Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information to

General interpretation and theory of apparent height in dynamic atomic force microscopy

Chia-Yun Lai, Sergio Santos, Matteo Chiesa

Laboratory for Energy and NanoScience (LENS), Institute Center for Future Energy (iFES), Masdar Institute of Science and Technology, Abu Dhabi, UAE

A. Equation of motion

In AM AFM the equation of motion can be written as

$$\frac{k}{\omega_0^2}\ddot{z}(t)+\frac{k}{Q\omega_0}\dot{z}(t)+kz=F_0\cos(\omega t)+F_{ts} \tag{S1}$$

where higher flexural modes of oscillation are ignored, z is the instantaneous tip position, k is the spring constant, Q is the Q factor due to dissipation with the medium, ω_0 is the angular natural frequency, the effective mass is $m=k/(\omega_0)^2$, ω is the angular drive frequency and F_0 is the magnitude of the driving force (typically $\omega=\omega_0$).

B. Tip displacement

The general response z can be written as a Fourier series as

$$z(t)=z_0+A\cos(\omega t-\phi)+O(\varepsilon) \tag{S2}$$

where z_0 is the mean cantilever deflection.

C. Transfer function

By neglecting higher harmonics O(ε) and by first multiplying (1) by z(t) and its derivative ż(t) and by then integrating over a cycle one arrives to the transfer function[1-3]

$$A_r = \frac{1/Q}{\sqrt{\left(-2\frac{V}{kA}\right)^2 + \left(\frac{1}{Q} + \frac{E_{ts}}{\pi k A^2}\right)^2}} \qquad \text{(S3)}$$

where $A_r = A/A_0$ is the normalized amplitude, A_0 is the free oscillation amplitude, V stands for Virial ($V = \langle F_{ts} \times z \rangle$) and E_{ts} stands for the energy dissipated per cycle in the interaction. From (S3) it follows that V and E_{ts} control A_r. The terms E_{ts} and V are defined as

$$E_{ts}(z_c) = \oint F_{ts}\,\dot{z}\,dt \approx \frac{\pi k A(z_c) A_0}{Q}\left[\sin\phi(z_c) - \frac{A(z_c)}{A_0}\right] \qquad \text{(S4)}$$

$$V_{sur}(z_c) = \frac{1}{T} = \oint F_{ts} z dt \approx -\frac{kA(z_c)A_0}{2Q}\cos\phi(z_c) \qquad \text{(S5)}$$

where z_c is the cantilever separation.

D. The virial

In the absence of the sample the virial of (5) gives (accounting for z_0 and the fundamental frequency)

$$V_{sur}(z_c) \approx \frac{R_t H_{sur}}{6A}\left[\left(\frac{z_c}{A}\right)^2 - 1\right]^{-3/2}\left[1 - \frac{z_c z_0}{A^2}\right] \quad \text{(S6)}$$

where R_t is the radius of the tip and H_{sur} is the Hamaker of the tip-surface system. Then, from (S5) and (S6)[1]

$$z_c \approx A\left(D\left[1 - \frac{z_c z_0}{A^2}\right]^{2/3} + 1\right)^{1/2} \quad \text{(S7)}$$

where

$$D = \sqrt[3]{\frac{\left(\frac{Q R_{tip} H}{3 k A_0^3}\right)^2}{\left(A_r^4 - A_r^6\right)}} \quad \text{(S8)}$$

The resulting net virial from (9) accounting from the net interaction in the presence of the sample, i.e. $V_{sur\text{-}sam}(z^*_c, h) = V_{sur}(z^*_c, h) + V_{sam}(z^*_c)$, is

$$V_{sur-sam}(z_c^*, h) = \frac{R_t H_{sur}}{6A}\left[\left(\frac{z_c^* + h}{A}\right)^2 - 1\right]^{-3/2}\left[1 - \frac{(z_c^* + h) z_0}{A^2}\right] + \frac{R^* H_{sam}}{6A}\left[\left(\frac{z_c^*}{A}\right)^2 - 1\right]^{-3/2}\left[1 - \frac{z_c^* z_0}{A^2}\right] \quad \text{(S9)}$$

where $V_{sur}(z^*_c, h)$ accounts for the tip-supporting surface interaction and $V_{sam}(z^*_c)$ for the tip-sample interaction in the presence of the sample.

The result is that (S7) and (S9) are the expressions that together with the main constraint in (4) give place to the two separations that can be employed to compute the error in apparent height when the mean deflection cannot be neglected, for example in liquid environments and/or where samples or surfaces are very compliant[4].

Reference

1. A. S. Paulo and R. Garcia, Physical Review B **64**, 193411-193414 (2001).
2. J. P. Cleveland, B. Anczykowski, A. E. Schmid and V. B. Elings, Applied Physics Letters **72** (20), 2613-2615 (1998).
3. J. R. Lozano and R. Garcia, Physical Review Letters **100**, 076102-076105 (2008).
4. A. Raman, S. Trigueros, A. Cartagena, A. P. Z. Stevenson, M. Susilo, E. Nauman and S. A. Contera, Nature Nanotechnology **6**, 809–814 (2011).