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STM "TIP CHANGES" - A POSSIBLE TOOL FOR TIP CHARACTERIZATION

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ABSTRACT. A method based on the detailed analysis of STM tip changes is proposed for the investigation of tip cluster structure. As proposed by Mizes et al [2] the tunneling current for a multiple tip is considered to be produced by the superposition of currents corresponding to the individual tip atoms. Good agreement is found between experimental results for PtIr tips and computer simulations for a Pt_{15} [110] tip cluster. From the modification of the acquired image during imaging HOPG the modifications of the tip structure may be inferred.
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Introduction

Scanning tunneling microscopy (STM) opened a new era in surface science by allowing to study the topography, and various characteristics of metallic, and semiconducting surfaces in atomic scale. Several challenging problems in theories of surface physics have been induced by STM. On the other hand a frequently met problem is the interpretation of "strange or abnormal" images (i.e., sudden changes of the image during the scan - tip changes -, periodical appearance of hillocks, etc).

In the present paper a possible explanation is proposed for *Highly Oriented Pyrolythic Graphite* (HOPG) images showing *tip changes*, *left-right asymmetry* (cf. fig.1). These images were taken at our laboratory in atmospheric conditions, and at room temperature with a *PtIr* tip. The interpretation of these phenomena is based on the work of Mizes et al [2]. According to this paper an image given by a two atom tip may be considered as a superposition of two shifted images. The authors suggest to interprete the obtained images as a consequence of changes of the physical state of the microtip participating in the acquisition of the image.

Experimental results, and discussion

A mechanically sharpened *PtIr* tip was scanned in air at room temperature over HOPG. Constant current topographs were recorded when applying tunneling currents in the range of *1 nA* at a bias of *100 mV*, at a scan speed of *986 Å/sec* (the scan speed does not have a marked influence on the image structure). In fig.1 a tip change is shown where before the change the upper regions of the left and right image are identical and the atomic details are poorly resolved. After the tip change an improved resolution is found and the left and right images are negative to each other. (It should be emphasized that in several cases similar differences between the left, and right images have been received, the image in fig.1 is only one example of these images.)

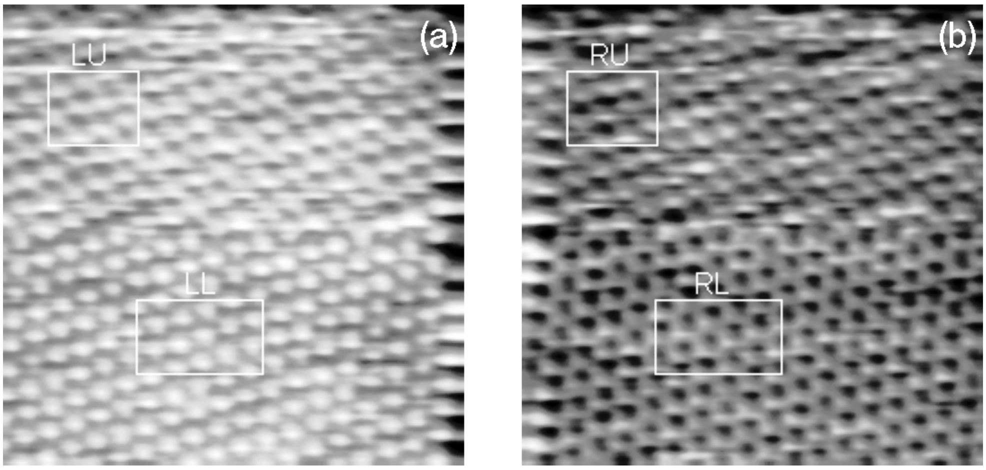

Fig.1 STM image ((50x50)A2) of HOPG with tip change
a) scanning from right to left, b) scanning from left to right.

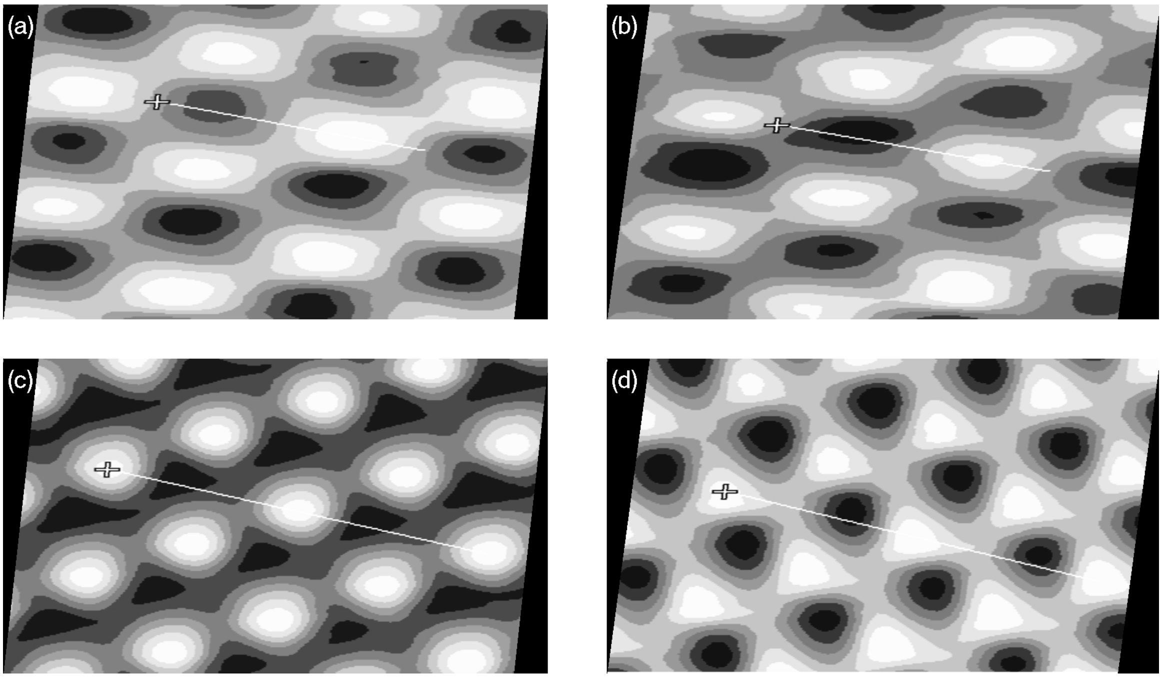

Fig.2 Skew corrected results of the calculation of kernel averages for the four image regions separated from fig. 1a and fig. 1b; a) left upper, b) right upper, c) left lower, d) right lower.

The exact location of the tip change was determined using autocorrelation technique. The two images were separated into four parts: left upper (LU), left lower (LL), right upper (RU) and right lower (RL) ones. For each of these four images autocorrelation analysis was done and unit cell averages were calculated.

The results are shown in fig.2. The local maxima and minima determined by a special program allowed us to draw accurate line cuts. The kernel averages received in this way show more clearly that LU is coincident with RU and RL is the negative of LL. This statement is also supported by the line cuts shown in fig 3.

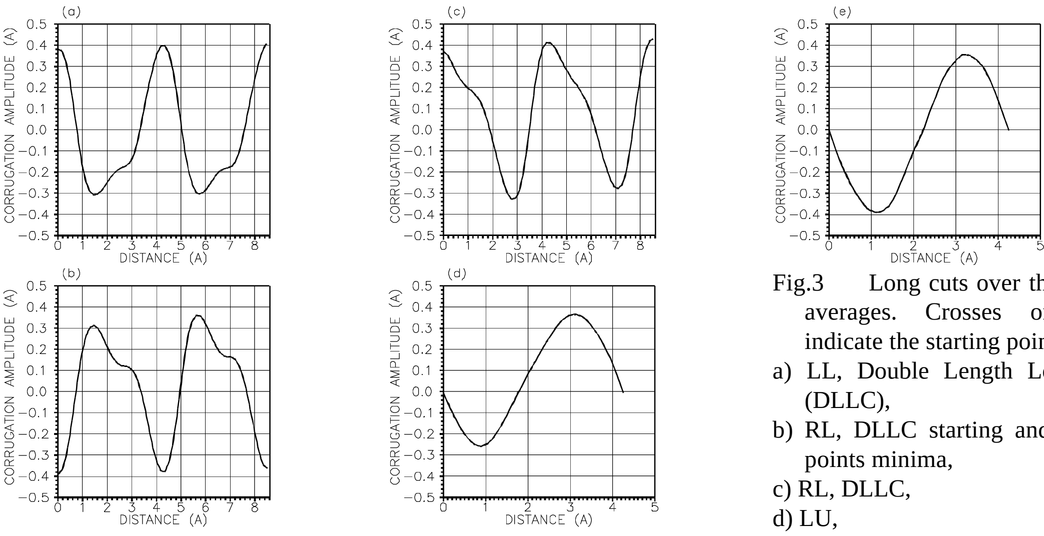

Fig.3 Long cuts over the kernel averages. Crosses on fig.2 indicate the starting point;

a) LL, Double Length Long Cut (DLLC),
b) RL, DLLC starting and ending points minima,
c) RL, DLLC,
d) LU,
e) RU

Inverted images of HOPG very similar to our RL one are frequently observed when using *Pt* tips (ref [3]). A possible explanation of these images may be based on the model calculations carried out by Tsukada, et al [1].

Let us examine the calculated tunnel current intensities from ref [1] for clusters $W_{10}[111]$ and a $W_{9}[111]$ scanned over HOPG. The line cuts in the "normal" directions, i.e. those joining a maximum with one of its closest neighbours - *"short cuts"* - show only little difference (fig. 4a.). In fig. 4b the line cuts in a direction joining a maximum with its neighbour from the second sphere of coordination - *"long cut"* -. Here the difference between the two image structures is more clear. These leads to the conclusion that for evaluation of images the long cuts are necessary, too.

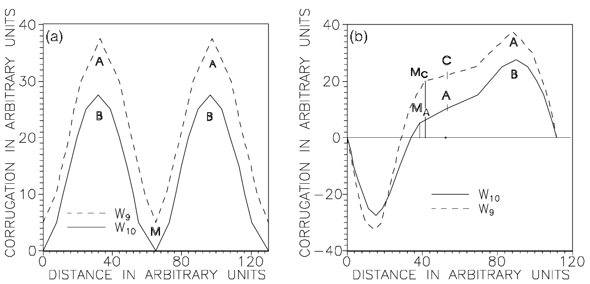

Fig.4 Line cut profiles from calculated data of ref. [1] for W_{10} and W_{9} clusters scanning over HOPG;

a) short cuts,
b) long cuts.

The right hand side of fig. 1a, and the left hand side of fig.1b show that there is a strong interaction between the tip and the sample i.e. when changing course, the tip has to suffer an increased friction. Let's assume the active microtip to be a cluster oriented along the *[110]* direction with a one atom apex. The cluster is built up of 16 atoms. If the apex atom is removed a Pt_{15} cluster is formed with a plane of four identical atoms at the corners of a rectangle with the dimensions of a and $a / \sqrt{2}$, where $a = 3.9158$ Å is the lattice constant of *Pt*. This means that $a / \sqrt{2} = 2.7688$ Å, close to the value of *2.46 Å* which is the distance of the B sites in HOPG. When assuming each tip atom as an individual microtip and the global image as a superposition of the four individual images, normal and abnormal HOPG images may be produced as a function of the rotation of the *Pt [110]* plane relative to the graphite lattice.

In order to reproduce the experimentally observed images a HOPG image was simulated applying the superposition of three plane waves with propagation vectors at angles *120*^{o} as used in ref [2,4]. The four atom *[110] Pt* plane, and the simulated normal HOPG image were convoluted. The images obtained for different angles of rotations of the *Pt* Fourier transform with respect to the HOPG Fourier transform are shown in fig.6 and fig. 7. These images are in good agreement with the experimental images.

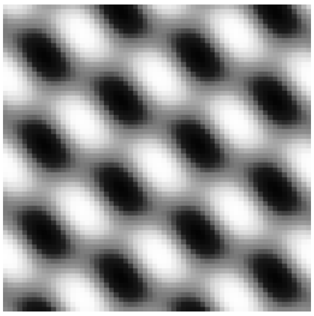

Fig.6 Simulated image corresponding to LU (RU). Rotation angle of HOPG FT 46^{o}.

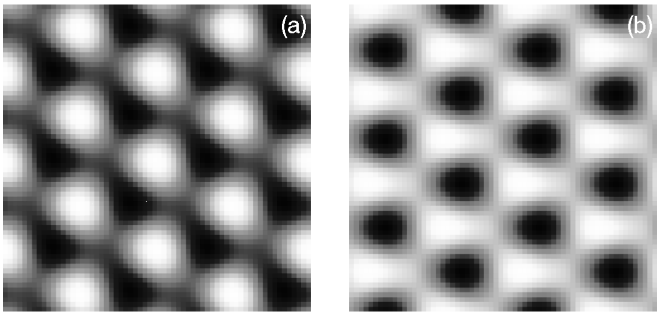

Fig.7 Simulations corresponding to the two metastable states responsible for the positive negative images;
a) LL, rotation angle 5^{o}, b) RL, rotation angle 19^{o}.

All the images were generated using the same wave combination, the only difference is the angle of rotation of the *Pt* plane. The LU (RU) type structure is generated at a rotation angle of *46*^{o}, the negative image (RL) at *19*^{o} and the nearly normal image (LL) at *5*^{o}.

At the points where the tip is turned due to the strong friction of adhesive nature the cluster orientation is changed. The oscillation between two metastable states of the tip cluster was observed for about 6 minutes after which the image structure characteristic for the upper parts is found again, and no more negative images were observed.

In the images of the type of LU and RU the lattices of the maxima and of the minima have an identical symmetry to that of HOPG, but they are shifted with respect to each other. Hence the global structure does not have the symmetry of normal HOPG. Consequently a minimum has four maxima in its neighbourhood instead of only three as in a normal HOPG picture.

Conclusions

Taking into consideration the additional information furnished by the observed tip changes and the structure of line cuts drawn in a nonconventional direction, we succeeded to overcome the difficulty mentioned by Mizes, et al. [2]. The detailed investigation of formerly neglected tip changes allows us to make assumptions concerning the tip structure and changes in it during the scan.

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