Scanning tunneling microscopy

Objective: to explain the basic operational principles of Scanning Tunneling Microscopy (STM) and the types of measurements that can be performed with it. To achieve this, the module reviews quantum mechanical tunneling through potential barriers and the behavior of tunneling current in different voltage regimes. It also includes modeling of the scanning process and manipulation of real STM data to help students understand how STM images are generated and used to analyze atomic-scale surface features.

Activity with the interface
https://qtechedu.centralesupelec.fr/EN/ex5.html

1. The **Introduction** presents the concept of Scanning Tunneling Microscopy (STM), highlighting the quantum-mechanical phenomenon phenomenon it is based on, and briefly describing its main operational modes and potential areas of application. Please answer the following questions to summarize the key concepts covered in this section.

(1) What quantum mechanical phenomenon underlies the operating principles of STM?

(2) Describe the main components of an STM setup and explain its basic operating principle.

(3) Briefly describe the operational modes of STM. What type of information about the sample can be obtained in each mode?

(4) Explain the difference between constant-current and constant-height modes in STM:

- Which mode is safer for imaging rough surfaces;
- Which mode offers faster scanning over atomically flat regions? Explain your reasoning.

(5) Describe $I(V)$ - spectroscopy in STM:

- What information about the local electronic structure can you obtain from the shape of the I(V) curve?
- Sketch the expected I(V) and dI/dV(V) curves, and explain how you would identify the local density of states peak.

!!! *By default the materials for tip is platinum and for sample – carbon. The work function data for other materials can be found at the end of lab reports**.

2. The paragraph "**Tunneling a Single Particle Through a One-Dimensional Potential Barrier**" focuses on the quantum mechanical phenomenon that underlies the operation of the Scanning Tunneling Microscope.

If you need to adjust the parameters of the barrier or the particle use the data input box and click the "Run Calculation" button for recalculation. To return to the default settings, use the "Reset to Default" button.

(1) What is quantum tunneling, and how does it differ from classical particle behavior? The answer can be supported by schematic drawing.

(2) Explain why electron tunneling can occur even if the electron's energy is less than the height of the potential barrier.

(3) Write the solution of the Schrödinger equation for a particle (electron) in three regions (before, within, and after a rectangular potential barrier), assuming the particle's energy is less than the barrier height ($E<U$). To obtain the values of the coefficient A, B, C, D, which correspond to the wave function components in the regions before, within, and after the barrier, use the graphic interface and the following parameters:

(a) U = 1 eV, E = U/2, d = 10 A;

(b) U = 1 eV, E = 0,8 eV, d = 5 A;

(c) U = 2 eV, E = U/2, d = 10 A;

(4) Write the formula for tunneling probability through a one-dimensional rectangular potential barrier for the following cases: $E<U$, $E=U$, $E>U$. Describe the behavior of the particle in each scenario.

(5) Plot in graphical interface the transmission probability $T(E)$ as a function of electron energy E, ranging from below to above the barrier height U, assuming fixed barrier parameters (d = 1.5 nm, U = 1 eV). Discuss the transition from quantum tunneling (when $E<U$) to classical transmission (when $E>U$).

(6) Calculate the tunneling probability T for particles with energies E_1 = 0.5 eV and E_2 = 2 eV, using the corresponding expression from the graphical interface.

(7) Analyze how changing the barrier width d or the potential height U affects the tunneling probability and the spatial decay of the wave function, assuming constant particle energy E = *1*.5 eV:

Part A: Plot the dependence of the transmission probability T on the barrier width d, for a fixed barrier height U=2eV, and the given particle energy E

Part B: For fixed particle energy E and the barrier width constant d = 0.6 nm, compute and plot the transmission probability T as a function of barrier height.

Part C: How does the spatial decay of the wavefunction inside the barrier change with increasing barrier width d? How does this relate to a transmission probability? Illustrate your answer by plotting the real part of ψ(x) as a function of position for both cases.

3. In the paragraph **"Tunneling current density in a metal-insulator-metal system,"** the calculation of the tunnel current density as a function of the applied bias voltage is proposed. This allows modeling the operation of the Scanning Tunneling Microscope in spectroscopy mode, where the tunneling current is monitored as a function of the voltage V (at z-const). The sensitivity of the STM method will also be investigated.

The voltage range for current density calculations is selected via the interface.

(1) Examine how the tunnel current density depends on the applied voltage. What key parameters influence the current and how can the tunneling behavior be characterized in each voltage range?

(2) Using the interface, determine the $I(V)$ characteristics for the selected tip–surface pair.

(3) Based on the tunneling current expression valid in the low-voltage regime, estimate the dependence of the current on the tip–surface distance. Use the graphical interface to evaluate the vertical sensitivity for selected work function and barrier parameters.

(4) In STM, the tunneling current I varies with tip-sample distance d as: $I \propto e^{-2\kappa d}$. If $\kappa = 10^{10} m^{-1}$, by what factor does the tunneling current change if the tip retracts by 0.1 nm?

(5) Which parameters of a scanning tunneling microscope influence its lateral sensitivity? Provide a justification for each identified parameter.

(6) Estimate energy resolution of STM in spectroscopy mode. Using interface simulate the $I(V)$ curves and than calculate the differential conductance dI/dV as a function of bias and estimate the energy resolution based on the smallest detectable changes in the conductance curve.

4. In the **conclusion**, discuss the potential applications of Scanning Tunneling Microscopy and its prospects for future development.

(1) Review the examples of STM applications presented in the section "**Some Aspects of STM Applications**." For each of them, identify the mode(s) of STM operation used. Additionally, provide your own examples of STM applications, specifying the operational modes involved. Don't forget to provide appropriate citations for any external information used.

(2) List the promising areas for the development of Scanning Tunneling Microscopy (STM). For selected area provide a detailed description of its significance, challenges, and potential impact.

(3) Discuss how STM has contributed to the study of surface physics and chemistry.

(4) What are the main advantages and limitations of Scanning Tunneling Microscopy.

(5) An STM is used to scan a carbon surface (graphite) using a tungsten tip. The surface exhibits a narrow peak in the density of states at the Fermi level.

Part A. Calculate the tunneling decay constant κ (in m^{-1}) at room temperature, assuming the effective barrier height is given by the average work function of the tip and sample.

Part B. Estimate by what factor the tunneling current changes if the STM tip is moved 0.1 nm closer to the sample.

Part C. Discuss qualitatively how would the **measured *dI/dV* spectrum** change when the temperature is increased?

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* Work functions of elements.

Material	Ag	Al	Au	Si	Cu	Li	Pb	Cr	Graphite	W	Pt
Work Function (eV)	4.26	4.06	5.1	4.60	4.65	2.9	4.25	4.5	4.6	4.32	5.3