STM LDOS reconstruction of HOPG surface

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Atomic resolution in scanning microscopy requires the probe size, the probe-surface distance and the interaction decay length, respectively, of atomic size. The image resolution is limited mainly by the size of the probe aperture that determines the scale of probe-surface interaction. In the case of tunneling microscopy (see, for example, the review [1]) it is a single atom on the very tip of the probe. The probe-surface interaction in STM can be considered as the wave function overlap of empty and filled states of a tip and sample. The well-known theory of symmetric “s-wave tip” of Tersoff and Hamman [2] leads to interpretation of STM image as an image of the local density of states (LDOS) for metal surfaces. However, for semimetal (in particular, for highly oriented pyrolytic graphite (HOPG) chosen for our research) or semiconductor surfaces the image may deviate from LDOS. The true LDOS structure is not seen in STM because of the smoothing property of the probe transfer function. It was found out in [3] that for these media the total tunneling current image can be expressed as the surface LDOS convoluted with the tip transfer function.

In our previous paper [4] we have proposed to take into account this smoothing property of the transfer function and a method based on Tikhonov’s deconvolution have been worked out to solve the inverse problem of true LDOS image retrieval. Using this method, an image of graphite surface with much thinner details has been obtained, but the hexagonal lattice symmetry in this image appeared to be disturbed because of the high enough level of measurements noise. In this paper we present results of retrieval of HOPG image after the preliminary averaging over the lattice period, which effectively reduced the noise level.

In our measurements (see [4]) the 2-D distribution (128×128 pixels) of the tunneling current between the probe and the surface is used (so-called constant-height or current-imaging mode). The initial tunneling current was set at about 2.5 nA at the bias voltage of 20 mV. The scanning rate was 4100 Å/s for the pixel size of about 0.1 Å.

It is well-known that in the case of HOPG measurements the tunneling current is considerably smaller at surface atomic sites which have nearest neighbors directly below them (so-called A-sites) than at sites with no such neighbors (B-sites). So, location of the three carbon atoms without neighbors in the second layer shows up as spots in the carbon hexagon image, the other three are like shadows between B-sites [5].

The relationship between the measured 2-D distribution (image) of the tunneling current and the true distribution can be (at least, approximately) expressed as a 2-D convolution [3]:

$$j_{\mathrm{m}}(x,y)=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}K(x-s,y-t)\,j(s,t)\,ds\,dt\ ,$$

where the kernel $K(w,W)$ is the transfer function, $j_{\mathrm{m}}(x,y)$ is the measured STM image, $j(s,t)$ is the true distribution to be found. This distribution is (to a factor) the same as LDOS distribution. The solution of this integral Fredholm equation of the 1-st kind is known as an ill-posed problem, and in this paper Tikhonov’s method of generalized discrepancy is applied for the solution. The only parameter of the Tikhonov’s retrieval method of generalized discrepancy (that determines the value of the regularization parameter) is the measurements error δ estimated in L_2-space [6]. This parameter determines the degree of smoothing of the retrieved image. The smaller the value of δ, the thinner details of the image can be retrieved. As the error reduces, the retrieved image converges (uniformly in the Tikhonov’s method) to the true one. We have used the theory [2] of the probe transfer function $K(w,W)$ in our calculations.

In Fig.1 one can see the measured distribution of the tunnel current on the HOPG lattice. It was easy to estimate the measurement accuracy just from the measurements data. The error in the neighbor pixels was practically uncorrelated with the *rms* value 0.08 nA (10% of the maximum overfall of the signal). However, there is an obvious (but not realized before) possibility of a significant improvement of the measurement accuracy by spatial averaging of the STM data over the lattice period. In Fig.2a an averaged (over 40 atoms) image of the HOPG lattice is shown; one can see an obvious quality improvement in this image. The *rms* error is reduced nearly 6-fold after averaging, so it is less than

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0.015 nA. In Fig.2b the retrieved image at the error value of 0.015 nA is presented. At this low level of noise the lattice image retrieval yields more detail. The results of LDOS modeling [5] has been inserted in this picture for the comparison.

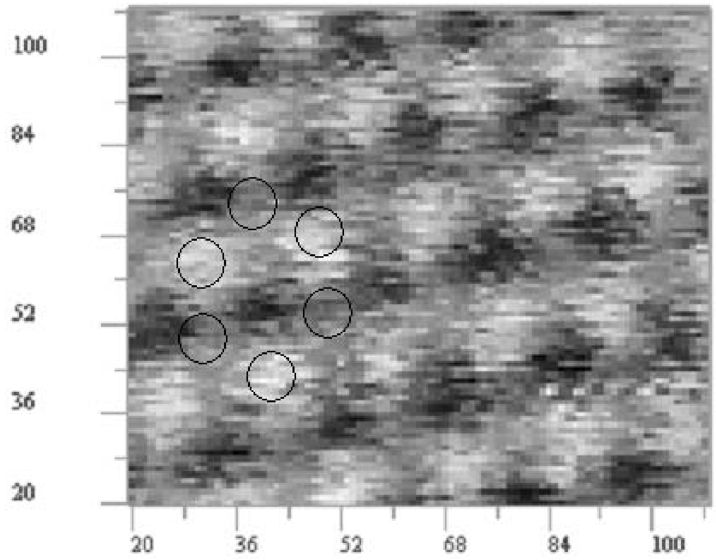

Fig.1. Initial STM image. Circles – atoms position in the HOPG lattice.
Angstrom per pixel (X): 0.135; (Y): 0.101.

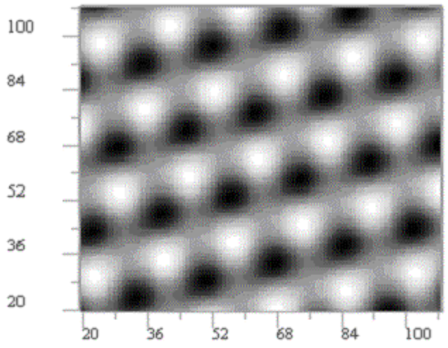

Fig.1. Averaged image.

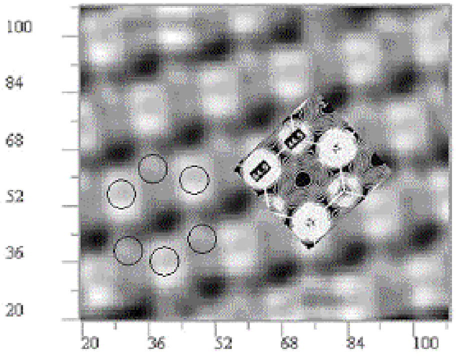

Fig.2. Retrieved image. Circles – atoms position in the HOPG lattice. Insertion – results of modeling [5].

First, the retrieved image reveals a true hexagonal structure of the lattice: both of the above-mentioned types of atoms are clearly seen. Second, one can see a thinner, sub-atomic structure instead of spots (see in Fig.1). The size of the smallest retrieved details in Fig.2b is about 0.4 Å. Better results can be achieved by improvement of the measurement accuracy, in particular, by means of averaging of the measured images over a lager number of atoms.

This work was supported by the RFBR, Grant *No*. 01-02-16444.

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