

Energy dissipation processes in scanning tunneling microscopy

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Energy dissipation associated with assisted tunneling processes in scanning tunneling microscopy is analyzed and compared with the normal tunnel current. We find that, for high voltages, greater than one volt, the tunneling processes associated with electron-hole pair excitation control the increase in temperature at the microscope's interface.

Recently, much theoretical and experimental work¹⁻⁶ has been concerned with the use of scanning tunneling microscopy as a tool to analyze surface properties. The wide potential applicability of this technique clearly justifies much needed experimental and theoretical work to improve our understanding of the complicated physical phenomena associated with the electron tunneling processes.

This paper addresses inelastic assisted processes and energy dissipation at the microscope's interface. Its contents are related to some broad fields of solid state physics, scanning tunneling spectroscopy, electron theory of surfaces, and heat transport in microscopic small objects.⁷ Phonons and electron-hole-pair-assisted tunneling at low voltages, and plasmons at high enough voltages, will lead to energy dissipation in the short distance of the interface region. This is in contrast to the dissipation of energy associated with the direct current which occurs inside the crystals forming the interface at distances of the electron mean free path, typically several hundred angstroms. On these grounds one could expect a temperature rise at the surface region, due to assisted tunneling processes, at least comparable to the one created by the direct current. In this paper, we compare both effects and analyze under which conditions assisted processes control and give an important increase to the temperature at the interface of the microscope.

For the transition probability of a tunneling process from state $\psi_1(\mathbf{r})$ at the metal surface 1 to state $\psi_2(\mathbf{r})$ at the metal surface 2, assisted by the emission of an interface quasiparticle of energy ω_s , we write the following⁸

$$\frac{\langle P_{1 \rightarrow 2}^A \rangle}{P_{1 \rightarrow 2}^{\text{direct}}} = \frac{1}{2\phi_1} \int_{E_{F2}}^{E_1} d\omega_s \int dz dz' \exp[-(z+z')(\sqrt{2\phi_1} - \sqrt{2\phi_2})] \text{Im}[W^{\text{int}}(z, z'; \omega_s)] , \tag{5}$$

where $\langle \rangle$ is the value of $P_{1 \rightarrow 2}^A$ integrated in the final state 2, such that $\phi_2 = \phi_1 + \omega_s$,

$$\frac{d^2 I^A}{dV^2} \sim \int dz dz' \exp[-(z+z')(\sqrt{2\phi_1} - \sqrt{2\phi_2})] \times \text{Im}[W^{\text{int}}(z, z'; \omega_s)] , \tag{6}$$

for $\omega_s = V$ (atomic units are used throughout this paper).

The response functions for the surface phonons and electron-hole pairs have been taken from Refs. 9 and 11.

(for zero temperature and first-order perturbation theory):

$$P_{1 \rightarrow 2}^A = \int d\mathbf{r} d\mathbf{r}' \psi_1^*(\mathbf{r}) \psi_2(\mathbf{r}) \text{Im}[W^{\text{int}}(\mathbf{r}, \mathbf{r}'; \omega_s)] \psi_2^*(\mathbf{r}') \psi_1(\mathbf{r}') . \tag{1}$$

The total assisted current I^A is obtained by integrating over initial (1) and final (2) states,

$$I^A = \int_{E_{F,2}}^{E_{F,1}} d1 \int_{E_{F,2}}^{E_1} d2 P_{1 \rightarrow 2}^A , \tag{2}$$

showing that $d^2 I^A / dV^2$ is proportional to $P_{1 \rightarrow 2}^A(\omega_s = V)$.

In calculating the screened interaction, $W^{\text{int}}(\mathbf{r}, \mathbf{r}'; \omega_s)$, we assume, for the sake of simplicity, that the surfaces are effectively decoupled, so that

$$\text{Im}(W^{\text{int}}) \approx \text{Im}(W^{\text{int}(1)}) + \text{Im}(W^{\text{int}(2)}) . \tag{3}$$

To proceed further, we assume translational invariance in the direction parallel to the surface and write

$$\text{Im}(W^{\text{int}(i)}) = \int \frac{d\mathbf{Q}}{(2\pi)^2} \frac{2}{Q} \exp[-Q(z+z')] \text{Im}g_{(i)}(\mathbf{Q}, \omega_s) , \tag{4}$$

where $g_{(i)}$ is the surface response function.⁹

We compare these results with the direct processes calculated by means of a Bardeen Hamiltonian.¹⁰ We use for simplicity a one-dimensional model, take for the wave functions ψ_1 and ψ_2 , $\psi_1 \sim \exp(-z\sqrt{2\phi_1})$ and $\psi_2 \sim \exp \times [- (d-z)\sqrt{2\phi_2}]$ (see Fig. 1), and obtain the following results:

For phonons, we neglect the small asymmetry between the two surfaces associated with the small energy transfer of a phonon mode; this yields

$$\frac{d^2 I^{\text{ph}}}{dV^2} \sim \begin{cases} \left[\frac{V}{\omega_0} \right] \left[1 - \frac{V^2}{\omega_0^2} \right]^{1/2} , & V < \omega_0 , \\ 0 , & V > \omega_0 , \end{cases} \tag{7}$$

ω_0 being the maximum phonon frequency.¹¹ For electron-hole ($e-h$) pairs we obtain different results for

surfaces 1 and 2:

$$\frac{d^2 I^{e-h}}{dV^2} \sim \begin{cases} (1) \frac{V}{\omega_P} \exp\left[-\frac{\sqrt{2}Vd}{\sqrt{\phi_1}}\right], & V \sim \phi_1 \ll \omega_P, & (8a) \\ (2) \frac{V}{\omega_P}, & V \sim \phi_1 \ll \omega_P, & (8b) \end{cases}$$

where ω_P is the plasma frequency.²

On the other hand, we have obtained the following results for the transition probabilities: For phonons,

$$\langle P_{1 \rightarrow 2}^{\text{ph}} \rangle / P_{1 \rightarrow 2}^{\text{direct}} \approx \begin{cases} 10^{-3} \left(\frac{E_1 - E_{F2}}{\omega_0} \right)^4 \frac{\omega_0}{\phi_1} \ln\left(\frac{\pi}{a} d\right), & (E_1 - E_{F2}) < \omega_0, \\ 10^{-3} \frac{\omega_0}{\phi_1} \ln\left(\frac{\pi}{a} d\right), & (E_1 - E_{F2}) > \omega_0, \end{cases} \quad (9)$$

where π/a is a measure of the reciprocal vector associated with the surface Brillouin zone edge. And for $e-h$ pairs

$$\langle P_{1 \rightarrow 2}^{e-h} \rangle / P_{1 \rightarrow 2}^{\text{direct}} \sim \begin{cases} \frac{(E_1 - E_{F2})^2}{4\pi\omega_P k_F \phi_1} \ln(2k_F d), & (E_1 - E_{F2}) < \frac{\phi_1^{1/2}}{2^{1/2}d} \ll \omega_P \text{ (surface 1)}, \\ \frac{\ln(2k_F d)}{8\pi\omega_P k_F d^2}, & \frac{\phi_1^{1/2}}{2^{1/2}d} < (E_1 - E_{F2}) \ll \omega_P, \end{cases} \quad (10a)$$

$$\langle P_{1 \rightarrow 2}^{e-h} \rangle / P_{1 \rightarrow 2}^{\text{direct}} \sim \frac{(E_1 - E_{F2})^2}{4\pi\omega_P k_F \phi_1} \ln(2k_F d), \quad (E_1 - E_{F2}) \ll \omega_P \text{ (surface 2)}, \quad (10b)$$

where k_F is the Fermi wavelength.

Typical values ($\phi_1 \sim 2$ eV, $d \sim 5$ Å, $\omega_P \sim 12$ eV, $k_F \sim 0.35$ Å⁻¹, $\pi/a \sim 0.25$ Å⁻¹, $\omega_0 \sim 0.05$ eV) yield

$$\langle P_{1 \rightarrow 2}^{\text{ph}} \rangle / P_{1 \rightarrow 2}^{\text{direct}} \sim 3 \times 10^{-5} \quad (V > \omega_0), \quad (11a)$$

and

$$\langle P_{1 \rightarrow 2}^{e-h} \rangle / P_{1 \rightarrow 2}^{\text{direct}} \sim \begin{cases} 10(E_1 - E_{F2})^2 \text{ (surface 2)}, \\ 10(E_1 - E_{F2})^2 \text{ (surface 1 for } E_1 - E_{F2} < 0.5 \text{ V)}, \\ 5 \times 10^{-3} \text{ (surface 1 for } E_1 - E_{F2} > 0.5 \text{ V)}. \end{cases} \quad (11b)$$

The energy dissipated by these modes can be calculated by including in the previous results the energy associated with each mode. Proceeding, in this way, we have obtained the ratio between the power losses W for the assisted processes and the normal current: For phonons,

$$W^{\text{ph}} / W^{\text{direct}} \sim 10^{-3} \frac{\omega_0^2}{\phi_0 V} \ln\left(\frac{\pi}{a} d\right) \quad (V > \omega_0), \quad (12)$$

and for $e-h$ pairs,

$$W_{(1)}^{e-h} / W^{\text{direct}} \sim \begin{cases} \frac{V^2 \ln(2k_F d)}{4\pi\omega_P k_F \phi_0} \text{ for } V < \frac{\phi_0^{1/2}}{2^{1/2}d} \ll \omega_P \text{ (surface 1)}, \\ \frac{\phi_0^{1/2} \ln(2k_F d)}{2^{1/2} 8\pi\omega_P k_F V d^3} \text{ for } \frac{\phi_0^{1/2}}{2^{1/2}d} < V \ll \omega_P, \end{cases} \quad (13a)$$

$$W_{(1)}^{e-h} / W^{\text{direct}} \sim \frac{\phi_0^{1/2} \ln(2k_F d)}{2^{1/2} 8\pi\omega_P k_F V d^3} \text{ for } \frac{\phi_0^{1/2}}{2^{1/2}d} < V \ll \omega_P, \quad (13b)$$

$$W_{(2)}^{e-h} / W^{\text{direct}} \sim \frac{V^2 \ln(2k_F d)}{4\pi\omega_P k_F \phi_0} \quad (V \ll \omega_P) \text{ (surface 2)}. \quad (13c)$$

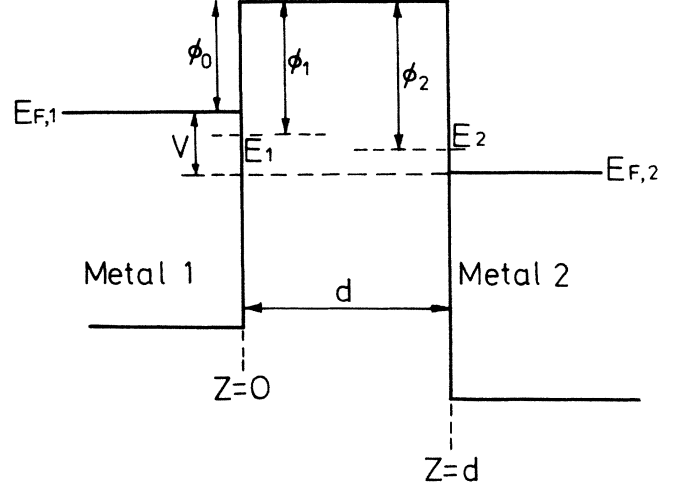


FIG. 1. Model used to calculate the assisted tunneling process. V is the applied voltage. An electron tunnels from level E_1 to level E_2 .

The energy dissipated by phonons is negligible: $e-h$ pairs can, however, be important in that respect, producing an important increase in the surface temperature. It is also possible that surface plasmon modes characterized by eigenfrequency $\omega_Q \sim \omega_P(Qd/2)^{1/2}$ may be excited in the tip-sample region. An estimate of the probability of such an excitation indicates that it is appreciably smaller than the corresponding probability of an electron-hole excitation.

The pairs excited at the surface can decay into other pairs at a very quick rate (the mean collision time for a pair of 1 eV is around 10^{-15} s). During these processes the pairs do not have the time to flow away from the interface, since the time needed for this process is 10^{-14} s; so the pairs can be thermalized, creating a region of local thermal equilibrium. Notice in this respect that the requirement of charge neutrality implies that the separation of $e-h$ pairs would be strongly inhibited, resulting in a highly localized deposition of energy to $e-h$ pair cascades. In a second step, this energy is taken away from the interface. Two mechanisms compete here: (i) the pairs can take away the energy themselves, and (ii) the pairs can excite phonons at the interface,¹² these modes then taking away the deposited energy. The first case can be analyzed by assuming that a steady state is reached at the interface, and by balancing the energy dissipated in regions⁶ of radius r ($r \sim 5 \text{ \AA}$), with the heat flux; this yields the following increase in temperature:

$$\Delta T_s \sim \frac{W^{e-h}}{2\pi r K_s},$$

where K_s is the surface thermal conductivity. It is important to note that the small contact region reduces the bulk thermal conductivity K by a factor of r/λ , λ being the bulk mean free path for electrons¹³ ($\lambda \sim 500 \text{ \AA}$).

The second case can be analyzed by noting that the mean collision time of electrons with acoustic phonons is around 2.5×10^{-14} s. This shows that the pairs are strongly coupled to the phonons, which can dissipate ballistically the energy deposited at the interface. In this respect, it is of interest to note that the time of flight for the crossing of the interface by the acoustic phonons is around 3×10^{-13} s. Now, this time of flight, the number of phonons excited at the interface, and the mean energy taken away by the acoustic phonons, ~ 0.03 eV, have to be compared with the power loss associated with the excitation of pairs. If the power dissipated by the phonons is greater than the power loss at the interface, the mechanism associated with ballistic phonons can very efficiently dissipate the energy; otherwise, phonons are thermalized with the pairs, and, finally, the first mechanism discussed above is the dominant one.

Consider now two microscope configurations having the following contact resistances: $R = 10^5$ and 10^9 \Omega . For $V = 1$ V, we obtain the following power losses.

R (Ω)	I (nA)	W^{direct} (eV/s)	$W^{e-h(2)}$ (eV/s)
10^5	10^4	$10^{14}/1.6$	1.2×10^{12}
10^9	1	$10^{10}/1.6$	1.2×10^8

For these values, and noticing that $K \sim 10^{11} \text{ eV/AsK}$, we obtain the following results if we assume that the first mechanism is dominant:

$$\Delta T_s \sim \begin{cases} 30 \text{ K} & (R = 10^5 \text{ \Omega}, V = 1 \text{ V}), \\ 3 \times 10^{-2} \text{ K} & (R = 10^9 \text{ \Omega}, V = 1 \text{ V}). \end{cases}$$

Now, for $R = 10^5 \text{ \Omega}$ and $V = 1$ V, the intensity is 10 \mu A and the pairs are excited about every 8×10^{-13} s. This is greater than the time of flight for phonons, 3×10^{-13} s, so that we conclude that the mechanism of ballistic phonons controls the dissipation of energy.

For $V = 2$ V, we obtain the following surface temperature for the first mechanism:

$$\Delta T_s \sim \begin{cases} 480 \text{ K} & (R = 10^5 \text{ \Omega}, V = 2 \text{ V}), \\ 4.8 \times 10^{-2} \text{ K} & (R = 10^9 \text{ \Omega}, V = 2 \text{ V}). \end{cases}$$

For this case, $e-h$ pairs are excited every 10^{-13} s, and acoustic phonons become quite ineffective for dissipating energy. This means that the energy is dissipated in this case by the first mechanism. It is worth noticing that for this voltage ($V = 2$ V) the locally deposited energy is around 6 eV, this quantity being much greater than the mean energy of the excited $e-h$ pairs (~ 1 eV); this implies that a steady state is reached for $e-h$ pairs and acoustic phonons at the interface.

On the other hand, assuming that the direct current is dissipated over distances of 100 \AA (this is the mean free path for electrons having energies around 1 eV above the Fermi level), we obtain the following increase in temperature for those distances of 100 \AA :

$$\Delta T_b \sim \begin{cases} 32 \text{ K} & (R = 10^5 \text{ \Omega}, V = 2 \text{ V}), \\ 3.2 \times 10^{-3} \text{ K} & (R = 10^9 \text{ \Omega}, V = 2 \text{ V}). \end{cases}$$

We see that at high voltages $e-h$ pairs at the surface increase the temperature more effectively. Notice in that respect ΔT_s increases with V^4 , while ΔT_b only increases with V^2 . This shows that the surface temperature can be increased by a thousand degrees for an applied voltage of a few volts if the contact resistance is low enough ($R \sim 10^5 \text{ \Omega}$). Let us finally comment that our results for ΔT_b are similar to those found by Persson and Demuth¹⁴ for the inelastic tunneling current assisted by the excitation of an adsorbed molecule. The deposition of energy in the small region of the contact point due to the $e-h$ pair excitation and the corresponding reduction in the thermal conductivity explains the high values calculated here for ΔT_s .

In conclusion, energy dissipation associated with assisted tunneling processes can be very important in scanning tunneling microscopy. Important increases of temperature can be obtained from these processes in very localized regions: One could take advantage of these effects to prepare etched surfaces.

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