Introduction to Nanotechnology (2013-2014)

Practical session: Theoretical simulations for the STM and the AFM

Short Theoretical Introduction

The most general expression for the current between tip and sample is:

$$I = \frac{4\pi e}{\hbar}\int_{-\infty}^{\infty} dE\ \mathrm{Tr}\big[\rho_{SS}(E)D^r_{SS}(E)t_{ST}\rho_{TT}(E-eV)D^a_{TT}(E-eV)t_{TS}\big]\times(f_T(E-eV)-f_S(E)) \tag{1}$$

where ρ_{TT},ρ_{SS} are the density of states for tip and sample, V the bias voltage, and $f_{S,T}$ the corresponding Fermi distributions. The terms D^a_{TT},D^r_{SS} are given by:

$$D^a_{TT}(E-eV) = [1-t_{TS}\ g^a_{SS}(E)\ t_{ST}\ g^a_{TT}(E-eV)]^{-1} \tag{2}$$

$$D^r_{SS}(E) = [1-t_{ST}\ g^r_{TT}(E-eV)\ t_{TS}\ g^r_{SS}(E)]^{-1} \tag{3}$$

These denominators $D^r_{SS}(E)$, $D^r_{TT}(E)$ include the multiple scattering effects and are responsible for the saturation of the current at short distances. In fact, we can define $\tilde{t}_{TS} = D^a_{TT}t_{TS}$ as effective hoppings, that are renormalized by the inclusion of the multiple scattering effects.

$$\tilde{t}_{TS} = \frac{t_{TS}}{1-t_{TS}\ g^a_{SS}\ t_{ST}\ g^a_{TT}} = t_{TS}+t_{TS}\ g^a_{SS}\ t_{ST}\ g^a_{TT}\ t_{TS}+\cdots \tag{4}$$

The influence of the temperature (included in the Fermi distributions) can be neglected for most metallic systems. Taking the limit $T\to 0\ K$:

$$I = \frac{4\pi e}{\hbar}\int_{0}^{eV} dE\ \mathrm{Tr}\big[\rho_{SS}(E)D^r_{SS}(E)t_{ST}\rho_{TT}(E-eV)D^a_{TT}(E-eV)t_{TS}\big]. \tag{5}$$

Considering the limit of small bias voltages, and assuming that the tip-sample distance is large enough to neglect the multiple scattering terms, the current is described by:

$$I = \frac{4\pi e}{\hbar}eV\ \mathrm{Tr}\big[\rho_{SS}(E_F)t_{ST}\rho_{TT}(E_F-eV)t_{TS}\big] \longrightarrow_{V\to 0} \frac{4\pi e^2}{\hbar}V\ \mathrm{Tr}\big[\rho_{SS}(E_F)t_{ST}\rho_{TT}(E_F)t_{TS}\big] \tag{6}$$

and the expression for the conductance, $G=\frac{dI}{dV}$, is:

$$G = \frac{dI}{dV} = \frac{4\pi e^2}{\hbar}\ \mathrm{Tr}\big[\rho_{SS}(E_F)t_{ST}\rho_{TT}(E_F)t_{TS}\big] \tag{7}$$

Approximate study of the tunneling currents and forces

1. Write a program to calculate the conductance dI/dV between a tip (initially including just a single atom) and a (100) surface of an FCC metal with a lattice parameter of 4 Å(represented initially by a single plane with the right periodicity and symmetry), summing up the contributions from the different atoms in the surface. We assume that there is only an *s* orbital in both tip and sample that contributes to the tunneling. The metal work function is 5 eV. Suppose that the multiple scattering effects can be neglected.

   a) What should the distance dependence of the tip-sample hoppings be in order to make sure that the conductance (or the current) have the expected distance decay?. Show that $T_{ss}(d)\propto\frac{1}{d}e^{-d\sqrt{2\Phi}}$ in order to fulfill $I\propto e^{-2d\sqrt{2\Phi}}$ (all the expressions are in atomic units).

   b) Assume, to begin with, that the tip is on top of one of the surface atoms and study the convergence as a function of the distance to the farthest surface atoms included in the calculation of the current.
   In order to get realistic values for the current, normalize the hoppings such that the conductance for a tip-sample distance equal to the interplane spacing in the (100) direction is equal to the quantum of conductance $G_0 = 2e^2/h$.

   c) Plot the conductance (in units of $2e^2/h$) as a function of distance when the tip is on top and hollow positions.

2. Generalize the program to simulate STM images at constant height and constant current.

   a) Study the conductance along two different symmetry directions (*top-hollow-top*, *top-bridge-top*) for tip heights between 10 and 2 Å. Could you resolve the atoms?. How is the corrugation changing with the tip-sample distance?.

   b) Calculate constant–current images for conductances equal to 0.1 G_0 y 0.01 G_0. (You should start the study with line profiles along the symmetry directions in order to check that the code is working and then move on to calculate the 2D image).

   c) Include the multiple *scattering* effects in the conductance-distance and corrugation-distance curves assuming that:

$$I = \frac{4e^2}{\pi\hbar} V \frac{x}{(1+x)^2} \quad \text{con} \quad \mathrm{x} = \pi^2 \mathrm{Tr}\left[\rho_{\mathrm{SS}}(\mathrm{E_F})\mathrm{t_{ST}}\rho_{\mathrm{TT}}(\mathrm{E_F})\mathrm{t_{TS}}\right] \tag{8}$$

   At what distance are these effects relevant?

3. Re-write the STM program to simulate AFM images. Assume that the tip-sample interaction has (1) a long-range van der Waals contribution described by a sphere-plane model $F = -AR/6D^2$ with D distance between the border of the sphere and the surface, $R = 10$ nm and $A = 2 \times 10^{-19}$ J; and (2) a short-range chemical contribution described by a Morse Potential:

$$V(r) = V_0 \left[\left(1 - \exp[-2b\frac{r - R_c}{R_c}] \right)^2 - 1 \right] \quad , \tag{9}$$

   with r interatomic distance , $\mathrm{V_0} = 2{,}273$ eV, $b = 1{,}497$ and $\mathrm{R}_c = 2{,}357$ Å.

   Perform an study analogous to the one done for the STM:

   a) Calculate force-distance curves when the tip is on the *top* and *hollow* positions. At what distance do you find the maximum of the force F_{max}?.

   b) Calculate the force along the two symmetry directions as a function of the tip height (tip-sample distance). How is the corrugation changing with distance?. Are you achiving atomic resolution?. At what distance?.

   c) Analize how the corrugation changes when you include or not the long-range contribution. What happens if $R = 100$ nm?.

   d) Calculate AFM images at constant force equal to 0.1 F_{max} and 0.5 F_{max}.

4. (OPTIONAL) Combined calculation of forces and currents: Repeat the study for the STM and AFM including now the possible relaxation of the atoms on the tip and sample induced by the tip-sample interaction. Consider that the atoms are connected to their nearest neighbours by springs with elastic constant $k = 20$ N/m. What happens if $k = 5$ N/m?.