Theory of Single-Atom Imaging in the Scanning Tunneling Microscope

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The tunneling-current density is computed in the vacuum region between two planar metal electrodes, on each of which is an adsorbed atom. Scanning of one atom (taken as the tip) past the other (the sample) permits plotting of tip displacement versus lateral separation for constant current. The calculation shows the extent to which scanning-tunneling-microscope images of an individual atom are visible. It confirms that for low bias, the microscope images the Fermi-level local density of states of the sample at the position of the tip.

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I present in this paper a discussion of the current flow in the scanning tunneling microscope.[1–9] The vacuum tunneling current between two planar metallic electrodes with a small bias voltage between them is studied in the instance in which there is an adsorbed atom on each electrode, with one electrode corresponding to the tip, and the other to the sample (a surface with a chemisorbed atom). This is the first calculation in which the tip and the sample are treated realistically and on an equal footing.

The method developed in Ref. 9 (equivalent to a spatial decomposition of the Bardeen tunneling-Hamiltonian formalism) is used to calculate the current density distribution in terms of the wave functions determined separately for each electrode in the absence of the other. These wave functions are calculated starting with the results of Lang and Williams[10] on atomic chemisorption, as described in Ref. 9. The jellium model for the metal surface is used ($r_s = 2$); it can be expected to be adequate for a discussion of many of the properties that depend on the wave functions well outside the surface.

Let us consider an atom A adsorbed on the left-hand electrode and an atom B adsorbed on the right-hand electrode. Let us take Y to be the lateral separation (i.e., that parallel to the surface) of the atoms, and s to be the z-axis separation (i.e., that along the surface normal), with all distances measured from the nucleus of one atom to the nucleus of the other. Let I_{AB} be the total current flowing between the two electrodes with adatoms, and let I_A be the total current flowing for this same arrangement in the absence of atom B (but with the electrode on which atom B had been adsorbed remaining in place). Then we will concentrate on the quantity $\delta I = I_{AB} - I_A$, which picks out atom B as the tip, in the sense that for large lateral separations Y, this difference excludes the current flow between atom A on the left-hand side and the metal surface on the right-hand side, since such an extended surface would not be present in most tip models one would consider. (This difference also, of course, subtracts out the current between the two bare metal electrodes.)

Let us first discuss results for the total current obtained when the same atom (Na) on the right-hand electrode, taken as the tip, is scanned past several *different* atoms on the left electrode: Na, S, and He. These chemically very different atoms produce characteristically different tunneling-current behaviors. I construct a table of values of δI for various values of Y and s, so that by interpolation in this table, we can plot curves of tip distance s versus lateral separation Y for constant current δI. Such a set of curves is shown in Fig. 1. For each case in this figure, δI is held constant at the value it has for $s = 16$ bohrs (8.5 Å) and $Y = \infty$.

We note first in Fig. 1 that the maximum change in tip distance Δs is much smaller for S than for Na. In part this is because S sits closer to the surface than Na, and in part because the Fermi-level state density for S is appreciably smaller than that for Na, as seen in Fig. 2. (For the case of low bias considered here, only states near the Fermi level participate in the tunneling

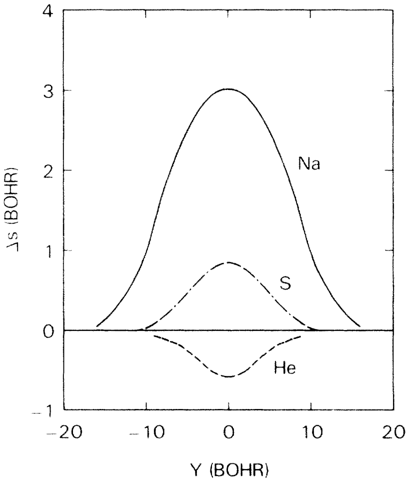

FIG. 1. Change in tip distance $\Delta s = s(Y) - s(\infty)$ vs lateral separation Y for constant δI, with $s(\infty) = 16$ bohrs. Tip atom is Na; sample adatoms are Na, S, and He. (1 bohr = 0.529 Å.)

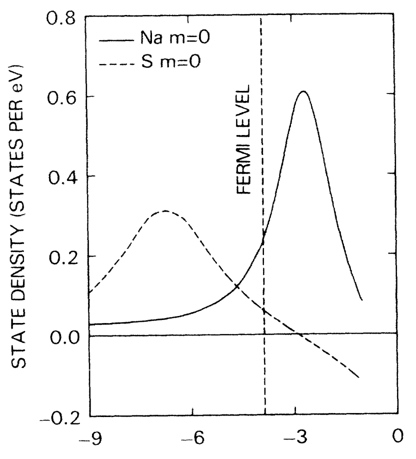

FIG. 2. Curves of the difference in eigenstate density between the metal-adatom system and the bare metal. The $3s$ resonance for Na and the $3p$ resonance for S are clearly visible. Only the component with azimuthal quantum number $m=0$ is shown, because $m\neq 0$ components make a much smaller contribution to the tunneling current (for lateral separation Y not too large)—cf. discussion in Ref. 9.

process.) Even more striking, however, is the fact that the change in tip distance for He is slightly negative. The He atom sits rather far from the surface, and so would cause a large enhancement of the tunneling current if there were to be even a small increase of the Fermi-level state density due to broadened levels of the atom. The closed valence shell is very far down in energy, however, and its only effect is to polarize metal states away from the Fermi energy, producing a decrease in Fermi-level state density (not visible on the scale of Fig. 2), which leads to the negative tip displacement. For analogous cases of adsorbed molecules that have practically no states of σ symmetry (this being most important in our problem—see Ref. 9) in the vicinity of the Fermi level, the tip displacement might be similarly small or even smaller (whether negative or positive). This could make such adsorbed molecules difficult to see in the scanning tunneling microscope.

Let us now discuss the spatial distribution of the current in our problem. We begin by considering the case in which the atom on the right-hand metal surface is absent, with the surface itself remaining. I show in Fig. 3 a contour map of j_z/j_0 for Na, with j_z the z component of the current density and j_0 the current density that would be present without the atom. Results are given only in a strip in the center of the vacuum barrier; much closer to the surfaces, the equation used is not adequate (see Ref. 9). Note that the highest-density contour shown only extends part way across the figure. This is a direct result of the fact that for a given nonzero ρ, the ρ component of the current density is largest at the left (see Ref. 9). A contour map of j_z/j_0 for the case of S is given in Fig. 4; the current

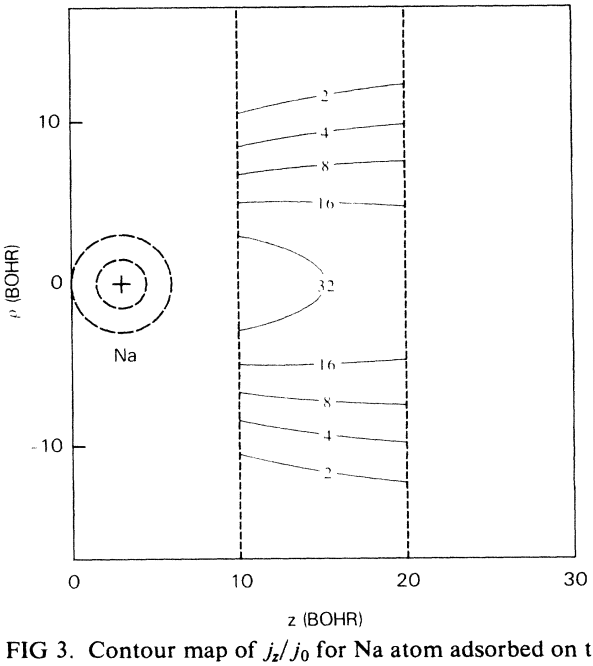

FIG 3. Contour map of j_z/j_0 for Na atom adsorbed on the left-hand electrode. Left- and right-hand edges of box correspond to the positive background edges of the two electrodes. The presence of the adsorbed atom is indicated schematically by two dashed circles with a cross at the equilibrium distance of its nucleus. The larger of the two circles is given a radius equal to this distance. (Corrects corresponding figure in Ref. 9.)

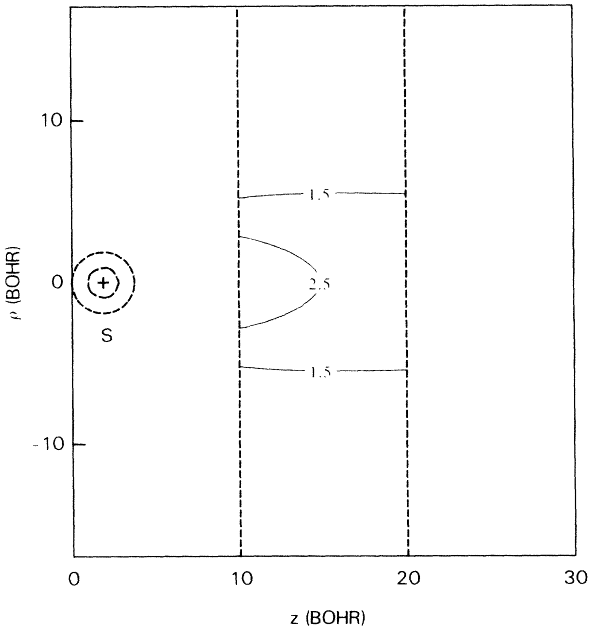

FIG. 4. Contour map of j_z/j_0 for S atom adsorbed on the left-hand electrode. (Corrects statements concerning this map in Ref. 9.)

here is much lower than for the Na case, for the reasons mentioned earlier. A similar map for He (not shown) exhibits only contours less than unity.

Current-density maps for the full two-atom case, with S on the left and Na on the right, are shown for several values of Y in Fig. 5. At the largest Y shown, the map is very similar to that given in Fig. 3 for Na alone; obviously the presence of the S atom would lead to a rather small z-axis displacement of an Na tip at this lateral separation. As Y is decreased, the fact that the z-axis displacement of the tip would have to grow to maintain constant current is clear. The spatial narrowing of the central channel roughly midway between the electrodes, in the bottom two contour maps, has the same explanation as the fact that the largest contour in the maps of Figs. 3 and 4 only extends part way across the figure (this channel can be thought of as composed of two such contours, one from each electrode).

Finally, in Figs. 6 and 7, I compare the tip-displacement curves of Fig. 1 with contours of both constant local density of states at the Fermi level and constant total density. Such a comparison was discussed by Tersoff and Hamann.[5] They showed that for the case in which the tip wave function is an s wave, the tip for constant current will follow a contour of constant Fermi-level local density of states, evaluated at the origin of the s wave (the atomic nucleus of the tip atom in our case). Since calculations of Fermi-level local densities of states at large distances are often not available, the total (energy-integrated) density, or even a superposition of free-atom densities,[5] is sometimes used as a rough approximation.

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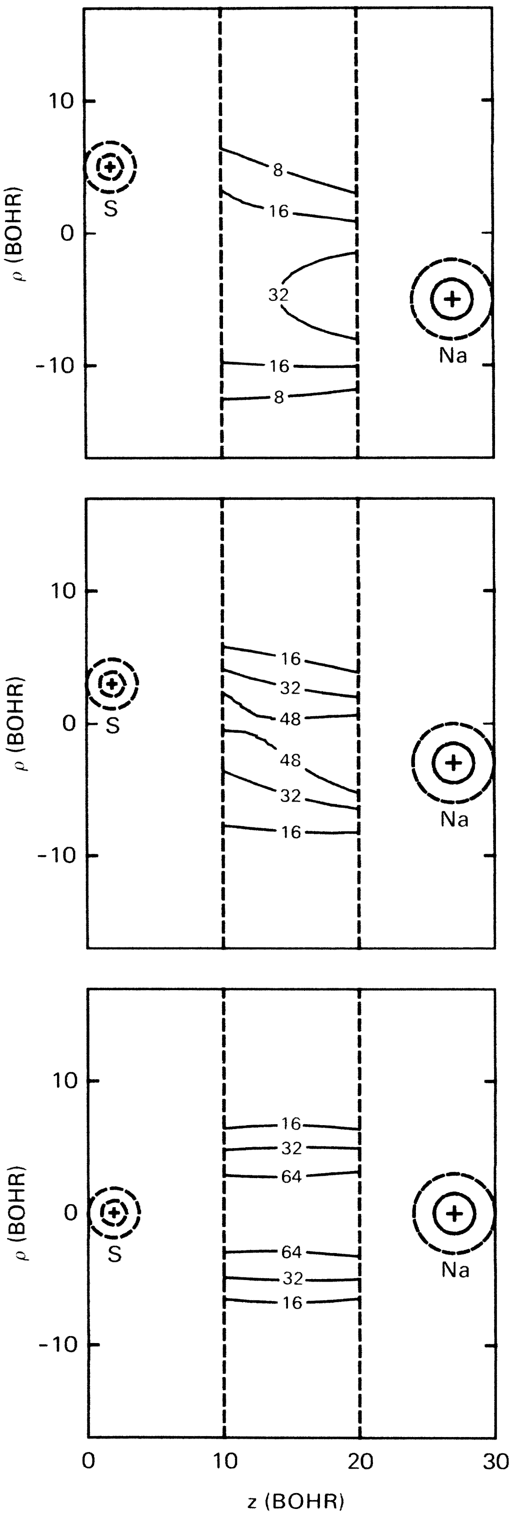

FIG. 5. Contour maps of j_z/j_0 for S adatom on the left-hand electrode and Na adatom on right-hand electrode for three values of lateral separation Y (10, 6, and 0 bohrs), in the plane normal to the surface that includes both atomic nuclei.

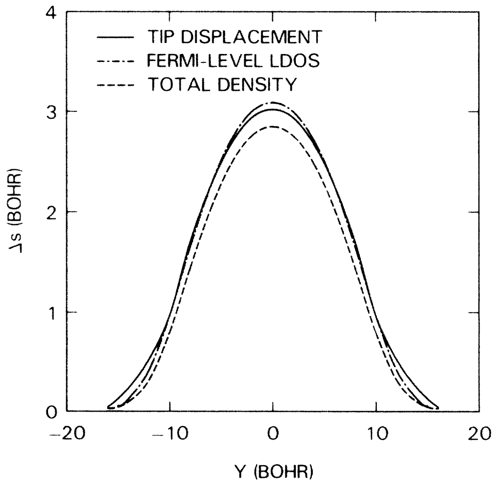

FIG. 6. Comparison of tip-displacement curve from Fig. 1 for Na adatom sample (and Na tip) with contours of constant Fermi-level local density of states and constant total density.

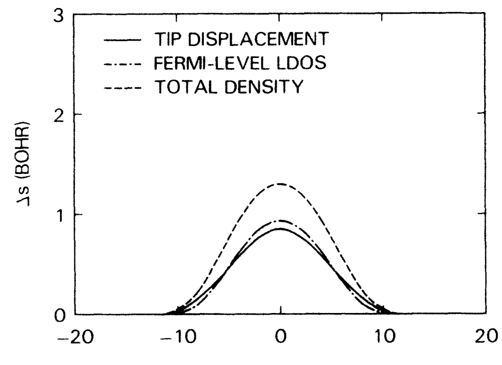

FIG. 7. Comparison of tip-displacement curve from Fig. 1 for S adatom sample (and Na tip) with contours of constant Fermi-level local density of states and constant total density.

tip) shown in Fig. 6, the tip-displacement curve, and the contours of constant Fermi-level local density of states, and constant total density, due to the sample, are all seen to be quite close. (The contour shown in each case is that at the position of the tip center when $Y=\infty$.) This will also be true for the case of the He sample, because the $1s$ wave function of the He valence shell, being quite deep in energy, is negligible at the tip position (so long as the tip is several angstroms away), leaving at this position only the polarized metal wave functions near the Fermi level. The case of the S adatom sample shown in Fig. 7 is slightly more complicated. The contour of constant local Fermi-level state density indeed follows the tip-displacement curve, but the total-density curve is somewhat higher. The reason for this is simply that the center of the largely filled valence resonance corresponding to the $3p$ state is not so far below the Fermi level that it cannot make a contribution to the total density at the tip position for reasonable tip-sample distances (see Fig. 2), unlike the He case. The curves are nonetheless not that far from one another.

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