The origins of friction and the growth of graphene, investigated at the atomic scale

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Appendix A

Theoretical description of the Q-factor of the cantilever

In Chapter 4, the Q-factor of the cantilever was discussed. The Q-factor was estimated via the frequency spectrum of the lateral force on the cantilever. At the very beginning of the discussion, a theoretical expression of the Q-factor was given in Equation 4.4. Here, we will derive this equation. But first, we motivate the need for an alternative expression with respect to known versions present in the literature.

A.1 Motivation

In Reference [15], a derivation of the Q-factor was made by Maier et al. in an attempt to explain the Q-factors that were estimated based on their experiments. One of the assumptions made in this derivation, was that the tip apex followed the motion of the cantilever. The results of our numerical calculations do not justify this assumption: we have shown that the tip apex is oscillating most of its time in the lower part of the substrate potential wells. At the same time, the stiff cantilever oscillates with its own charactiristic frequency. The relatively soft spring between the cantilever and the tip apex makes the tip apex significantly decoupled from the cantilever.

Our alternative derivation is meant to incorporate the effect of the presence of the substrate potential and the effect of the decoupling between the tip apex and the cantilever.

A.2 Derivation of Equation 4.4

The Q-factor of the cantilever is defined as

$$Q = 2\pi \frac{E}{\Delta E}, \tag{A.1}$$

where E is the energy stored in the oscillator, and ΔE is the energy loss per oscillation cycle of the cantilever. Here, we are interested in the case where the cantilever is coupled to the flexible tip apex, which turns our system into a 2-mass-2-spring system.

For the sake of simplicity, we treat the symmetric case, in which the equilibrium positions of the support, the cantilever and the tip apex are coinciding with a local minimum in the substrate potential.

We will calculate the energy loss per oscillation cycle of the cantilever ΔE, under the following assumption:

Assumption 1: We assume that the intrinsic damping of the cantilever is so weak that it can be ignored completely.

This assumption simplifies our derivation of ΔE, as the energy dissipation is now only concentrated in the tip apex:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\gamma_{\mathrm{diss}}(\dot{x}_{\mathrm{d}}(t))^2. \tag{A.2}$$

Now, we have to establish a relation between the motion of the cantilever and that of the tip apex. First, we define the motion of the cantilever as follows:

$$x_{\mathrm{cant}}(t) = A_{\mathrm{cant}} \sin\left(\omega_{\mathrm{cant}} t\right). \tag{A.3}$$

The motion of the tip apex, x_{d}, is coupled to the time-dependent position of the cantilever and to the substrate. This coupling can be made explicit via the combined potential that is experienced by the tip apex:

$$V_{\mathrm{d}}(x_{\mathrm{d}}(t)) = \frac{1}{2} k_{\mathrm{d}} \left(x_{\mathrm{d}}(t) - x_{\mathrm{cant}}(t)\right)^2 - U_0 \cos\left(\frac{2\pi}{a} x_{\mathrm{d}}(t)\right), \tag{A.4}$$

in which the two terms on the right-hand side represent the tip-cantilever spring potential and the tip-substrate interaction potential, respectively. As the tip apex is a very dynamic element, especially with respect to the much heavier cantilever, we can describe its motion as a rapid oscillation around the time-dependent minimum x_{d}^* of V_{d}. The position of this minimum is given by

$$x_{\mathrm{d}}^*(t) = x_{\mathrm{cant}}(t) - \frac{2\pi U_0}{k_{\mathrm{d}} a} \sin\left(\frac{2\pi}{a} x_{\mathrm{d}}^*(t)\right). \tag{A.5}$$

Assumption 2: As the amplitude of the tip apex oscillation is small with respect to width of the substrate potential wells, we can approximate the shape of the substrate potential by a parabola, so that $\sin(ax) \approx ax$.

This assumption simplifies Equation A.5 to:

$$x_{\mathrm{d}}^{*}(t) = \left(1 + \frac{4\pi^2 U_0}{k_{\mathrm{d}} a^2}\right)^{-1} x_{\mathrm{cant}}(t) = \varepsilon x_{\mathrm{cant}}(t). \tag{A.6}$$

We can describe the motion of the tip apex as a rapid oscillation around this time-dependent potential energy minimum:

$$x_{\mathrm{d}}(t) = A_{\mathrm{d}} \sin\left(\omega_{\mathrm{d}} t\right) + \varepsilon A_{\mathrm{cant}} \sin\left(\omega_{\mathrm{cant}} t\right). \tag{A.7}$$

From this we obtain the velocity of the tip apex:

$$\dot{x}_{\mathrm{d}}(t) = A_{\mathrm{d}} \omega_{\mathrm{d}} \cos\left(\omega_{\mathrm{d}} t\right) + \varepsilon A_{\mathrm{cant}} \omega_{\mathrm{cant}} \cos\left(\omega_{\mathrm{cant}} t\right). \tag{A.8}$$

This can be used to calculate the energy dissipation rate at the tip apex:

$$\begin{aligned} \frac{\mathrm{d}E}{\mathrm{d}t} &= -\gamma_{\mathrm{diss}} \dot{x}_{\mathrm{d}}^2 \\ &= -\gamma_{\mathrm{diss}} \big(A_{\mathrm{d}}^2 \omega_{\mathrm{d}}^2 \cos^2\left(\omega_{\mathrm{d}} t\right) \\ &+ \varepsilon^2 A_{\mathrm{cant}}^2 \omega_{\mathrm{cant}}^2 \cos^2\left(\omega_{\mathrm{cant}} t\right) \\ &+ 2\varepsilon A_{\mathrm{d}} A_{\mathrm{cant}} \omega_{\mathrm{d}} \omega_{\mathrm{cant}} \cos\left(\omega_{\mathrm{d}} t\right) \cos\left(\omega_{\mathrm{cant}} t\right) \big). \end{aligned} \tag{A.9}$$

If we integrate this over one full oscillation period of the cantilever, we obtain the total energy loss per cycle:

$$\Delta E = \left(\frac{\pi}{\omega_{\mathrm{cant}}}\right) \gamma_{\mathrm{diss}} (A_{\mathrm{d}}^2 \omega_{\mathrm{d}}^2 + \varepsilon^2 A_{\mathrm{cant}}^2 \omega_{\mathrm{cant}}^2). \tag{A.10}$$

In the integration, the cross term in $\mathrm{d}E/\mathrm{d}t$ leads to a zero contribution. The two remaining terms can be associated with the dissipation due to the separate contributions from the rapid tip apex motion and the much slower motion of the tip apex's equilibrium position due to the cantilever oscillation. It is the latter term that we associate with the modest dissipation of the cantilever motion via the tip apex. This is the cantilever energy loss per oscillation cycle that we need to determine:

$$\Delta E = \pi \gamma_{\mathrm{diss}} \omega_{\mathrm{cant}} \varepsilon^2 A_{\mathrm{cant}}^2. \tag{A.11}$$

The energy of the cantilever oscillation is equal to:

$$E = \frac{1}{2} m_{\mathrm{cant}} \omega_{\mathrm{cant}}^2 A_{\mathrm{cant}}^2 \tag{A.12}$$

Using these expressions for E and ΔE, we can now calculate the corresponding Q-factor to be:

$$Q = \frac{m_{\text{cant}}\omega_{\text{cant}}}{\gamma_{\text{diss}}\varepsilon^2} \tag{A.13}$$

Using Equation 2.7, which stated that $\gamma_{\text{diss}} = 2\sqrt{m_{\text{d}}k_{\text{d}}}D$, we can rewrite Equation A.13 as

$$Q = \frac{1}{2D\varepsilon^2}\frac{m_{\text{cant}}\omega_{\text{cant}}}{\sqrt{m_{\text{d}}k_{\text{d}}}}. \tag{A.14}$$

This relation can be further simplified, which results in the expression of the Q-factor given in Equation 4.4:

$$Q = \frac{1}{2D}\left(1 + \frac{4\pi^2 U_0}{k_{\text{d}}a^2}\right)^2\sqrt{\frac{m_{\text{cant}}}{m_{\text{d}}}\frac{k_{\text{cant}}}{k_{\text{d}}}} = \frac{1}{2D}\left(1 + \frac{k_{\text{TSI}}}{k_{\text{d}}}\right)^2\sqrt{\frac{m_{\text{cant}}}{m_{\text{d}}}\frac{k_{\text{cant}}}{k_{\text{d}}}}. \tag{A.15}$$

What the equation shows is that the mass ratio between the cantilever and the tip apex makes the damping of the cantilever motion via the forced motion of the tip apex extremely inefficient. In addition it shows that the effectiveness of this weak dissipation channel depends strongly on the amplitude of the tip-substrate interaction potential.

The form derived here for the Q-factor was tested by numerical calculations that comprised ringdown tests using our 2-mass-2-spring model with various, realistic amplitudes of the graphite substrate potential, including the extreme case of a flat potential. The Q-factor in these calculations, that was estimated via the decay of the cantilever oscillation amplitude, was (within the statistical error margin of the calculations) identical to the Q-factor calculated via Equation 4.4.

Appendix B

List of symbols

List of all symbols used in the first part of this thesis. The symbols are put in alphabetical order. Greek symbols are put at the end of the list.

a	lattice constant of the substrate
D	relative damping rate of the friction contact, $D = 1$ corresponds to the critically damped case
F_{diss}	the dissipative force on the dynamic mass m_{d}
k_{at}	spring constant associated with each of the atomic bonds in the tip
k_{B}	Boltzmann's constant
k_{cant}	(torsional) cantilever spring constant
k_{d}	spring constant with which the dynamic tip mass m_{d} is connected to the rigid remainder of the tip plus the cantilever
k_{eff}	effective spring constant of the entire system (from support to substrate)
k_{subs}	spring constant associated with the stiffness of the substrate
k_{tip}	spring constant of the tip
k_{TSI}	spring constant associated with the tip-substrate interaction
m_{at}	atomic mass of the atoms in the tip
m_{cant}	effective mass of cantilever
m_{d}	dynamic mass, i.e. the mass associated with the N_{d} dynamic atoms
m_{eff}	effective mass present in the 1-mass-1-spring model, which is pulled through the substrate potential

N_c	number of atoms making physical contact with the substrate
N_d	number of dynamic atoms, i.e. the effective number of atoms moving at same speed as the N_c contact atoms
Q	quality factor of an oscillator, which is in our work the cantilever
T	the temperature of the system
t_diss	timescale set by the damping rate η_diss
t_slip	timescale for a slip event of the dynamic mass
U_0	corrugation amplitude of the periodic substrate potential V_subs
V_subs	substrate potential
v_supp	velocity of the support
x_cant	x-coordinate of the cantilever
x_d	x-coordinate of the dynamic mass
x_supp	x-coordinate of the support
x_t	x-coordinate of the tip apex

Greek symbols

γ	dissipation rate [kg/sec]
γ_at	dissipation rate of one single atom in the contact [kg/sec]
γ_diss	dissipation rate of the entire contact [kg/sec]
η_at	damping rate of one single atom in the contact [sec^{-1}]
η_diss	damping rate of the dynamic mass [sec^{-1}]
μ	macroscopic friction coefficient
ξ	Gaussian distributed random noise term
σ_F	standard deviation of the random force
ω_at	typical (angular) frequency for vibrations of an atom in the tip
ω_d	(angular) eigenfrequency for vibrations of the dynamic mass