}{\sqrt{Hz}} \text{ cm} \tag{10}$$

Therefore, the quantum 1/f fluctuations in this spatial direction are 0.006 Angstroms per square root of Hertz. This means that the piezoelectric crystal in the STM contributes 10 times more error in tip sample separation distance compared with the quantum 1/f fluctuations occurring in a stationary needle without the feedback loop engaged [4].

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