

Influence of the atomic and electronic structure of the tip on STM images and STS spectra

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Abstract

Theoretical studies of the influence of electronic and atomic structure of a tip on STM images and STS spectra are presented. This is discussed for the scanning of clean Al(001) surface performed within aluminium tips of a different geometry. The influence of d states of a tip on STS spectra for the Ni-tip/Al(001)-sample system is also studied. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

We have discussed how the electronic and atomic structure of different tips could change the topography of STM images. This important problem has been studied previously by several authors; for example the influence of the tip was discussed was discussed for the STM images of graphite or Mo(001)+S(2×2) surfaces [1,2]. Our work presents studies of this problem for the scanning of clean Al(001) surface. In the case of Al, the STM images of Al(111) [3] show an unexpected high corrugation – this effect has been considered in some theoretical papers [4–6]. In our present studies we want to show how the properties of the tip could influence the variation of the conductance along the surface of the nearly-free-electron metal.

Our calculations have been performed for Al tips of a different geometry; an Al tip could be

obtained via the mechanical contact of another kind of tip (Ni, W etc.) with an Al surface.

We have also discussed the influence of d states of a transition metal tip on the STS tunneling spectra, which represents a complex convolution among the tip and sample electronic states [7,8]. It seems that the influence of localized d states of the tip on STS spectra is still not clear – this problem has been considered here for Ni-tip/Al(001)-sample system.

2. Model and method of calculations

For description of the tunneling current we have used the non-equilibrium Keldysh–Green-function method described in detail in Ref. [9]. This approach is very useful for the studies of the coherent tunneling through different orbitals in

tip–sample system. The method applied is not based in a perturbation theory, and therefore it is accurate even at small distances (contrary to the Tersoff–Hamann approach [10], for example).

In our studies, the calculations of the Green functions and the density of states of the sample (necessary for the calculation of the tunneling current) have been done within the self-consistent LCAO approach.

The tip has been described self-consistently using the cluster–Bethe-lattice approach with the top of the tip represented by the cluster of a few atoms, while the influence of the rest of the tip is simulated by the Bethe lattice. We have assumed that the tip has a form of pyramid with a single atom at the apex and three atoms at the basis. We have also considered a tip without the apex atom, i.e. with a flat top formed by three atoms. In all cases the geometry of the system is determined by the fcc structure and distances between the atoms forming the tip are equal to those in the bulk of a metal.

3. Results and discussion

3.1. Scanning of clean Al(001) surface

We shall discuss first the results obtained within sharp pyramidal tip.

Fig. 1(a) presents the evolution of the conductance along Al(001) surface for tip–sample distance $d=3.64 \text{ \AA}$, but this form of evolution also

occurs for greater d (d is defined as the distance between the top atom of the tip and the surface Al layer). For such distances the most effective tunneling is via s and p_z orbitals of the apex atom (p_z is oriented perpendicular to the surface), and it takes place mainly from the region located directly below the tip, which gives the image with the normal topography (maxima above surface atoms).

For smaller distances (see Fig. 1(b)), when the tip is above surface atom, the s and p_z contributions quickly reach saturation and their values above the hollow and bridge points became higher than above surface atoms. This effect, together with a growing contributions from the tunneling via p_{xy} orbitals, leads to the image with the inverted topography (maxima above the hollow points). The inverted STM topography at very small d was also found by Doyen for Pd(001) [5].

In the case of a flat tip (without apex atom) the top is built by three atoms, which are equally active in the tunneling between tip and sample. We have considered here two different orientations of this triangle top with respect to the atomic structure of Al(001) surface (see Fig. 2(a) and (b)). The images presented in Fig. 2(a) and (b) were calculated for $d=3.64 \text{ \AA}$ (a greater d gives the same form of topography). The evolution of conductance is now determined by the superposition of the tunneling via s , p_z and p_{xy} orbitals of three Al atoms from the triangle top. As a consequence the images strongly depend on the orienta-

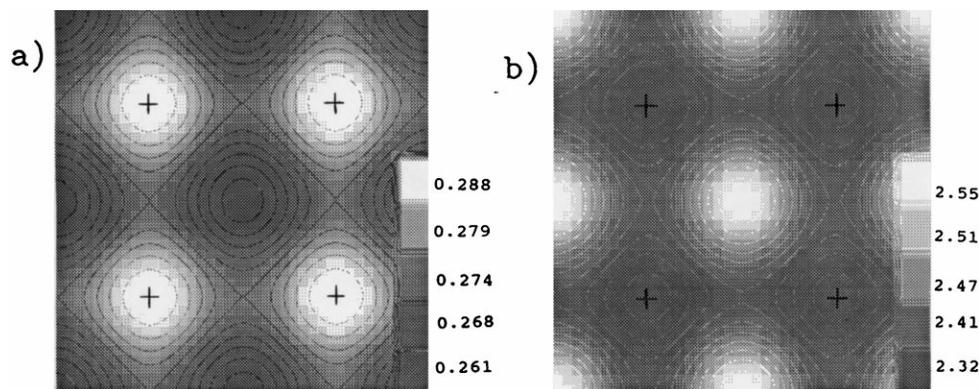


Fig. 1. Image of the clean Al(001) (constant height mode) obtained within sharp aluminium tip for: (a) $d=3.64 \text{ \AA}$, (b) $d=2.35 \text{ \AA}$. Black crosses denote the positions of surface atoms. Conductance is given (gray-scale definition) in $2e/h$ units.

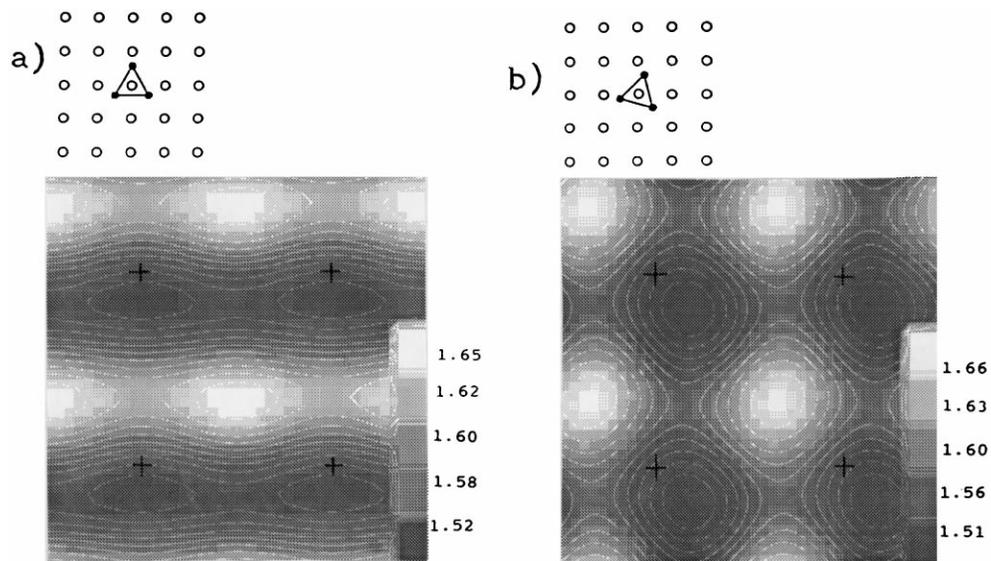


Fig. 2. Images of clean Al(001) obtained within flat triangle aluminium tip for $d=3.64$ Å. These two images correspond to two different orientations of the tip with the respect to the surface structure (shown schematically above corresponding images). Conductance is given in $2e/h$ units.

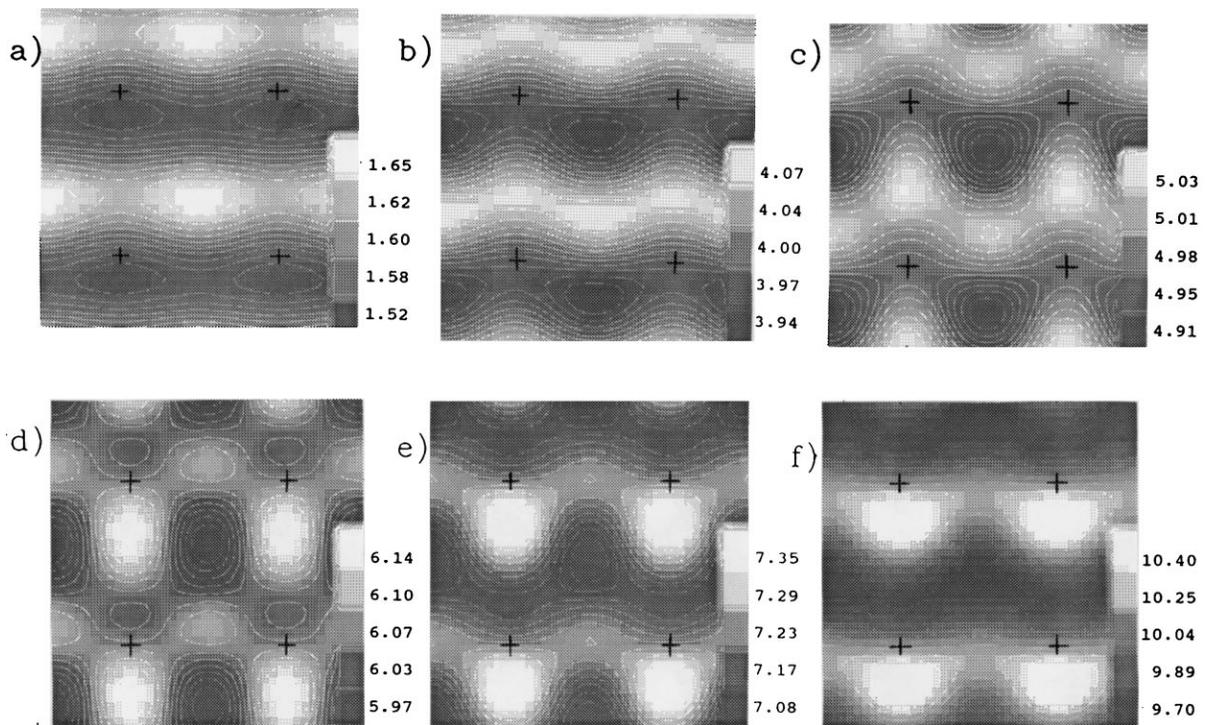


Fig. 3. The set of images of clean Al(001) obtained within flat triangle aluminium tip (orientation as in Fig. 2(a)) for different distances d : (a) 3.64 Å, (b) 3.13 Å, (c) 2.98 Å, (d) 2.84 Å, (e) 2.7 Å, (f) 2.34 Å. Conductance is given in $2e/h$ units.

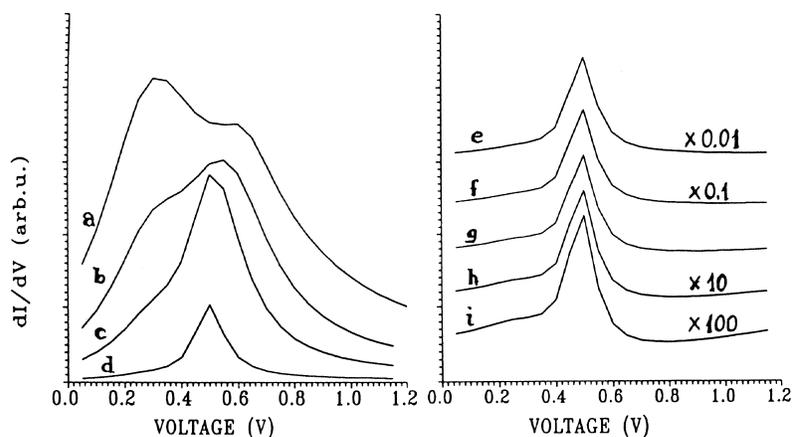


Fig. 4. Differential conductance vs. applied voltage for the Al(001)/Ni-tip system with the maxima caused by d states of the apex atom from the tip. Different curves correspond the following values of d : (a) 2.56 Å, (b) 2.9 Å, (c) 3.2 Å, (d) 3.9 Å, (e) 4.7 Å, (f) 5.75 Å, (g) 6.4 Å, (h) 7.05 Å, (i) 7.7 Å.

tion of the tip. For greater distances the tunneling takes place mainly through s and p_z orbitals, from the regions located directly below the respective tip atoms; then the orientation as in Fig. 3(a) gives the image with untrue structure of rows. Rotation of the tip by 15° changes considerably this topography: instead of rows the image shows the structure of peaks reproducing the geometry and distances of the surface structure (see Fig. 2(b)). In both cases the positions of conductance maxima do not correspond to the true positions of surface atoms.

Fig. 3(a)–(f) presents the set of images of Al(001) surface for a few decreasing distances d ; calculations were performed within the same flat tip as before (triangle top), oriented as in Fig. 2(a). As already mentioned, when d decreases, the tunneling through s and p_z from the region of the surface located directly below the tip atom becomes less effective than from that the surroundings. This effect, as well as the more significant tunneling via p_{xy} orbitals, leads to important changes in topographies of images obtained for decreasing d . As a consequence, these images could show complicated topographies, very different from the true surface structure (Fig. 3(a)–(f)).

3.2. STS: Ni-tip/Al(001)-surface system

In this section we shall discuss the influence of d orbitals of the tip atoms on the LDOS spectra

detected by STS. These calculations have been performed for the system of a clean Al(001) surface and a sharp pyramidal Ni tip. The d orbitals of the apex atom form a structure of sharp peaks located just below the Fermi level. To check their influence on STS spectra we have computed the differential conductance as a function of applied voltage (see Fig. 4). Assuming that the tip is located above a surface atom, different distances between the tip and sample surface have been considered. The strong localization of d orbitals on Ni apex atom causes the tunneling via these orbitals to be most effective for very small tip–sample distances. Therefore, for $d < 3$ Å Fig. 4 shows a structure of peaks and shoulders connected with particular d states. For greater distances this structure disappears and d states are represented only by a single sharp peak. Anyway, the d states from the apex atom always appear in the STS spectra even for large distances.

4. Conclusions

We have found that flat tips (i.e. without an apex atom) give the images of Al(001) with atomic resolution. On the other hand, topographies of these images could have untrue structures and features – they are caused by the geometry of the flat top of the tip, its orientation with the respect

to the surface structure, and electronic properties of the tip atoms. Our calculations show also that d states of the apex atom from the tip could considerably modify the LDOS spectra detected by STS.

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