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INFLUENCE OF ATOMIC AND ELECTRONIC STRUCTURE OF A TIP ON STM IMAGES

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Theoretical studies of the influence of electronic and atomic structure of a tip on scanning tunneling microscopy images are presented. Results are discussed for the scanning of Al(001) and Al(001)+Xe surfaces performed within aluminum and nickel tips of a different geometry.

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1. Introduction

This article presents some theoretical studies related to a general problem of interpretation of scanning tunneling microscopy (STM) results. More specifically, we have investigated the influence of electronic properties of a tip as well as its geometry on the multichannel tunneling of electrons in a tip-sample system.

In particular, we have discussed how the electronic and atomic structure of different tips could change the topography of STM images. This problem has been considered in detail for STM images of a single Xe atom adsorbed on an Al(001) surface as well as for those of a clean Al(001) surface; our calculations have been performed for Al and Ni tips of a different geometry.

2. Model and method of calculation

To calculate the tunneling current in a tip-sample system, we have used the non-equilibrium Green-function method developed by Keldysh [1]. This approach was used by Caroli et al. in theoretical investigations of the tunneling phenomena in microstructures [2, 3]. Later it was also adopted for STM study [4, 5]. A detailed description of this method is presented in [6]. It is shown there that for calculation

of a tunneling current, the matrices of the Green functions and the density of states for the tip and the sample are needed.

In our study, calculations of the Green functions and the density of states of the sample have been done within the self-consistent LCAO approach, described in detail in [7]. On the other hand, the tip has been described using the cluster-Bethe-lattice method: the top of a tip is represented by a cluster of a few atoms, while the influence of the rest of the tip is simulated by a Bethe lattice connected to this cluster (cf. Fig. 1).

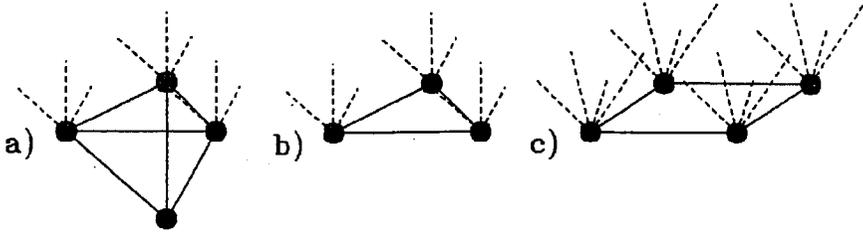


Fig. 1. Different geometries of the top part of a tip considered: sharp tip with a single atom located at the apex (a), and flat tips (i.e., without the apex atom) formed by three (b) or four (c) atoms.

Such a model enables us to consider different geometries of the top of a tip. We have assumed it has a form of pyramid with a single atom at the apex and three atoms at the basis (cf. Fig. 1a). For comparison, we have also considered two tips without the apex atom, i.e., with a flat top formed by three or four atoms (cf. Figs. 1b and c, respectively). In all the cases shown in Fig. 1 the geometry of the tip is determined by the fcc structure of a considered metal (i.e., Al or Ni), with distances between the atoms forming the tip equal to those in the bulk.

3. Results and discussion

3.1. Al(001)+Xe surface

First we shall discuss the influence of the tip properties on STM images of a single Xe adatom on Al(001) surface. The results obtained within the sharp aluminum tip (as in Fig. 1a) are shown in Fig. 2a, where the conductance evolution along the line passing above the adsorbed Xe atom is presented for different tip-sample distances d (constant height mode for each d is assumed). It follows that for large enough d the protrusion of Xe adatom has a typical shape with one maximum located exactly above the adsorbed atom. For $d \approx 4.2 \text{ \AA}$ the conductance-dependence curve becomes flat at the top, and for still smaller d ($d < 4 \text{ \AA}$) it starts to exhibit a crater-like shape with a minimum located above the adatom.

This behavior is due to electronic properties of the aluminum tip. Indeed, Figs. 2b-d present evolution of the conductance resulting from the tunneling via s , p_z , and p_y orbitals of the apex atom, respectively. As it can be seen, for greater tip-sample distances the main contribution to the total conductance comes from

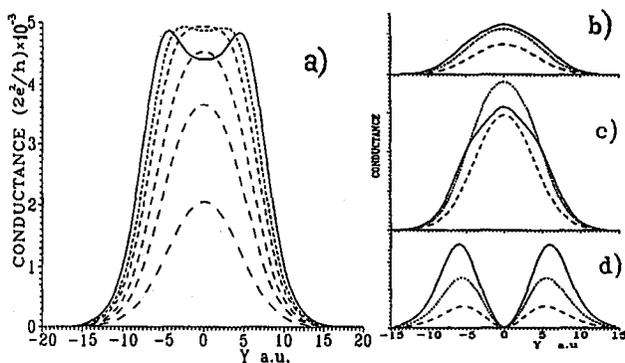


Fig. 2. (a) Evolution of the conductance along the line passing above Xe atom adsorbed on Al(001) surface and located at $y = 0$, obtained within a sharp Al tip (as in Fig. 1a). Different curves correspond to different heights d of the tip above Xe adatom: $d = 3.1$ Å (solid curve), $d = 3.48$ Å, $d = 3.76$ Å, $d = 4.2$ Å, $d = 4.6$ Å, and $d = 5.33$ Å (dashed curves with an increasing length of dash corresponding to an increasing value of d). (b), (c), and (d) represent the s , p_z , and p_{xy} orbital contribution to the total conductance, respectively. Solid, dotted, and dashed curves correspond to $d = 3.1$ Å, $d = 3.76$ Å, and $d = 4.6$ Å, respectively.

the tunneling via s and p_z orbitals (p_z being perpendicular to the surface). Under such conditions the current flows mainly from the region located directly below the tip, thus the conductance reaches its maximum value just above the Xe adatom. On the other hand, p_y and p_x orbitals are parallel to the surface, so the tunneling via them takes place not from the region just below the tip, but rather from its surrounding. As a result, the conductance via p_{xy} orbital has two maxima situated symmetrically with respect to the position of Xe atom (cf. Fig. 2d). Since tunneling via p_y and p_x orbitals becomes more effective for smaller tip-sample distances, this considerably influences the evolution of the total conductance and creates a crater-like shape (cf. Fig. 2a for $d < 4$ Å).

Figure 3 presents the corresponding results obtained within a flat aluminum tip with a triangle top (as in Fig. 1b). Three topmost atoms are equally active in electron tunneling, which leads to a considerably higher conductance and a broader Xe protrusion (cf. Fig. 3a). For smaller tip-sample distances, the conductance-dependence curve shape is strongly influenced by the atomic structure of the flat top of the tip — as a consequence, the image of a single Xe adatom has a complicated and untrue structure (cf. Fig. 3b). For greater d , when the tunneling takes place again mainly via s and p_z orbitals, the effect of the atomic structure of the tip becomes less important.

3.2. Clean Al(001) surface

First, we shall discuss the results obtained within a sharp aluminum tip (cf. Fig. 1a). Figure 4a presents evolution of the total conductance along the Al(001) surface (constant height mode) for the tip-sample distance $d = 3.62$ Å, but this result is typical also of greater distances. Under such conditions, tunneling

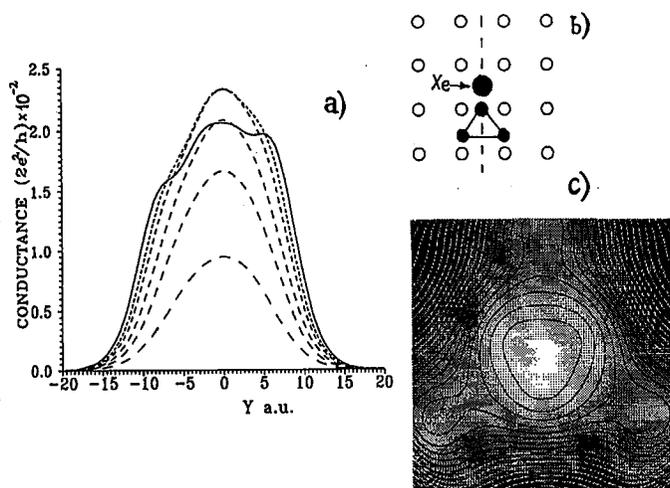


Fig. 3. (a) Evolution of the conductance along the line passing above Xe atom adsorbed on Al(001) surface, obtained within a flat Al tip with a triangle top (as in Fig. 1b). Different curves correspond to different heights d of the tip above Xe adatom: $d = 3.1 \text{ \AA}$ (solid curve), $d = 3.48 \text{ \AA}$, $d = 3.76 \text{ \AA}$, $d = 4.2 \text{ \AA}$, $d = 4.6 \text{ \AA}$, and $d = 5.33 \text{ \AA}$ (dashed curves with an increasing length of dash corresponding to an increasing value of d). (b) Tip orientation with respect to the sample surface. Solid and open circles denote the positions of atoms from the top of the tip and from the surface, respectively, while the dashed line shows the direction of a tip displacement. (c) Image of the Xe adatom calculated for $d = 3.48 \text{ \AA}$.

via s and p_z orbitals of the apex atom takes place mainly from the region located directly below the tip, hence the s and p_z contributions to the total conductance reach maximum whenever the tip is located above a surface atom (cf. Figs. 4b and c). Because the tunneling via p_x and p_y orbitals takes place not from the region located directly below the tip, but rather from its surrounding, the p_{xy} contribution has maximum above the hollow points of the surface structure (cf. Fig. 4d). For greater tip-sample distances, however, the tunneling via p_{xy} orbitals is not effective (10–16% of the total conductance), so the evolution of the conductance along the surface is determined by s and p_z contributions. Therefore, the obtained image (cf. Fig. 4a) shows a normal topography (conductance has maxima above surface Al atoms).

Figure 5 presents the corresponding results for $d = 2.34 \text{ \AA}$. For such small distances, when the tip is above a surface atom, the s and p_z contributions quickly reach saturation, so they become higher above the hollow and bridge points than above the surface atoms (cf. Figs. 5b and c). Moreover, the p_{xy} contributions are more important for smaller d (about 78% of the total conductance) and they show maxima above the surface atoms as well as the hollow points (cf. Fig. 5d). The superposition of all the contributions gives now the image with an inverted topography (cf. Fig. 5a — the conductance has maxima above the hollow points).

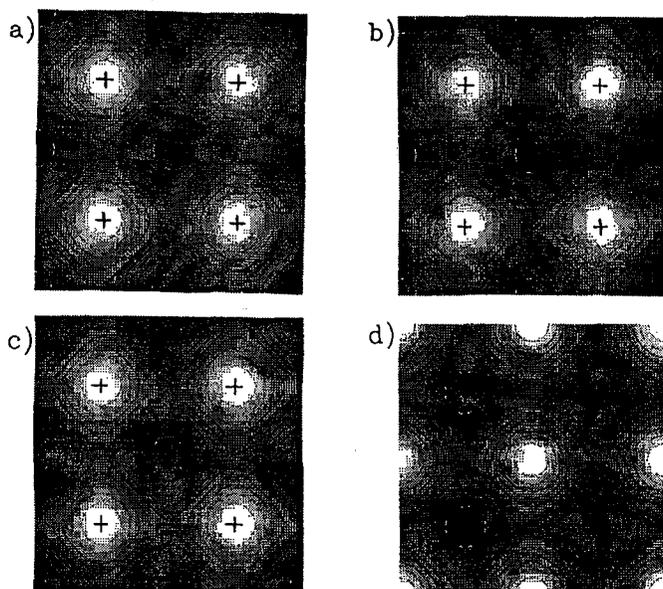


Fig. 4. (a) Image of a clean Al(001) surface (constant height mode), obtained within a sharp Al tip (as in Fig. 1a) for $d = 3.62 \text{ \AA}$. (b), (c), and (d) represent the conductance components connected with the tunneling via s , p_z , and p_{xy} orbitals, respectively. Black crosses denote the positions of surface atoms.

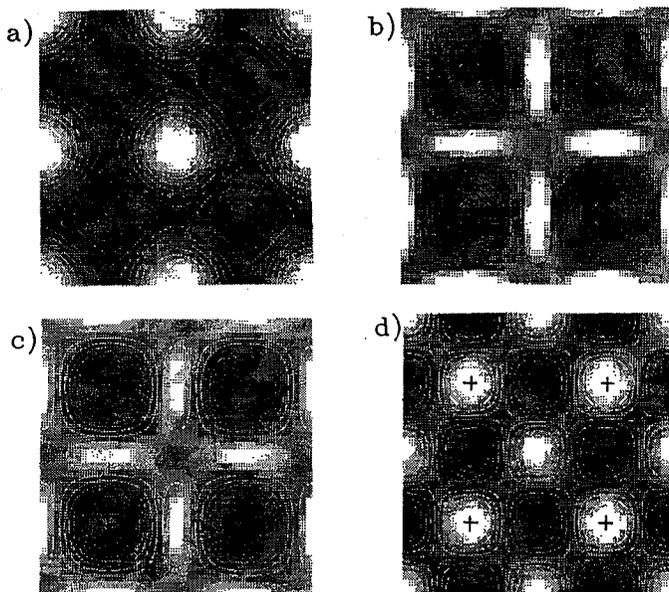


Fig. 5. The same as in Fig. 4, but for $d = 2.34 \text{ \AA}$.

The case of a flat Al tip (i.e., without the apex atom) has been studied for the tip with a triangle and square top (cf. Fig. 1b and c, respectively). The evolution of the conductance is determined now by the superimposed tunneling through s , p_z and p_{xy} orbitals of all the three or four atoms forming the top of a tip. Figure 7 presents the STM images calculated for $d = 3.62 \text{ \AA}$ (representative also for greater distances). Then the tunneling takes place mainly through s and p_z orbitals, from the regions located directly below the respective top atoms. The calculations have been performed for different orientations of the tip with respect to the surface structure, as it is schematically shown in Figs. 6a-c. It follows from the obtained

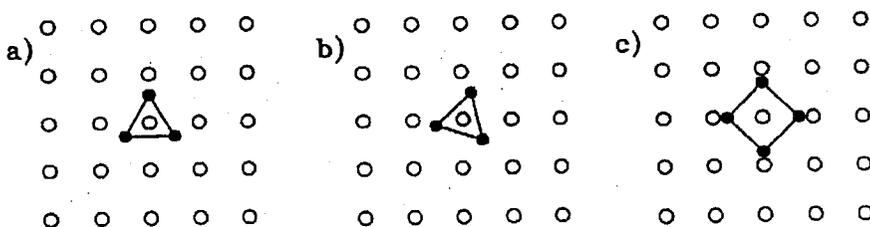


Fig. 6. Different orientations of a flat Al tip with respect to the surface atomic structure of Al(001). (a) and (b) correspond to the tip with a triangle top ((b) being rotated by 15 degrees as compared to (a)), while (c) represents the tip with a square top.

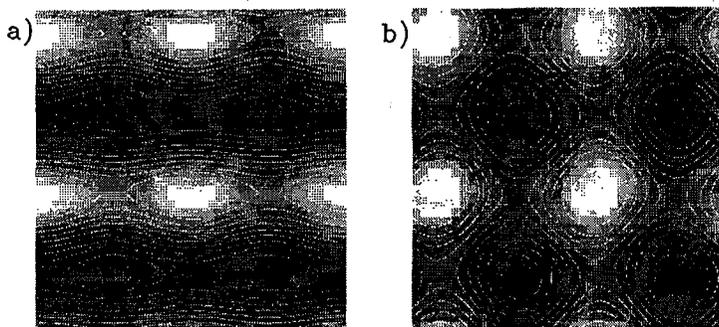


Fig. 7. Images of a clean Al(001) surface (constant height mode), obtained within a flat Al tip with a triangle top for $d = 3.62 \text{ \AA}$. (a) and (b) correspond to the tip orientations as in Fig. 6a and b, respectively.

results that the tip with a triangle top, oriented as in Fig. 6a, gives the image with an untrue structure of rows (cf. Fig. 7a). But rotating this tip by 15 degrees (i.e., as in Fig. 6b) leads to the image with a structure of peaks reproducing the geometry and distances of the surface structure (cf. Fig. 7b). It should be noticed, however, that in both cases the positions of conductance maxima do not correspond to the true positions of surface atoms.

Figures 8 and 9 present the images of a clean Al(001) surface for a variable tip-sample distance d , obtained within a flat Al tip with a triangle and square top,

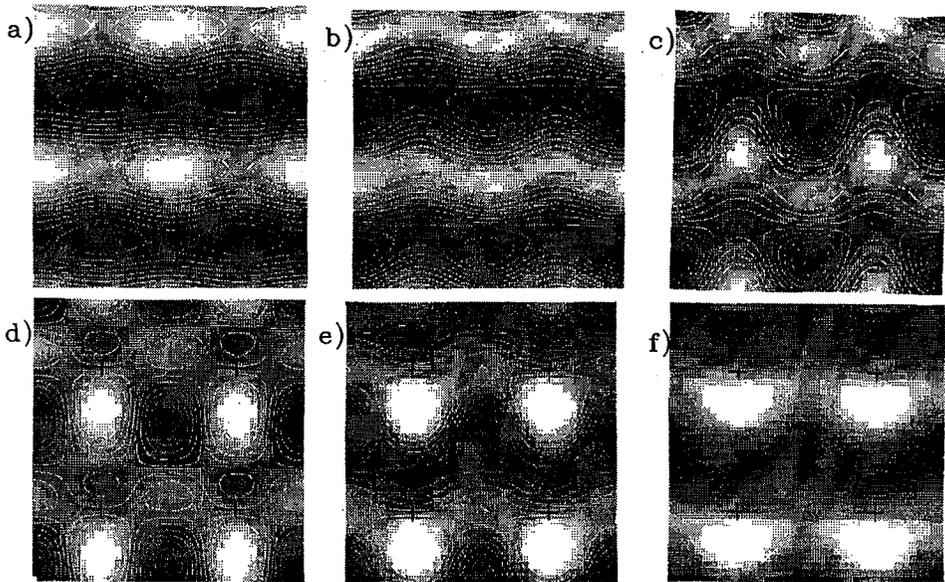


Fig. 8. Set of images of a clean Al(001) surface, obtained within a flat Al tip with a triangle top and oriented as in Fig. 6a, for a decreasing tip-sample distance d : (a) 3.62 Å, (b) 3.13 Å, (c) 2.98 Å, (d) 2.84 Å, (e) 2.7 Å, and (f) 2.34 Å.

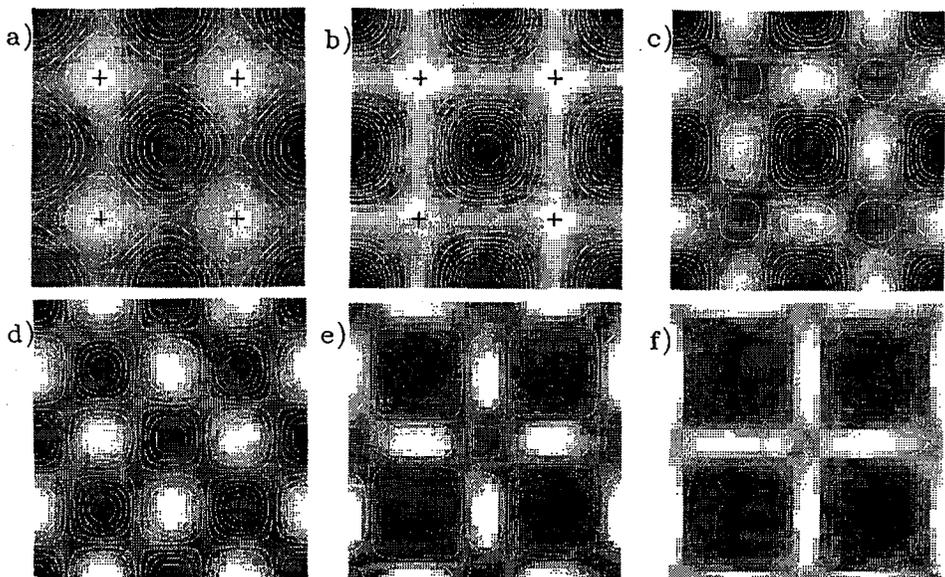


Fig. 9. Set of images of a clean Al(001) surface, obtained within a flat Al tip with a square top and oriented as in Fig. 6c, for a decreasing tip-sample distance d : (a) 3.62 Å, (b) 3.27 Å, (c) 3.13 Å, (d) 2.98 Å, (e) 2.7 Å, and (f) 2.34 Å.

and oriented as in Fig. 6a and c, respectively. For s and p_z orbitals, tunneling from the region located below the respective tip atom becomes — with decreasing d — less effective than from its surrounding. This effect, as well as the more significant tunneling via p_{xy} orbitals, cause important changes of the obtained images. As a result, they have complicated topographies, very different from a clean Al(001) surface atomic structure.

To study the influence of d orbitals of atoms forming the tip on STM images, calculations have been also performed for a triangle flat tip made of Ni atoms. The images obtained for $d = 3.62 \text{ \AA}$ are shown in Fig. 10 for two different orientations (as in Figs. 6a and b, respectively). For such a distance almost 85% of the current flows via s orbitals of Ni atoms. In contrast to the Al tip, however, the s orbitals of Ni atoms do not contribute to the current only from the regions located directly below these atoms — this is due to a greater radius of s orbital of Ni atom as compared to Al atom. As a consequence, the corrugation implied by s orbitals is very small, and the topography of the images shown in Fig. 10 is caused mainly by d and p_z orbitals of the topmost atoms. The tip orientation as in Fig. 6a gives,

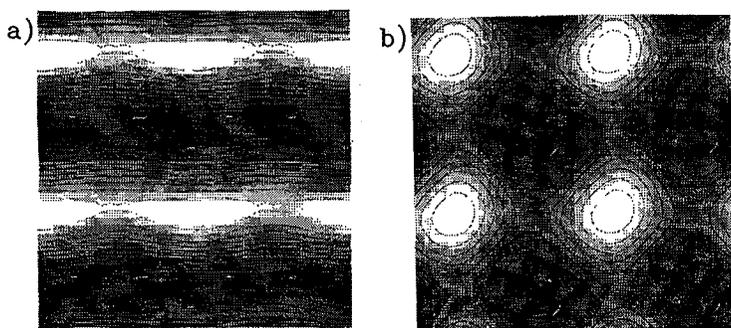


Fig. 10. The same as in Fig. 7, but for a Ni tip.

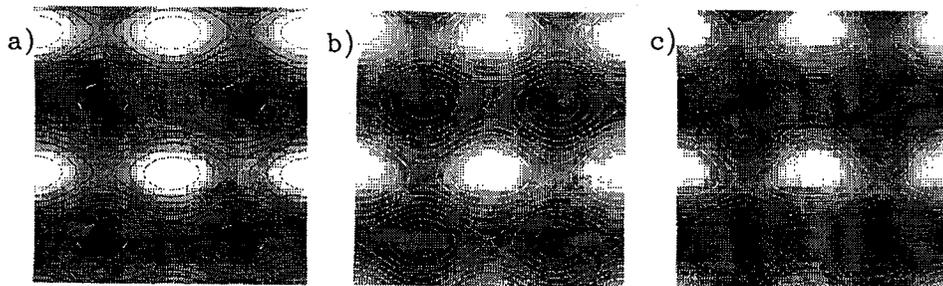


Fig. 11. Set of images of a clean Al(001) surface, obtained within a flat Ni tip with a triangle top and oriented as in Fig. 6a, for a decreasing tip-sample distance d : (a) 3.13 \AA , (b) 2.7 \AA , and (c) 2.34 \AA .

like in the case of Al tip, an image with the structure of untrue rows, while the tip rotation by 15 degrees changes completely this topography (cf. Fig. 10b).

For smaller distances (cf. Fig. 11), the tunneling current is dominated entirely by the contribution of d orbitals. Because of the strong localization of these orbitals, their current components come mainly from the regions located directly below the respective tip atoms. This explains the topographies of the obtained images (cf. Figs. 11a-c). As it can be seen — contrary to the case of Al tip — decreasing the tip-sample distance does not lead to any important changes of the STM images.

4. Conclusions

Theoretical studies presented in this paper indicate that the electronic and atomic properties of a tip considerably influence STM images. This effect seems to be important for the investigation of structural properties of sample surfaces within STM technique.

We have found that flat tips (i.e., without apex atom) give images of an Al(001) surface with an atomic resolution. On the other hand, their topographies could have untrue structures and features, which is caused by the geometry of the flat top of a tip, its orientation with the respect to the surface structure, and electronic properties of the atoms forming the tip. The d states of the tip atoms give an important contribution to electron tunneling in the tip-sample system, especially for small distances; a strong localization of d orbitals results in a local character of tunneling through them, so it takes place mostly from the regions located directly below the tip atoms.

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