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Application Notes

"Observed" Physical Quantities in STM

Current-Voltage Characteristic

Measurement of relation between tunneling current and probe-sample voltage is carried out in $J(V)$ spectroscopy mode. The $J(V)$ spectroscopy is based on the dependence of tunneling current on number of electron states *N*, forming a tunneling contact of conductors, in the energy range from the Fermi level μ to $\mu - eV$ (Fig. 1), which at $T = 0$ gives (see (7) in chapter "John G. Simmons Formula")

$$J \infty N = \int_{\mu - eV}^{\mu} \xi(E_z) dE_z \qquad (1)$$

Thus the tunneling current dependence *J(V)* at constant tip-sample separation δ_z represents an allocation of torn bonds as well as other electron states corresponding different energies, i.e. energy band structure of either tip or surface. Function $\xi(E_z)$, which was introduced in (6) of chapter "John G. Simmons Formula", depends on electron state density of phase space plane which is normal to tunneling direction at given E_z.

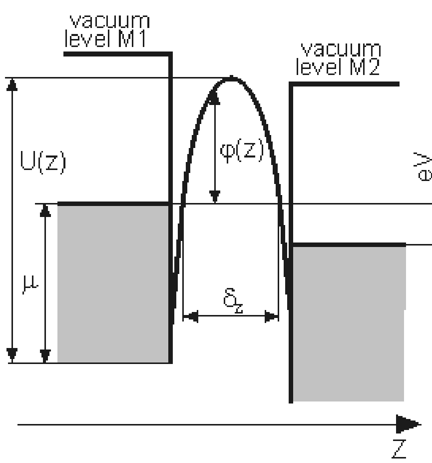

Fig. 1. Model of MIM system with an arbitrary shape potential barrier. Positive potential is applied to the right metal

Using expression (1) and $J(V)$ curve at constant tip-sample separation δ_z, it is possible to compute the density of electronic states:

$$\frac{dJ}{d(eV)} \infty \xi(\mu - eV) \qquad (2)$$

Thus, inspection of $J(V)$ and its derivative $dJ/d(eV)$ curves allows to investigate energy levels distribution with atomic resolution. It is possible to determine a conductivity type, in particular for semiconductors – to detect the valence band, conductivity band and impurity band. [1]–[3].

According to (2) and (3) from chapter "John G. Simmons Formula in a Case of Small, Intermediate and High Voltage (Field Emission Mode)" tunneling conductivity $G = dJ/dV$ does not depend on applied voltage *V* in case $eV << \bar{\phi}$.

$$G = \frac{\gamma\sqrt{\bar{\phi}}}{\delta_z} \exp\left(-A\delta_z\sqrt{\bar{\phi}}\right) \qquad (3)$$

at $eV < \phi_2$ relation between *G* and *V* is parabolic

$$G \approx \gamma\sqrt{\bar{\phi}} \exp\left(-A\sqrt{\bar{\phi}}\right)\left(1 + 3\sigma V^2\right) \qquad (4)$$

On Fig. 2, 3 experimental dependences *J(V)*, *G(V)*, which were measured for Pt and HOPG samples and Pt-Ro probe using STM Solver P47, is shown. Experimental data are in good agreement with the theoretical predictions (1)–(4).

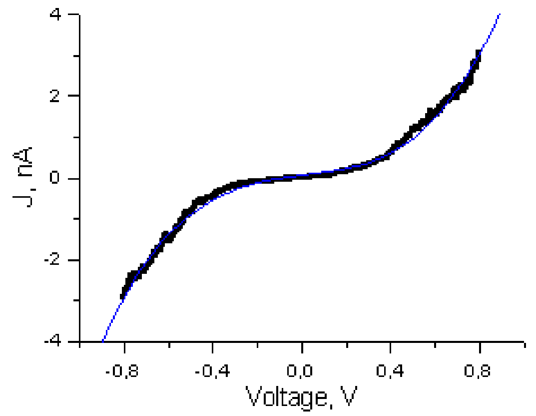

Fig. 1a. Experimental (points) and theoretical (solid line) dependences *J(V)* for Pt

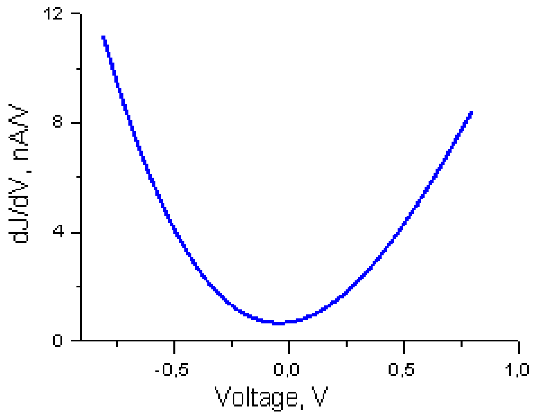

Fig. 1b. Experimental dependence *G(V)* for Pt

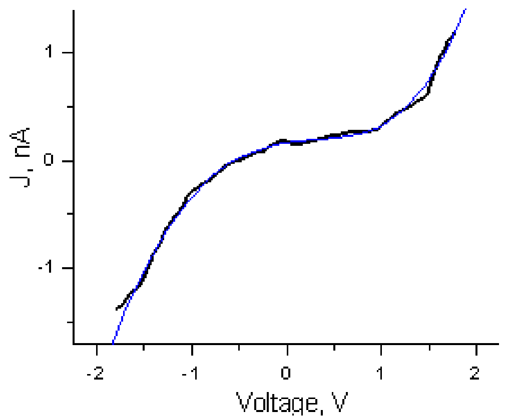

Fig. 2a. Experimental (points) and theoretical (solid line) dependences *J(V)* for HOPG

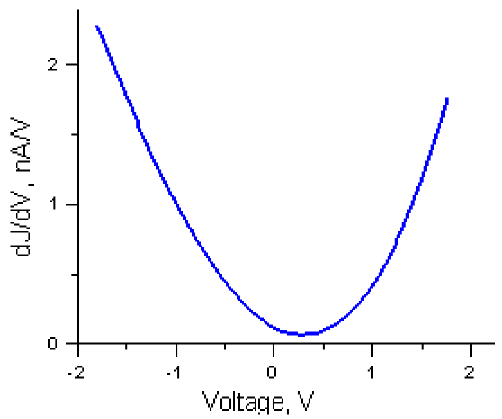

Fig. 2b. Experimental dependence *G(V)* for HOPG

Summary

- Tunneling current-voltage characteristic represents number of electron states and their distribution in energy spectrum of electrodes which creates tunneling contact.
- Differential conduction G is proportional an electron state density. For metals at low voltages G does not depend on applied voltage (3). At intermediate voltages the relation between G and applied voltage is parabolic (4).
- Experimantal current-voltage and differential characteristic are in good agreement with theory.

References

1. G. Binnig., H. Rohrer. Scanning tunneling microscopy. Helv. Phys. Acta. - 1982, - V. 55 726.
2. A. Burshtein, S. Lundquist. Tunneling phenomena in solid bodies. Mir, 1973 (in Russian).
3. E. Wolf. Electron tunneling spectroscopy principles. Kiev: "Naukova Dumka", 1990, 454 p. (in Russian).

Current-Distance Characteristic

Measurement of relation between tunneling current and tip-sample distance is carried out in $I(\delta_z)$ spectroscopy mode. According to (11) from chapter "John G. Simmons Formula", in absence of a condensate, a typical current-height relation is an exponential current decay (Fig. 1) with a characteristic length of a few angstrom [1], [2].

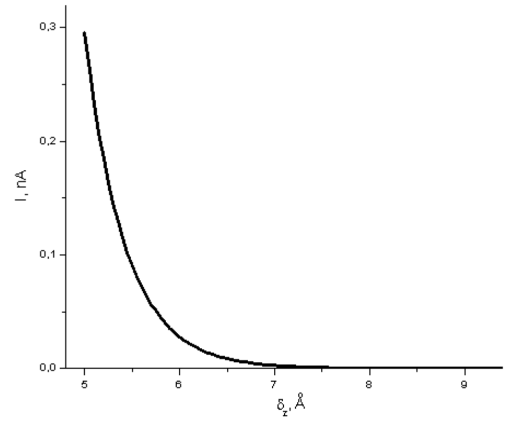

Fig. 1. Theretical $I(\delta_z)$ curve for Pt sample and Pt-Ro probe

Inspecting an experimental $I(\delta_z)$ curve, it is possible to estimate the potential barrier height $\overline{\phi}$. If tip-sample bias V is small enough, then according to [chapter "John G. Simmons Formula in a Case of Small, Intermediate and High Voltage (Field Emission Mode)"](), tunneling current can be written as

$$I = \frac{\gamma S \sqrt{\bar{\phi}} V}{\delta_z} \exp\left(- A\delta_z \sqrt{\bar{\phi}}\right) \qquad (1)$$

where $\gamma = \frac{e\sqrt{2m}}{4\beta\pi^2\hbar^2}$, $A = 2\beta\sqrt{\frac{2m}{\hbar^2}}$, S – contact area, m – free electron mass, e – elementary charge, $\hbar$ – Planck's constant.

From (1) $\bar{\phi}$ can be expressed through some analytical function of $d\ln(I)/d\delta_z$. Finding the natural logarithm of (1) and differentiate the result by δ_z one can obtain

$$\frac{d\ln(I)}{d\delta_z} = -\frac{1}{\delta_z} - A\sqrt{\bar{\phi}} \qquad (2)$$

If $\delta_z >> 1/A\sqrt{\bar{\phi}}$, then $\bar{\phi}$ can be expressed from (2) by following way

$$\bar{\phi} = \frac{1}{A^2}\left(\frac{d\ln(I)}{d\delta_z}\right)^2 \approx 10^{-20}\left(\frac{d\ln(I)}{d\delta_z}\right)^2 eV \qquad (3)$$

where $d\ln(I)/d\delta_z$ is experessed in m^{-1}.

Emphasize, that in most cases the condition $\delta_z >> 1/A\sqrt{\bar{\phi}}$ realizes practically always. For instance, if $\bar{\phi} = 4eV$, then expression (3) will be correct at $\delta_z >> 0{,}5Å$.

Experimental $I(\delta_z)$ curve for Pt-flim which was measured using Pt-Ro probe in STM (Solver P47) on air, is shown on Fig. 2.

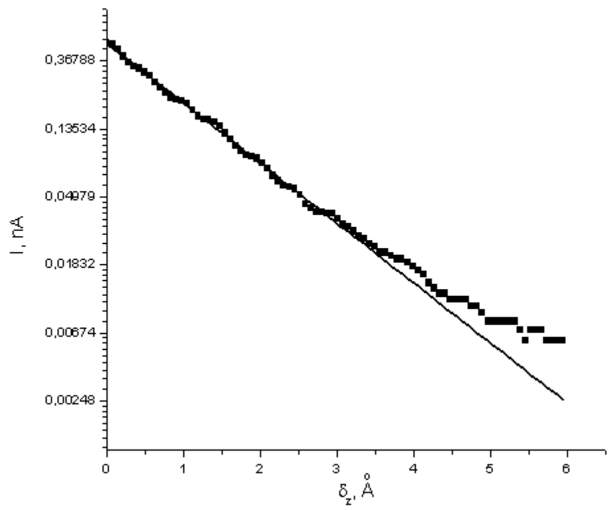

Fig. 2. Experimental $I(\delta_z)$ curve (semilogarithmic scale). Solid line – approximation $I = 0{,}47\exp(-10\delta_z/11)$.

Substituting value of approximated straight line slope $d\ln(I)/d\delta_z = -0{,}09nm^{-1}$ in (3), we obtain, that $\bar{\phi} \approx 0{,}8eV$. Theoretical value of $\bar{\phi}$, in case, then both electrodes are produced from Pt, equals $\bar{\phi} = 5{,}3eV$. Thus, experimental value of $\bar{\phi}$ is lower by a factor about 6 than theoretical one. Most probably, the main reason of this difference is condensate presence on electrodes surface. Even for fresh surfaces of pyrolitic graphite at maximum $d\ln(I)/d\delta_z$ values, the corresponding values of $\bar{\phi}$ are less than several tenths of eV. These values are deliberately less than those known from high vacuum and low temperature STM experiments for the same samples and tips [3]. Values of $\bar{\phi}$ derived from experiments in air are close to those obtained using STM configured for electrochemical measurements *in situ* when liquid polar medium exists between sample and tip [3]. A condensate in the STM operating in air is evidently the analogue of such a medium. Thus, the condensate occurence on the sample surface results in the STM image quality deterioration and values of $\bar{\phi}$ understatement.

Frequently $I(\delta_z)$ spectroscopy is used for a determination of tip quality (sharpness).
Experimental $I(\delta_z)$ curves, which are measured at investigation of HOPG surface using "good" and "poor" sharp tip of Pt-Ro probe, is shown on Fig. 3, 4.

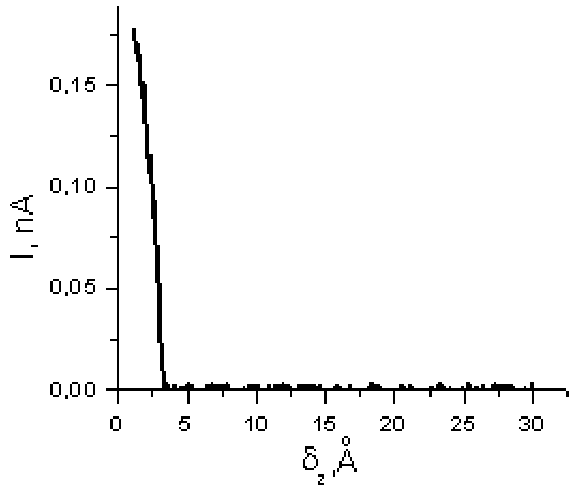

Fig. 3. $I(\delta_z)$ **spectroscopy for a "good-shape" STM tip**

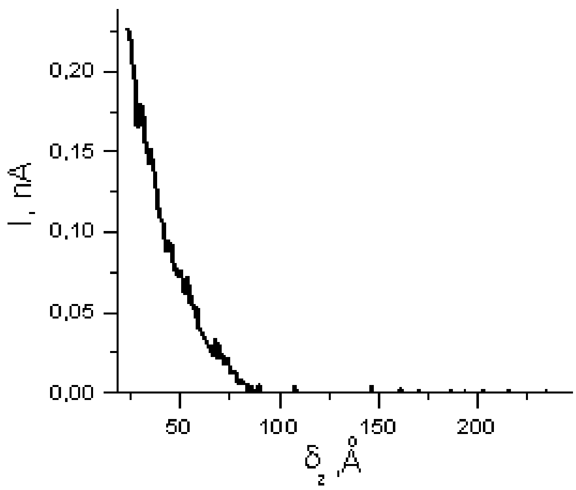

Fig. 4. $I(\delta_z)$ **spectroscopy for a "poor-shape" STM tip**

Tip quality criterion is following: 1) if tunneling current drops twice at tip-sample distance less than 3 Å, then tip quality is very good; 2) if this distance is about 10 Å, then atomic resolution can be still obtained on HOPG using such STM tip; 3) if the current drops at distance equals or more than 20 Å, then this STM tip should be replaced or sharpened [4].

Summary

- It is possible to estimate electron work-function of investigated material using $I(\delta_z)$ spectroscopy (3).
- The difference between experimental and table values of work-function is connected with the condensate presence on electrodes surface.
- In practice $I(\delta_z)$ curve is used for a determination of STM tip quality (sharpness).

Reference

1. John G. Simmons. J. Appl. Phys. – 1963. – V. 34 1793.
2. G. Binnig., H. Rohrer. Helv. Phys. Acta. – 1982, – V. 55 726.
3. S. Yu. Vasilev, A. V. Denisov. Journal of technical physics. – 2000, – vol. 70, num. 1 (in Russian).
4. NT-MDT. Solver P47 users guide.

Measurements of the Electronic States Density

In chapter Current-Voltage Characteristic we considered the spectroscopy of electronic states. Meanwhile, at given eV it is possible to measure the electronic states distribution across the sample surface.

The electronic states density distribution measurement is performed in parallel with surface topography imaging in the $J = const$ mode. Instead of constant tip bias V_0, the alternating voltage $V = V_0 + b\sin\omega t$ is applied between sample and tip, where $b\sin\omega t$ – the alternating signal having amplitude $b << V_0$ (Fig. 1). Then, the net tunneling current is proportional to the following

$$J \propto N_0 + N_{\approx} \qquad (1)$$

where $N_0 = \int_{\mu - eV_0}^{\mu} \xi(E_z)dE_z$

and $N_{\sim} = \xi(\mu - eV_0)eb\sin\omega t$.

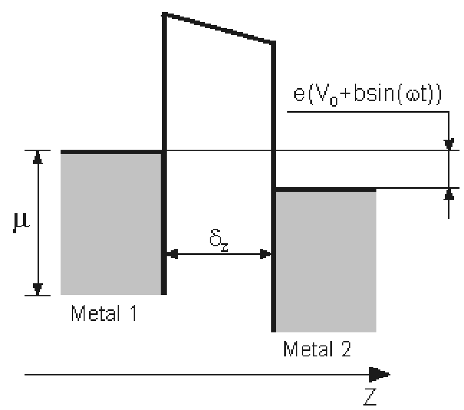

Fig. 1. Diagram of MIM system, when applied voltage is modulated as $V = V_0 + b\sin\omega t$

Thus, the total current flowing through the tunneling gap is equal to $J = J_0 + J_\sim$, where $J_\sim$ – alternating component. Because J_0 is held constant during the scan and $eb = const$, the alternating tunneling current amplitude is proportional to the electronic states density $\xi(\mu - eV_0)$. Hence, measuring the alternating current amplitude during scan allows for the mapping of the electronic states density in standard units. Since $b << V_0$, then $J_\sim / b$ is actually dJ/dV.

The frequency ω, as mentioned above, should be much more than the reciprocal feedback integrator time constant and be limited by maximum permissible scan frequency.

Summary

- Modulation of applied voltage V results in oscillations of tunneling current J. Amplitude of such oscillations depends on electron properties of electrodes, which create a tunneling contact.
- Using this method, it is possible to measure distribution of electron state density on investigated sample surface.

References

1. G. Binnig, H. Rohrer. Helv. Phys. Acta. – 1982, – V. 55 726.
2. A. Burshtein, S. Lundquist. Tunneling phenomena in solid bodies. Mir, 1973 (in Russian).
3. E. Wolf. Electron tunneling spectroscopy principles. Kiev: "Naukova Dumka", 1990, 454 p. (in Russian).

Work-Function Distribution Study

In chapter Current-Distance Characteristic we considered that it is possible to estimate average electron work-function of electrodes using current-distance experimental curves. However, these measurements give work-function values only in small region where one electrode is located over another. In STM there is another method which is able to measure distribution of work-function along all investigated sample surface.

The work function distribution measurement is performed in parallel with surface topography imaging in the $J = const$ mode. In this case, the Z-axis piezo tube motion is determined not only by the feedback signal but also by application of an alternating signal producing motion law $\Delta Z = a\cos(\omega t)$. Accordingly, the tip-sample separation is $\delta_z = \delta_{z0} + a\cos(\omega t)$, where parameter being $a << \delta_{z0}$, δ_{z0} – tip-sample separation held constant through the feedback, ω – Z-axis piezo tube resonant frequency (Fig. 1).

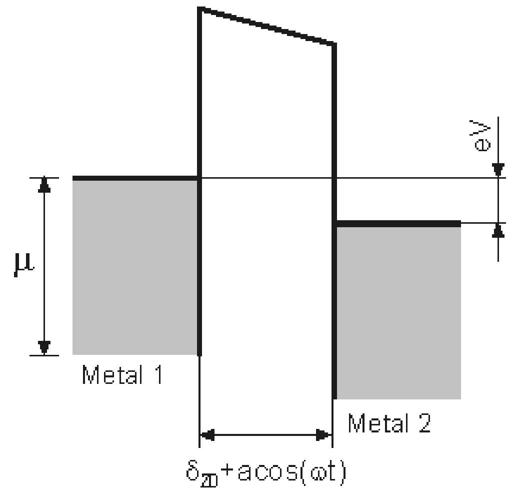

Fig. 1. Diagram of MIM system when tip-sample distance is modulated as $\delta_z = \delta_{z0} + a\cos(\omega t)$

If voltage applied between tip and sample is small $V \approx 0$, then according to designations introduced, expression (2) from chapter 1.2.2 can be transformed to the following

$$J = \frac{\gamma\sqrt{\bar{\phi}}V}{\delta_{z0} + a\cos(\omega t)}\exp\left(-A\sqrt{\bar{\phi}}\left(\delta_{z0} + a\cos(\omega t)\right)\right) \approx$$
$$\approx J_0\left[1 - A\sqrt{\bar{\phi}}\,a\cos(\omega t)\right] \qquad (1)$$

where $J_0 = J(\delta_{z0})$.

Thus, total current flowing through the tunneling gap in this case is equal to $J = J_0 + J_\sim$, where $J_\sim$ – alternating tunneling current. Because J_0 is held constant during the scan, the alternating tunneling current amplitude is proportional to the square root of the tip and the sample work function half-sum. Assuming that tip work function is constant during scanning, the $J_{\sim}$ amplitude will depend only on the studied surface work function.

The frequency ω, as mentioned above, should be much more than the reciprocal feedback integrator time constant and be limited by maximum permissible scan frequency.

Summary

- Modulation of tip-sample distance results in oscillations of tunneling current *J*.
- Using this method it is possible to measure the distribution of work-function along all investigated sample surface.

References

1. G. Binnig., H. Rohrer. Scanning tunneling microscopy. Helv. Phys. Acta. - 1982, - V. 55 726.
2. A. Burshtein, S. Lundquist. Tunneling phenomena in solid bodies. Mir, 1973 (in Russian).
3. E. Wolf. Electron tunneling spectroscopy principles. Kiev: "Naukova Dumka", 1990, 454 p. (in Russian).

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