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Correlation between charge and current corrugations in scanning-tunneling microscopy

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The aim of this paper is to investigate how charge and current corrugations in scanning-tunneling microscopy are compared. A Si(111) surface is analyzed and a method to calculate tunneling currents from localized states is proposed. The main result of this model is that charge corrugations are always greater than current corrugations, although they only differ significantly for large corrugations.

The key question concerning the recently developed technique of scanning-tunneling microscopy (STM) is the correlation between charge and current (measured) corrugations.[1] Some of the theoretical models proposed to interpret the STM images use the local density of states of the sample.[2,3] In a different approach a full calculation of the tunneling current through the matching of tip and sample wave functions[4,5] is performed. In these references[4,5] both the tip and sample were described by means of a jellium model.

The purpose of this paper is to present a full calculation of the tunneling current for a Si-metal configuration. Although the voltage drop controlling the total current is determined by a diffusive process inside the semiconductor,[6] the surface corrugation measured by STM only depends on the tunneling process between Si and the metal. Surface corrugations are studied by analyzing the local charge and the current densities as a function of the distance between the tip and the sample. We assume the tip's curvature to be large enough for the tip to scan with high accuracy the surface corrugation. The results given in Ref. 4 show that the total tunneling current has two factors: one is associated with an effective curvature of the tip and the sample (measuring the effective area for the total current), the other one is related to the terms appearing in the case of two planar surfaces located at the same distance as the tip and the sample (measuring the local current density at the tip's center). Assuming that the effective curvature of the microscope's interface is controlled by the tip's curvature allows us to reduce the analysis of the tunneling-current corrugation to consider a planar surface for the tip. On the other hand, as tunneling from Si is assumed to occur through surface states, a method suitable for this case will be proposed. Most calculations of tunneling currents in the parent experimental technique of field emission are based upon the WKB approximation.[7,8] Our method provides a new approach to the calculation of tunneling currents from localized states.

As stated above, the tungsten tip and the semiconductor will be taken as flat parallel surfaces. We shall consider a Si(111) unreconstructed surface and a jellium model for the tip.[4] Of course surface corrguations for this surface will not be similar to the large values found at the Si(111)7×7 surface.[1] Instead, our model will illustrate the kind of corrugations which can be expected at less corrugated surfaces or even regions of the 7×7 surface having a local structure similar to the ideal surface.[9] On the other hand, this system provides an appropriate case to compare charge and current corrugations.

The barrier height will be taken from recent experimental data,[10] according to which it depends significantly on the distance between the tip and the sample. Two abrupt barriers will be placed at the tip and the sample surfaces, adequately shifted to account for charge neutrality.[11,12] The vacuum potential in between will be taken constant and adjusted to give the actual barrier height.[10] The semiconductor band structure will be described by means of an empirical pseudopotential, including 27 plane waves in first-order perturbation theory. Details of the surface calculation can be found in Ref. 11. Electron-electron interaction will not be considered since it does not affect the electron density of states at the Fermi level,[13] the energy region actually contributing to the tunneling current.[1]

We turn now to discuss the method proposed here for calculating tunneling currents. It should be noticed that as surface states are localized, no current can be, in principle, built up through them. The source of charge is provided by conduction through the semiconductor bands; electrons or holes falling to the surface states maintain a constant current through the surface states. This process will be modeled by a δ function at z_0 (the position of the abrupt barrier for the semiconductor); its weight will be adjusted to provide the appropriate current.

The following equation defines the wave function $\phi_{\mathbf{k}}$ we are going to use in order to calculate tunneling currents:

$$-\tfrac{1}{2}\nabla^2\phi_{\mathbf{k}}+[V(\boldsymbol{\rho},z)-E]\phi_{\mathbf{k}}=Ce^{i\mathbf{k}\cdot\boldsymbol{\rho}}\delta(z-z_0)\ . \qquad (1)$$

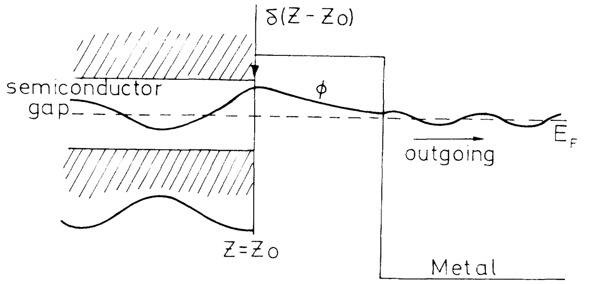

FIG. 1. Effect of the inhomogeneous term of Eq. (1) in one dimension. Note the outgoing wave function in the metal.

Here, $V(\rho,z)$ is the full crystalline potential of the metal-semiconductor interface and $Ce^{i\mathbf{k}\cdot\rho}\delta(z-z_0)$ is the kind of interface source creating the tunneling current we are looking for (C is a constant to be adjusted below, $\mathbf{k}$ is a two-dimensional reciprocal vector); Fig. 1 illustrates in one dimension the kind of wave function provided by Eq. (1). Notice that the boundary conditions in the metal have to be chosen such that $\phi_{\mathbf{k}}$ represents an outgoing wave function. Equation (1) has the following solution:

$$\phi_{\mathbf{k}}(\rho,z,E)=Ce^{i\mathbf{k}\cdot\rho}\sum_{g} e^{i\mathbf{g}\cdot\rho}G_s(\mathbf{k}+\mathbf{g},z;\mathbf{k},z_0;E)\ , \tag{2}$$

where $\mathbf{g}$ is a two-dimensional reciprocal-lattice vector. The Green's function G_s is that corresponding to the whole system and is calculated by means of the surface Green's-function method.[11,14,15] The current associated with $\phi_{\mathbf{k}}$ is given by (atomic units are used in this paper)

$$\mathbf{j}(\rho,z;\mathbf{k};E)=\mathrm{Im}[\phi_{\mathbf{k}}^{*}(\rho,z;E)\nabla_r\phi_{\mathbf{k}}(\rho,z;E)]\ , \tag{3}$$

and the corresponding local density of states,

$$D_{\mathbf{k}}(\rho,z;E)=|\phi_{\mathbf{k}}(\rho,z;E_1)|^2\delta(E-E_1)\ , \tag{4}$$

where E_1 is the energy of the surface state for a given $\mathbf{k}$. Equation (4) gives the local density of states associated with $\phi_{\mathbf{k}}$ which, in principle, would be different from the local density of the actual system. However, we can show that both quantities are the same if the constant C, introduced in Eq. (1), is appropriately chosen. The point to be noted is the following: The function $\phi_{\mathbf{k}}$ is a given component of the Green's function of the whole system; this Green's function is quite close to the Green's function of the vacuum-semiconductor interface. For this last case, the Green's function has poles at the surface-state energies, and at those energies the Green's function is determined by the surface-state wave function, i.e., the residue at the poles is $|\phi_{\mathbf{k}}(\rho,z;E_s|^2$. For the slightly changed Green's function given by Eq. (1), we can expect that with a high accuracy $\phi_{\mathbf{k}}$ behaves in the same way if we choose the energy to be close enough to the surface-state level $E_s(\mathbf{k})$. The constant C introduced in Eq. (1) can be chosen by analyzing the z component of the total current per unit area associated with $\phi_{\mathbf{k}}$; this can be calculated by multiplying Eq. (1) by $\phi_{\mathbf{k}}$ and subtracting the complex conjugate equation. The result is the following:

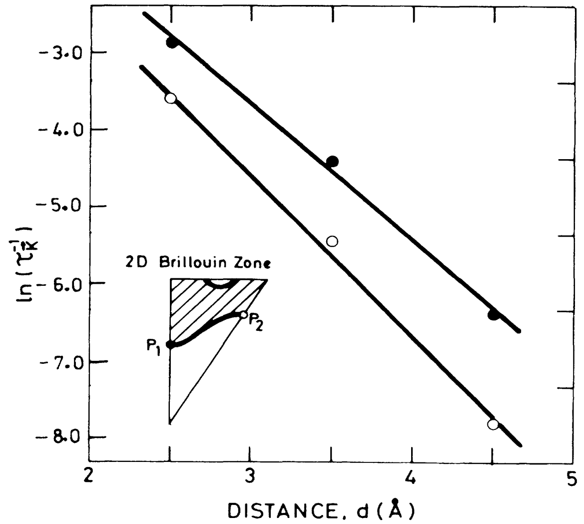

FIG. 2. Half-widths of surface states ($\tau_{\mathbf{k}}^{-1}$) in eV at points P_1 and P_2 of the two-dimensional Brillouin zone (irreducible part also shown in the figure) as a function of the distance between the tip and the semiconductor (d). The shaded area coincides with the filled part of the Brillouin zone.

$$J_z(\mathbf{k},E)=\int_{\substack{z\ \mathrm{const}\\ z>z_0}} d^2\rho \mathbf{j}_z(\rho,z;\mathbf{k};E)=2\pi|C|^2 n(\mathbf{k},z_0;E)\ , \tag{5}$$

where

$$n(\mathbf{k},z_0;E)=-\frac{1}{\pi}\mathrm{Im}G_s(\mathbf{k},z_0;\mathbf{k},z_0;E)\ .$$

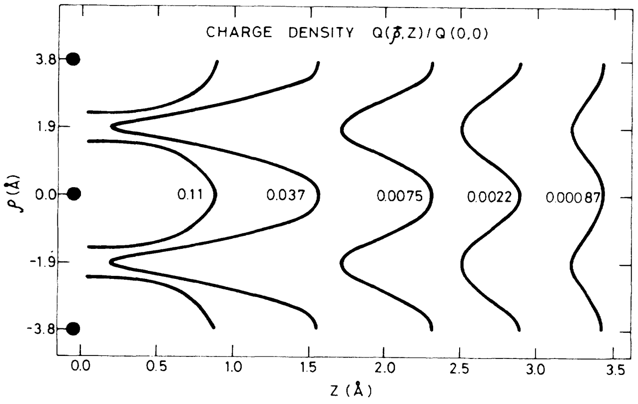

FIG. 3. Contours of constant charge as a function of ρ and z for $d=3.5$ Å. Values referred to the charge at $\rho=0$, $z=0$. Origin of z at the semiconductor midbond. The position of surface atoms is indicated by circles (atoms are actually a half bond behind $z=0$).

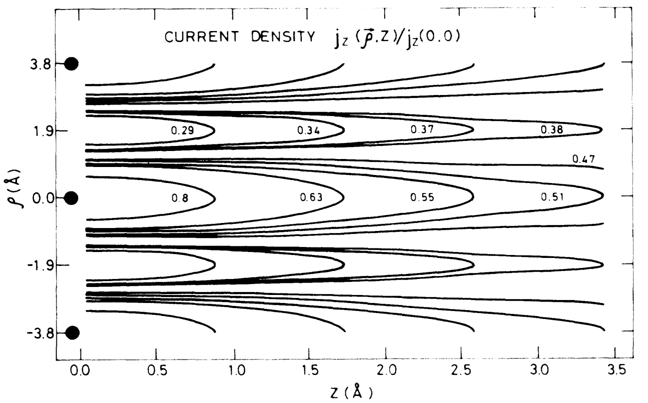

FIG. 4. Same as Fig. 2 for the z component of the current density.

Now, we choose $|C|^2$ in order to obtain the following general result:[16]

$$J_z(\mathbf{k},E)=n(\mathbf{k},E)/\tau_{\mathbf{k}} , \tag{6}$$

where $\tau_{\mathbf{k}}^{-1}$ is the state half-life (this time is obtained by calculating the broadening of the corresponding surface state in the metal-semiconductor interface) and $n(\mathbf{k},E)$ the density of surface states for a given $\mathbf{k}$ and E. Equations (5) and (6) yield

$$C=\left[\frac{n(\mathbf{k},E)}{2\pi\tau_{\mathbf{k}}n(\mathbf{k},z_0;E)}\right]^{1/2} . \tag{7}$$

This normalization factor provides the full wave function (2) and the current and charge densities (3) and (4). [In our calculation we have checked independently that the factor given by Eq. (7) is correct, by comparing Eq. (4) and the local density of states given by $n(\mathbf{k},z_0;E)$ after Eq. (5).]

The current and local charge density should be calculated by taking an average over the surface electron states at the Fermi level (E_F). The resulting mean value will be multiplied by the total density of states at E_F and by the voltage drop at the interface. In our calculations, we have only considered the two points at the Fermi surface shown in Fig. 2. For each point we have calculated $\phi_{\mathbf{k}}$ and $\tau_{\mathbf{k}}$. Figure 2 shows $\tau_{\mathbf{k}}^{-1}$ for those two points as a function of d (distance between the end of the tip's jellium and the plane passing through the midpoint of the broken semiconductor surface bonds). Note that $\tau_{\mathbf{k}}^{-1}$ decreases exponentially with d, being smaller for P_2, the point with larger $|\mathbf{k}|$, as expected. This means that for large d, points with the smallest $|\mathbf{k}|$ will give the largest contribution to current and charge densities.

We have performed calculations for $d=2.5$, 3.5, and 4.5 Å (actual distances between atomic planes should be around 2.5 Å larger). Note that calculations for smaller values of d are meaningless as the barrier height rapidly vanishes for d less than 2.5 Å.[9] Our results for the local charge and the z component of the current densities are illustrated in Figs. 3 and 4 ($d=3.5$ Å). As regards charge density the following results are worth being outlined: (i) For a given distance between the semiconductor and the tip, corrugation decreases for z closer to the tip (notice that corrugation is defined here by the curves of constant charge density; (ii) the corrugation nearest the tip surface decreases as d increases, being 0.63 Å for $d=2.5$ Å, 0.2 Å for $d=3.5$ Å, and 0.1 Å for $d=4.5$ Å; and (iii) corrugations as a function of z for $z \leqq 1.5$ Å are nearly independent of d. Contours of constant current j_z for $d=3.5$ Å are shown in Fig. 4 (corrugation is defined in this case by the tip's distance for which the current density is a constant). The result is rather intuitive: Near the semiconductor surface the current density is much higher on top of the surface atom. Then, current lines open, leading to an overall decrease of j_z on top of the atom, and increase midway between atoms. Similar results were obtained for other d.

Comparison between the corrugations yielded by the current can be alternatively (and more clearly) carried out by defining the ratios R_q (charge) and R_j (current) between their values on top of the surface atom and midway between atoms, for a given d and at the tip plane ($z=d$). We obtain

$$\begin{aligned} d&=2.5\ \text{Å},\quad R_q=1.9,\quad R_j=1.63 ,\\ d&=3.5\ \text{Å},\quad R_q=1.4,\quad R_j=1.35 . \end{aligned} \tag{8}$$

These results show that for $d=2.5$ Å charge corrugation is 14% greater than current corrugation (measured), whereas for $d=3.5$ Å it is only 3% larger. A case with larger corrugation can be considered by recalling that for $z \leqq 1.5$ Å corrugations are nearly independent of d. Then for $z=1.5$ Å, a plane for which charge corrugations is around 1 Å, our calculations lead to a ratio $R_q/R_j \sim 1.3$, showing again that the difference between charge and current corrugations increases for greater corrugations. These results show that for large corrugations current corrugations cannot be replaced by charge corrugations: Errors can be as large as 30% for corrugations of 1 Å.

In conclusion, we have presented a full calculation of tunneling currents from a crystal surface. In particular, we have studied the Si(111) surface in which tunneling is likely to occur through surface states. A method to perform a full calculation of tunneling currents through localized states has been proposed. The results suggest that while current corrugations (STM results) for weakly corrugated surfaces are very similar to charge corrugations, the latter are significantly greater than current corrugations for strongly corrugated surfaces.

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