Зондовая микроскопия: методы, теория, приложения

Лекция 9: Кельвиновская микроскопия
Сканирующая туннельная микроскопия

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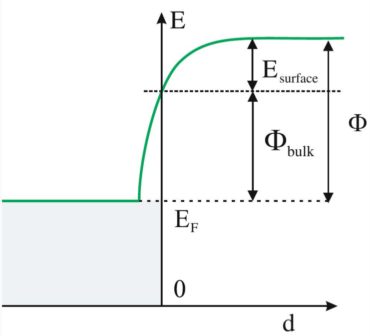
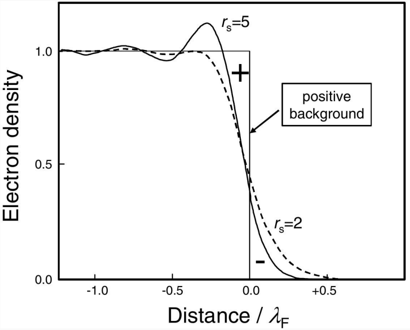
Факультет наук о материалах

Работа выхода

Зонная диаграмма

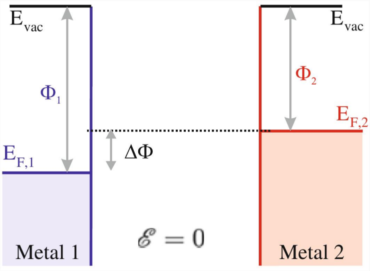


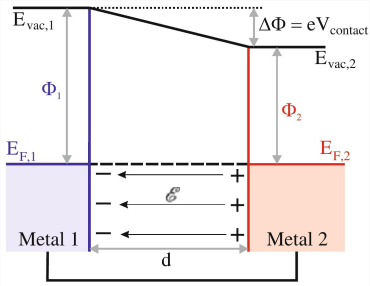
Эффект Смолуховского



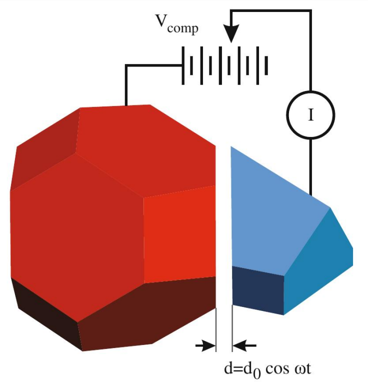
$$\Phi(d) = E_{\mathrm{out}}(d) - E_F$$

Контактная разность потенциалов





Метод Кельвина



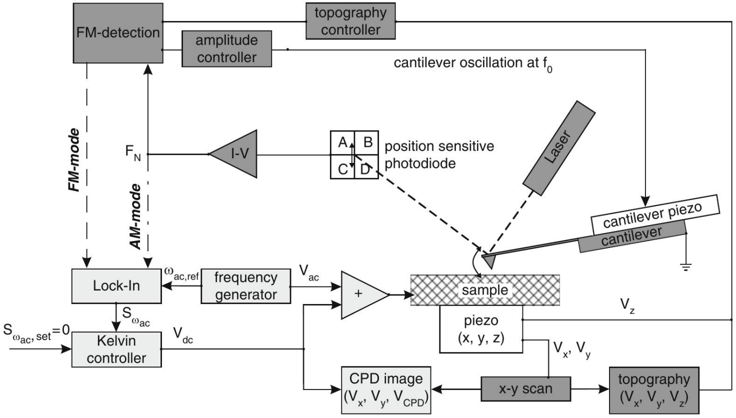
$$Q = CV = C(V_{\text{contact}} - V_{\text{comp}})$$

$$I = \frac{dQ}{dt} = \frac{dC}{dt}(V_{\text{contact}} - V_{\text{comp}})$$

$$I \to 0$$

$$V_{\text{comp}} = V_{\text{contact}} = \frac{1}{e}\Delta\Phi$$

Кельвиновская микроскопия

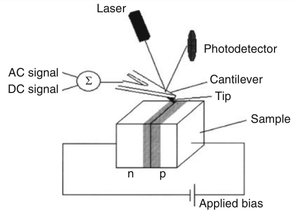


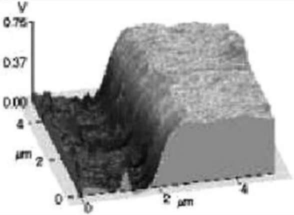
$$F = -\frac{1}{2}\frac{\partial C}{\partial z}(V_{\rm dc} - V_{\rm CPD} + V_{\rm ac}\sin(\omega_{\rm ac}t))^2; \quad F_{2\omega_{\rm ac}} = \frac{\partial C}{\partial z}\frac{V_{\rm ac}^2}{4}\cos(2\omega_{\rm ac}t)$$

$$F_{\omega_{\rm ac}} = -\frac{\partial C}{\partial z}(V_{\rm dc} - V_{\rm CPD})V_{\rm ac}\sin(\omega_{\rm ac}t); \; F_{\rm dc} = -\frac{\partial C}{\partial z}(\frac{1}{2}(V_{\rm dc} - V_{\rm CPD})^2 + \frac{V_{\rm ac}^2}{4})$$

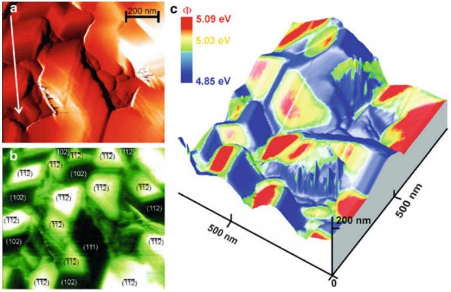
Кельвиновская микроскопия: примеры

GaP p-n переход

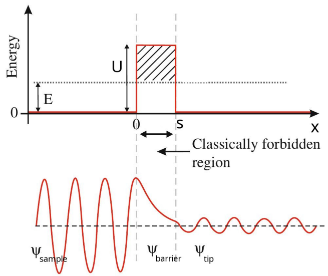




Пленка $CuGaSe_2$ на подложке $ZnSe(110)$



Туннелирование: наивный подход



$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) + U(x)\psi(x) = E\psi(x)$$

$$\psi_{\text{sample}} = e^{ikx} + Ae^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_{\text{barrier}}(x) = Be^{-\kappa x} + Ce^{\kappa x},$$

$$\kappa = \frac{\sqrt{2m(U-E)}}{\hbar}$$

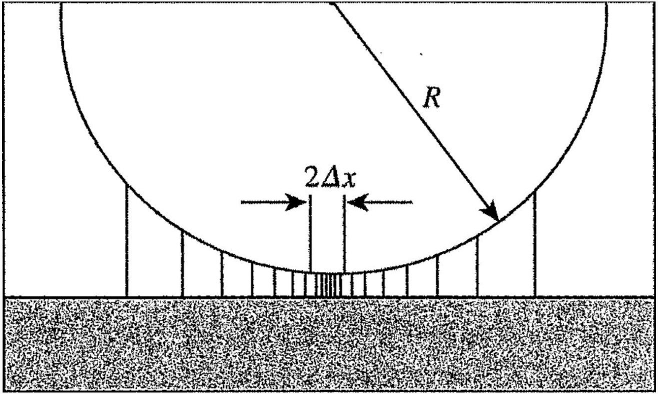
$$\psi_{\text{tip}} = De^{ikx}$$

$$I = -\frac{i\hbar}{2m}(\psi^*\partial_x\psi - \psi\partial_x\psi^*)$$

$$T = \frac{I_{\text{tip}}}{I_{\text{sample}}} = |D|^2 \sim \frac{16\kappa^2k^2}{(\kappa^2+k^2)^2}e^{-2\kappa s}, \ \kappa s \gg 1$$

$$\kappa = \frac{\sqrt{2m\Phi}}{\hbar} \approx 1\text{Å}^{-1}, \quad \Phi \approx 5eV$$

СТМ: оценка разрешения

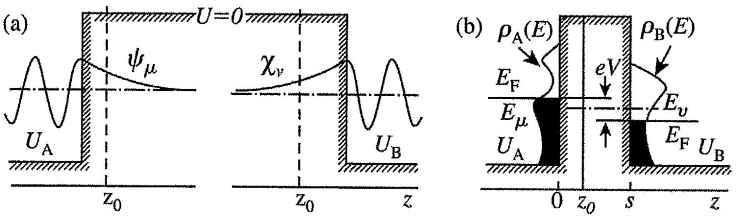


$$\Delta z \approx \frac{\Delta x^2}{2R}$$

$$I(\Delta x) \approx e^{-\kappa \frac{\Delta x^2}{R}}$$

$$R = 10\text{Å}, \quad \Delta x \approx 3\text{Å}$$

СТМ: теория Бардина



$$i\hbar\partial_t\Psi = \left[-\frac{\hbar^2}{2m}\partial_z^2 + U_A\right]\Psi, \qquad i\hbar\partial_t\Psi = \left[-\frac{\hbar^2}{2m}\partial_z^2 + U_B\right]\Psi$$

$$\Psi = \psi_\mu e^{-iE_\mu t/\hbar}, \qquad \Psi = \chi_\nu e^{-iE_\nu t/\hbar}$$

$$\left[-\frac{\hbar^2}{2m}\partial_z^2 + U_A\right]\psi_\mu = E_\mu\psi_\mu, \qquad \left[-\frac{\hbar^2}{2m}\partial_z^2 + U_B\right]\chi_\nu = E_\nu\chi_\nu$$

СТМ: теория Бардина

$$i\hbar\partial_t\Psi = \left[-\frac{\hbar^2}{2m}\partial_z^2 + U_A + U_B\right]\Psi$$

$$\Psi = \psi_\mu e^{-iE_\mu t/\hbar} + \sum_{\nu=1}^{\infty} c_\nu(t)\chi_\nu e^{-iE_\nu t/\hbar}, \quad c_\nu(0) = 0$$

$$\int \psi_\mu^* \chi_\nu \, d^3r \approx 0 \leftarrow \text{ модельное предположение}$$

$$i\hbar\partial_t c_\nu = \int\limits_{z>z_0} \psi_\mu U_B \chi_\nu^* \, d^3r \cdot e^{-i(E_\mu - E_\nu)t/\hbar}$$

$$M_{\mu\nu} = \int\limits_{z>z_0} \psi_\mu U_B \chi_\nu^* \, d^3r \leftarrow \text{ туннельный матричный элемент}$$

$$c_\nu(t) = M_{\mu\nu}\frac{e^{-i(E_\mu - E_\nu)t/\hbar} - 1}{E_\mu - E_\nu}$$

$$p_{\mu\nu}(t) = |c_\nu(t)|^2 = |M_{\mu\nu}|^2 \frac{4\sin^2[(E_\mu - E_\nu)t/2\hbar]}{(E_\mu - E_\nu)^2}$$

СТМ: теория Бардина

$$\lim_{t\to+\infty}\frac{1}{\omega^2 t}\sin^2(\omega t)=\pi\delta(\omega)$$

$$P_{\mu\nu}(t)=\partial_t|c_\nu(t)|^2=\frac{2\pi}{\hbar}|M_{\mu\nu}|^2\delta(E_\mu-E_\nu)\leftarrow \text{ золотое правило Ферми}$$

$$I_{A\to B}=\frac{4\pi e}{\hbar}\sum_{\mu\nu}f(E_\mu-E_F^A)(1-f(E_\nu-E_F^B))|M_{\mu\nu}|^2\delta(E_\mu-E_\nu)$$

$$I_{B\to A}=\frac{4\pi e}{\hbar}\sum_{\mu\nu}f(E_\nu-E_F^B)(1-f(E_\mu-E_F^A))|M_{\mu\nu}|^2\delta(E_\mu-E_\nu)$$

$$I=\frac{4\pi e}{\hbar}\int_{-\infty}^{\infty}(f(E_F-eV+\epsilon)-f(E_F+\epsilon))\rho_A(E_F-eV+\epsilon)\rho_B(E_F+\epsilon)|M(\epsilon)|^2d\epsilon$$

$$\boxed{I=\frac{4\pi e}{\hbar}\int_{0}^{eV}\rho_A(E_F-eV+\epsilon)\rho_B(E_F+\epsilon)|M(\epsilon)|^2d\epsilon}\quad \text{при } T\to 0$$

СТМ: теория Бардина

$$M_{\mu\nu} = \int\limits_{z>z_0} \psi_\mu (E_\nu + \frac{\hbar^2}{2m}\partial_z^2)\chi_\nu^* d^3 r$$

Для случая упругого туннелирования ($E_\mu = E_\nu$),

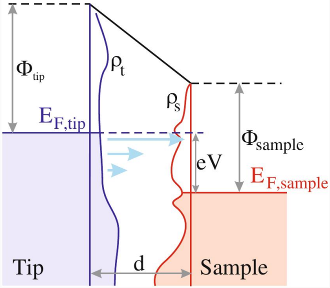
$$M_{\mu\nu} = \int\limits_{z>z_0} (\chi_\nu^* E_\mu \psi_\mu + \psi_\mu \frac{\hbar^2}{2m}\partial_z^2 \chi_\nu^*) d^3 r$$

$$= -\frac{\hbar^2}{2m} \int\limits_{z>z_0} (\chi_\nu^* \partial_z^2 \psi_\mu - \psi_\mu \partial_z^2 \chi_\nu^*) d^3 r \ .$$

$$\chi_\nu^* \partial_z^2 \psi_\mu - \psi_\mu \partial_z^2 \chi_\nu^* = \partial_z (\chi_\nu^* \partial_z \psi_\mu - \psi_\mu \partial_z \chi_\nu^*)$$

$$\boxed{M_{\mu\nu} = \frac{\hbar^2}{2m} \int\limits_{z=z_0} (\psi_\mu \partial_z \chi_\nu^* - \chi_\nu^* \partial_z \psi_\mu) dx dy}$$

СТМ: модель плоского интерфейса

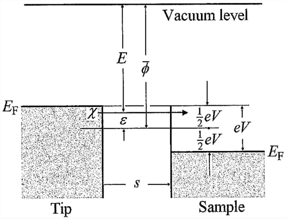


$$\psi_\mu(z) = \psi_\mu(0)e^{-\kappa_\mu z}, \quad \kappa_\mu = \sqrt{2m|E_\mu|}/\hbar$$

$$\chi_\nu(z) = \chi_\nu(s)e^{\kappa_\nu(z-s)}, \quad \kappa_\nu = \kappa_\mu$$

$$M_{\mu\nu} = \frac{\hbar^2}{2m}\int\limits_{z=z_0} 2\kappa_\mu\psi_\mu(0)\chi_\nu(s)e^{-\kappa_\mu z_0}e^{\kappa_\mu(z_0-s)}dxdy$$

$$= \left[\frac{\hbar^2}{2m}\int\limits_{z=z_0} 2\kappa_\mu\psi_\mu(0)\chi_\nu(s)dxdy\right]e^{-\kappa_\mu s}\,.$$



$$I = \frac{4\pi e}{\hbar} \int_{-\frac{1}{2}eV}^{\frac{1}{2}eV} \rho_S(E_F + \frac{1}{2}eV + \epsilon)\rho_T(E_F - \frac{1}{2}eV + \epsilon)|M(\epsilon)|^2 d\epsilon$$

$$\kappa = \frac{\sqrt{2m(\overline{\phi} - \epsilon)}}{\hbar} \approx \kappa_0(1 - \frac{\epsilon}{2\overline{\phi}}); \quad \kappa_0 = \frac{\sqrt{2m\overline{\phi}}}{\hbar}$$

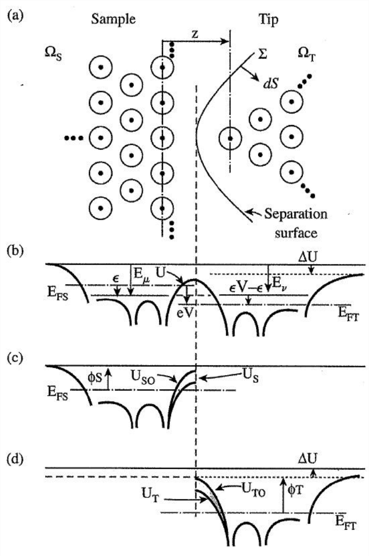
$$M(\epsilon) = M(0)\exp(\frac{\kappa_0 \epsilon s}{2\overline{\phi}})$$

$$I = \frac{4\pi e}{\hbar} \int_{-\frac{1}{2}eV}^{\frac{1}{2}eV} \rho_S(E_F + \frac{1}{2}eV + \epsilon)\rho_T(E_F - \frac{1}{2}eV + \epsilon)|M(0)|^2$$

$$\times \exp(\frac{\kappa_0 \epsilon s}{\overline{\phi}}) d\epsilon.$$

$$\kappa_0 = 10\ nm^{-1},\ \overline{\phi} = 5\ eV,\ s = 1\ nm,\ \epsilon = 0.5\ eV$$

СТМ: модель 3D интерфейса



$$U_S + U_T = U, \quad U_S U_T = 0$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U_S\right]\psi_\mu = E_\mu \psi_\mu$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U_T\right]\chi_\nu = E_\nu \chi_\nu$$

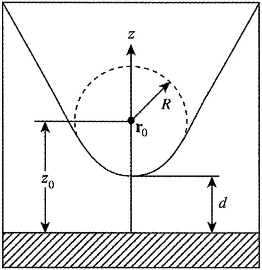
$$i\hbar\partial_t \Psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U_S + U_T\right]\Psi$$

$$M_{\mu\nu} = \int\limits_{\Omega_T} \psi_\mu U_T \chi_\nu^* \, d^3r$$

$$M_{\mu\nu} = \frac{\hbar^2}{2m}\int\limits_{\Omega_T} (\chi_\nu^* \nabla^2 \psi_\mu - \psi_\mu \nabla^2 \chi_\nu^*) d^3r$$

$$M_{\mu\nu} = \frac{\hbar^2}{2m}\int\limits_{\Sigma} (\psi_\mu \nabla \chi_\nu^* - \chi_\nu^* \nabla \psi_\mu) \cdot d\mathbf{S} = M_{\nu\mu}^*$$

СТМ: модель Терсоффа-Хаманна



$$-\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}) = -\phi\psi(\mathbf{r})$$

$$\Delta\psi(\mathbf{r}) = \kappa^2\psi(\mathbf{r}), \quad \kappa = \sqrt{2m\phi}/\hbar$$

$$\psi(\mathbf{r}) = \int d^2\mathbf{q}\, f(\mathbf{q}, z)e^{i\mathbf{q}\cdot\mathbf{x}},$$

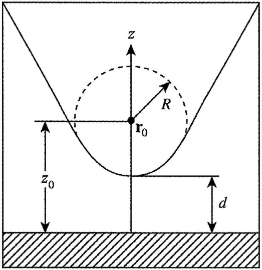
$$\mathbf{q} = (k_x, k_y), \quad \mathbf{x} = (x, y)$$

$$\partial_z^2 f(\mathbf{q}, z) = (\mathbf{q}^2 + \kappa^2)f(\mathbf{q}, z)$$

$$f(\mathbf{q}, z) = a(\mathbf{q})e^{-\sqrt{\mathbf{q}^2+\kappa^2}z}$$

$$\psi(\mathbf{r}) = \int d^2\mathbf{q}\, a(\mathbf{q})e^{-\sqrt{\mathbf{q}^2+\kappa^2}z+i\mathbf{q}\cdot\mathbf{x}}$$

СТМ: модель Терсоффа-Хаманна



$$r^2 = x^2 + y^2 + (z - z_0)^2$$

$$\frac{1}{r}\frac{d^2}{dr^2}[r\chi(r)] = \kappa^2\chi(r)$$

$$\chi(r) = \frac{1}{r}e^{-\kappa r} = \frac{1}{2\pi}\int d^2\mathbf{p}\frac{e^{-\sqrt{\mathbf{p}^2+\kappa^2}(z_0-z)+i\mathbf{p}\cdot\mathbf{x}}}{\sqrt{\mathbf{p}^2+\kappa^2}}$$

$$M = \frac{\hbar^2}{2m}\int\limits_{z=0}(\psi\partial_z\chi^* - \chi^*\partial_z\psi)dxdy$$

$$M \propto \int d^2\mathbf{q}d^2\mathbf{p}d^2\mathbf{x}\left[1 + \frac{\sqrt{\mathbf{q}^2+\kappa^2}}{\sqrt{\mathbf{p}^2+\kappa^2}}\right]a(\mathbf{q})e^{-\sqrt{\mathbf{q}^2+\kappa^2}z_0+i(\mathbf{q}+\mathbf{p})\cdot\mathbf{x}}$$

$$M \propto \int d^2\mathbf{q}\,a(\mathbf{q})e^{-\sqrt{\mathbf{q}^2+\kappa^2}z_0} = \psi(\mathbf{r}_0)$$

$$\boxed{G \propto |\psi(\mathbf{r}_0)|^2\rho_S(E_F) = \rho_S(E_F, \mathbf{r}_0)}$$

Литература

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Вопросы?