Lab work N4: Scanning tunneling microscope (STM)

During this practical you will study the Scanning Tunneling Microscope (STM) through two complementary approaches: simulation (using Nanonis) and practical (using the Nanosurf STM).

Based on the theoretical part of this text and on your STM lecture you must interpret the results obtained in both simulation and practical parts. Your report must contain at least the answers to all the parts marked by the following symbol: 

Theoretical part:

The functioning of the scanning tunnelling microscope (STM) is based on the tunnel effect established between a conductive tip and a conductive surface (Fig. 1a).

In first approximation, the tunnel effect of the STM can be simply described by the transmission of electrons through a potential barrier of width z and of height W as shown in Fig. 1 (b).

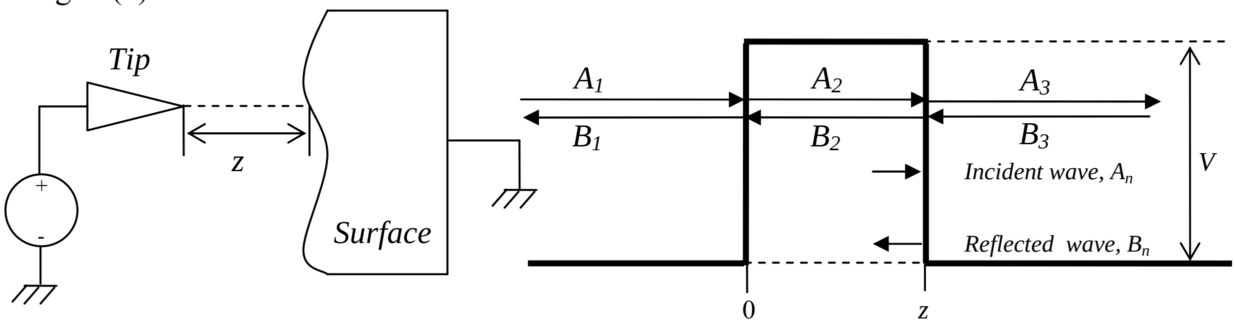


Figure 1: (a) Sketch of the STM system (b) First approximation model of the STM system

The 1D Schrödinger equation for this system $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+W\right)\psi(x)=E\psi(x)$ gives for each of the three zones, wave functions of the form:

$$\psi_n(x)=A_n e^{ik_n x}+B_n e^{-ik_n x}, k_n=\frac{1}{\hbar}\sqrt{2m(E-W_n)},$$

with k_n the wave-vector in the n zone and Wn is the potential value in the region n.

We consider that the B_3 coefficient is zero (the particle is coming from the left, $x=-\infty$). The boundary conditions in $x=0$ and in $x=z$ are the continuity of the wave-function and of its derivative.

In the case $E<W$ (tunnel effect), the analytical expression of the transmission coefficient is given by:

$$T(E)=\left|\frac{A_3}{A_1}\right|^2=\frac{4E(W-E)}{4E(W-E)+W^2\sinh^2\left(\frac{\sqrt{2m(W-E)}}{\hbar}\cdot z\right)}$$

1. Approximate the form T(E) for $z >> \dfrac{\hbar}{\sqrt{2m(W-E)}}$.
2. We can affirm that $I \propto T(E)$ in the approximation of single energy transport. Assuming a value of V-E of 4eV, calculate the variation of the current if the distance, *z*, decreases of 1Å. Use the approximated formula in 1.

In the mid-1980s, Tersoff and Hamann described theoretically the tunnel effect in a STM: the tunneling current is the result of a sum over all possible transitions between the tip and the sample[1]:

$$I = \frac{4\pi e^2}{\hbar} V \rho_{sub}(E_F)\rho_{tip}(E_F)|M|^2$$

In this model, *M* represents the matrix of transition probability, $\rho_{sub}(E_F)$ and $\rho_{tip}(E_F)$ are the density of states (DOS) of the surface and tip near the Fermi level and *V* is the applied bias.

Assuming that only s-like wave functions contribute to the tunnelling from the tip with radius R, the DOS of the tip near the Fermi level can be represented by:

$$\rho_{tip}(E_F) \propto |\Psi_n|^2 \propto e^{-2k(R+z))}$$

Where *z* is the distance from tip to sample and *k* is the inverse decay length given by[2]:

$$k = \sqrt{\frac{2m}{\hbar^2}\frac{\phi_{tip}+\phi_{sub}}{2} - E + \frac{eV}{2}}$$

(Assumption: only electron states near the Γ point of the Brillouin zone contribute to the tunnelling.)

Because the STM tip is usually a metal, the DOS of the tip can be assumed to be featureless. For illustrative purposes, we can write an approximate expression for the tunneling current as:

$$I \propto \int_0^{eV} \rho_{sub}(E) T(E,eV)\, dE$$

with $T(E,eV) = e^{-2kz}$ is the transmission probability of the electron.

All these theoretical considerations are correct when the applied voltage is negligible with respect to the work function. In high voltage configuration, the tip influences the wave function of the sample surface; the energy levels of electrons will be directly dependent on the applied potential and the current dependence is:

$$I = \alpha V + \beta V^3$$

[1] H.J.W. Zandvliet and A. van Houselt, Scanning Tunneling Spectroscopy; Annual Review of Analytical Chemistry 2009; pp 37-55.

[2] $(\Phi_{tip} + \Phi_{sub})/2$ represent the barrier height in this case.

Part I: Simulation of STM function using Nanonis simulator

This part will be performed using the documents describing the Nanonis simulator.

1. Approach the tip to the surface.
In the z-controller menu, increase the gains and explain the effect induced on the measured current.

2. Bring the gain values to the initial values (P ~ 200pm and I ~ 200nm/s).
In the scan control menu, start a scan on the surface (the surface under study is a Si (111) 7x7 reconstructed surface). Describe the obtained image.
In the tools menu, follow the evolution of a line during the scan measurement (line scan monitor A). Explain the observed topography of the surface. Correct the problem and scan the surface again.

3. Using the "Experiments" menu, start a bias spectroscopy.
Trace I(V) for different intervals of voltage. You should be able to observe two regimes. Explain the origin of the two regimes.

Start a z-spectroscopy measurement.
Explain the shape of the curve and its different regimes.

Part II: Experimental work

The experimental work done during this practical has three parts: large-area scan, reaching the atomic resolution and spectroscopy. You will realise each part using the EasyScan document present in the lab room. The scientific article in the lab room should help you to interpret the images obtained[3].

1. Large-area image

Approach the tip to the surface. Scan a large area surface (~ 200nm by 200 nm).
Measure the height of the step present in the image.
Compare the step height with the vertical distance between two consecutive atomic layers (334.8 pm for graphite).

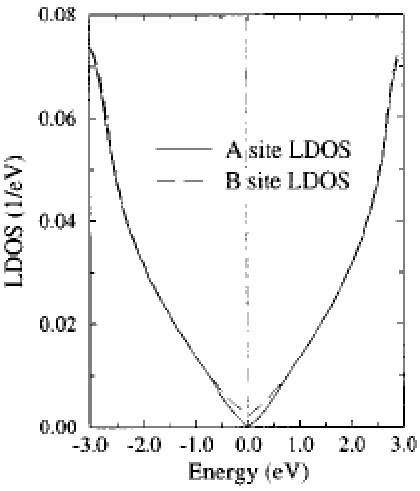
2. Atomic resolution

Decrease slowly the scan size in order to reach the atomic resolution.
Using the article available in the lab, describe the observed cell (lattice type), measure the lattice parameters and angles directly on your image. Explain the contrast obtained in the STM image.

3. Spectroscopy

Realize I(z) measurements for some values of applied voltage.
Give a method to estimate the work function for graphite. Compare your value with the theoretical value (4.5 – 4.7 *eV*). Give some elements that could explain the difference.

Trace I(V) curves.
Based on the obtained curves, explain the electrical behaviour of graphite (metallic...).
Using the figure below[4], explain the shape of your experimental I(V) curves.



[3] S. Hembacher, F.J. Giessibl, J. Mannhart and C.F. Quarte, Revealing the hidden atom in graphite by low-temperature atomic force microscopy; PNAS 2003; vol. 100, issue 22, pp 12539-12542.
[4] B.A. McKinnon and T.C. Choy, Electronic effects in scanning tunneling microscopy of graphite: A Green's function calculation based on the tight-binding model; Physical Review B 1996; vol. 54, issue 16, pp. 11777-11785.