Synthetic Atomic Force Microscope Data

Introduction

Throughout numerous fields, most especially within biomaterials, nanotechnology and solid state physics, atomic force microscopes are used to create three-dimensional images of samples. These particular microscopes can be used to deduce various properties of the sample material [1] – at nanoscale – with incredible accuracy.

However, these microscopes must be calibrated correctly in order to operate as expected. Currently, the calibration process is somewhat unsystematic and requires a great deal of determination to master.

In this research, various Python code blocks have been written in order to:
- Calculate the surface-tip separation force from the '12-6' Lennard-Jones potential;
- Plot the surface-tip separation force vs. the separation of the tip from the surface;
- Calculate the numerical integrals representing the frequency shifts in z;
- Plot projections of frequency shifts as a result of the cantilever motion.

Methodology

To establish the motion of the cantilever clearly, the first point to note was that the cantilever acts as a simple harmonic oscillator. By definition then, the cantilever obeys Hooke's law ($F_{spr.} = -kx$) – that is, the cantilever can be modelled simply as a spring.

In order to further simplify the model initially, we assume no other forces other than that from the surface-tip interaction act on the cantilever. To find this force, we use the '12-6' Lennard-Jones potential

$$U_{LJ}(z) = -4\varepsilon\left[\left(\frac{\sigma}{z}\right)^{12} - \left(\frac{\sigma}{z}\right)^{6}\right] \qquad [2]$$

and differentiate with respect to z. Taking the negative of this derivative finds the surface-tip interaction force by definition of potential energy,

$$F_{LJ}(z) = \frac{24\epsilon\sigma^6}{z^7} - \frac{48\epsilon\sigma^{12}}{z^{13}}$$

where the positive and negative terms represent the repulsive and attractive regimes of the force respectively.

To obtain a more realistic plot, the above force can be summed with another force derived from the surface energy of a (periodic) crystalline surface. Using the sample force,

$$F_{sur.}(z) = e^{-az}[\cos(bx) + \cos(by)] \qquad \text{with } a, b \in \mathbb{R}$$

we can obtain a sample plot (see Fig. 1). However, any force could be used instead of the above.

Now the model is well-established, we calculate the frequency shifts and plot the projections of contour maps.

The oscillations of the cantilever are forced – driven by an excitation signal – which can be described by the second-order differential equation

$$\ddot{z} + \frac{{\omega_0}^2}{k}\alpha\dot{z} + {\omega_0}^2 z - \frac{{\omega_0}^2}{k}F(z+h) = \frac{{\omega_0}^2}{k}F_{ext.} \qquad [3]$$

This can be simplified, since the external forces can be assumed to cancel any damping. The simplified differential equation is solved using a Fourier series for z, producing a system of non-linear equations solvable by the Newton-Raphson method. The final result is an integral, describing the frequency shifts from the cantilever oscillations as below

$$\Omega^{\,2} = 1 - \frac{1}{\pi k A_1}\int_0^{2\pi} F(z+h)\cos(\tau)\,d\tau \qquad [3][4]$$

with k being the spring constant; A_1 the amplitude of the driven oscillation. By re-writing the force in terms of cosine ($z = h - A_1\cos(\tau)$) , it is possible to compute the frequency shifts, iterated over some range of z (over different distances of separation).

Using contours, simulating the cantilever tip in a straight path back and forth from the surface, as well as across the surface, it is possible to plot these shifts (see Fig. 2 & 3).

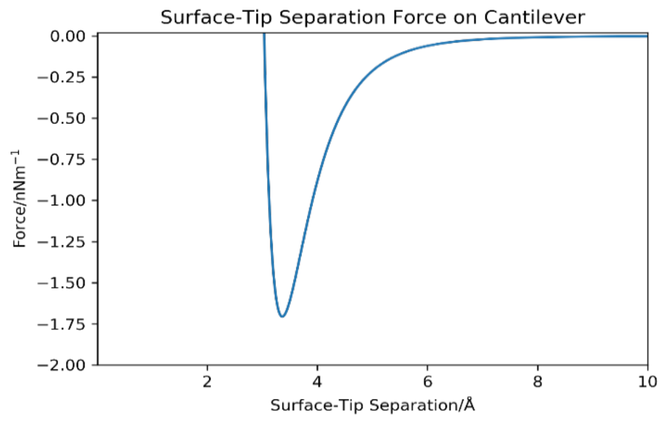

Figure 1: A graph of the separation-dependent force acting on the cantilever from some crystalline surface, along with the force from the Lennard-Jones potential.

Results

In Fig. 1 (above), we see that at very small distances, the force acting on the cantilever tip becomes greatly attractive – at the point of 'contact', the surface force becomes greatly repulsive before decreasing exponentially as the separation increases.

Computation shows us as the height separation of the tip from the (atoms constituting the) surface increases, the frequency shift decreases (as the cantilever tip enters the exponential repulsive regime). However, in Fig. 3 (below), the frequencies shift unexpectedly.

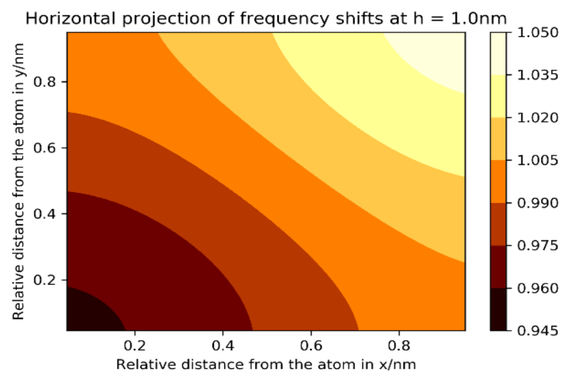

Figure 2: Contour map. Moving linearly relative from one atom constituting the sample surface. The frequency shift from that specific atom changes proportional to the displacement of the cantilever tip relative to the atom (as expected).

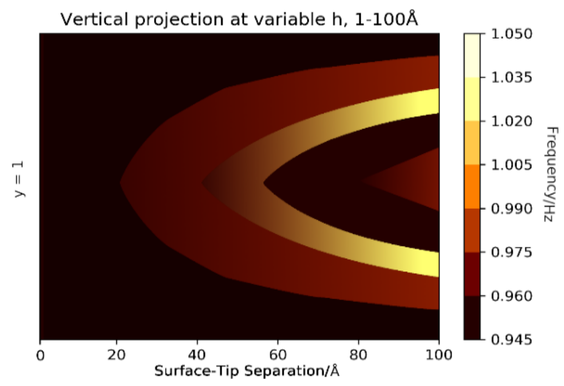

Figure 3: Contour map. As the repulsive regime is entered, due to the nature of this particular crystalline surface, the frequencies alternatively shift every 20 Ångströms, increasing and then decreasing over this period.

Conclusion

Through computation and concise code blocks, the methodology provides a framework for more consistent calibration methods of atomic force microscope cantilevers. The method could be extended further to utilise a neural network, which can machine-learn the required calibration for specific cantilever tips depending on the frequency shifts obtained from the simulated motion.

References

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