Image Retrieval in Scanning Probe Microscopy with Regard for the Probe-Surface Interaction Nonlocality

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The higher resolution in the scanning tunneling and atomic force microscopy is achieved by deconvolution of measured 2-D distributions using Tikhonov's method taking into account the smoothing property of the probe transfer function. This method makes it possible to resolve a sub-atomic structure in the tunneling microscopy and to obtain much better sharpness of images in the atomic-force microscopy.

1. Introduction

The image resolution in various kinds of scanning microscopy is limited by the size of the probe aperture that determines the size of probe-surface interaction. So, the smoothing of the real picture could take place, and, moreover, its distortion in cases when the transfer function has a complicated structure. To obtain a better image sharpness, it is possible to take into account the microscope transfer function and consider the inverse problem of image retrieval. This problem in its simplest form consists of the solution of integral Fredholm equation of the 1-st kind of 2-D convolution type, which is known as an ill-posed problem. In this paper Tikhonov's method of generalized discrepancy [1] is applied for the solution. The same approach has been used successfully in the problem of 2-D currents distribution retrieval on the superconductor film by measurements of magnetic field above its surface [2].

If some 2-D distribution (image) is measured, then the relation between the measured and true distribution in most cases can be (at least, approximately) expressed as 2-D convolution:

$$z_{\mathrm{m}}(x,y)=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}K(x-s,y-t)\mathrm{z}(s,t)\,ds\,dt \qquad (1)$$

where the kernel $K(w,W)$ is the transfer function, $z_{\mathrm{m}}(x,y)$ is the measured signal, $z(s,t)$ is the true distribution to be found. The solution of (1) relative to $z(s,t)$ make it possible to retrieve the surface image with a higher resolution. It is known that the accuracy of retrieval for ill-posed equations can be determined on the basis of numerical simulation only, and these results are presented in [3].

In this paper this method is applied to the retrieval of scanning tunneling microscopy (STM) and atomic-force microscopy (AFM) images.

2. Scanning tunneling microscopy

In tunneling microscopy the 2-D distribution of tunnel current between the probe and the surface is used as a measured value (so-called z=const mode). The retrieval makes possible to resolve not only positions of single atoms but also more thin structure of atomic lattice. The form of transfer function in this case is, in general, unknown, but it is obvious that the width of this function is comparable to atomic size. So, it was reasonable to start with Gauss form of transfer function $K(x,y) = \frac{1}{\pi\sigma_x\sigma_y}\exp[-(\frac{x^2}{\sigma_x^y} + \frac{y^2}{\sigma_y^2})]$ with σ_x , σ_y of atomic size. Then it is possible to apply this transfer function to retrieval using the solution of the equation (1).

In Fig.1 there is the initial distribution of the tunnel current and in Figs.2-4 the retrieval results at $\sigma_x = \sigma_y = 1$Å are shown at different values of proposed measurements error (a parameter of Tikhonov's method that determines the value of regularization parameter). As the error reduces in the range of its possible values, one can see more and more thin subatomic structure, related perhaps to electron density distribution. Finally, it is some hexagonal structure, where individual atoms are not seen. This procedure can be considered as similar with "image focusing". The same results for the retrieval of a single atom are shown in Figs. 5-8. In Fig.9 the transfer function *K(x,y)* is seen.

3. Atomic-force microscopy

In the atomic-force microscopy the surface relief is measured using a thin probe, which interacts with a surface. For the strong interaction mode (contact mode) to take into account the probe shape geometrical methods have been developed [4]. According to [5] in the whole interaction energy *E* between the tip and the sample is calculated (taking into account the retarded effects in the electromagnetic theory) by summing the pair interaction as

$$E = A\iiint_{tip} \iiint_{surface} \frac{n'(r')n''(r'')d^3r'd^3r''}{(r'-r'')^7}, \qquad (2)$$

where *A* is the Hamaker constant, n', n'' are the respective densities of atoms of the materials and $(r' - r'')$ represents the distance between two atoms.

In the weak interaction mode the relation between the measured and the real shape of the surface could be obtained from (2) and expressed by the formula (1). In this case the information about the instrument transfer function one can obtain just from measurements, choosing the smallest elements in the structure of measured surface shape. Such elements appear on the point (comparing with the transfer function width) relief details, which effect like the δ-function and give, in fact, the transfer function of the probe. In Fig.10 an example of initial relief of the surface is given, and in Fig.11 one can see the retrieval result. It is clear, that the solution of the equation, similar with (1), makes possible to improve the observed resolution.

4. Conclusion

The results presented in this paper open new possibilities in various kinds of scanning microscopy. It appeared possible to retrieve from measured images a thin subatomic structure in tunneling microscopy, which make possible new research opportunities. In the atomic-force microscopy the retrieval makes it possible to improve the resolution and the sharpness of images. A similar approach is very effective in the scanning near-field optical microscopy [6].

Acknowledgements

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References

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Captures to the figures

Fig.1. Initial image. Angstrom per pixel (X): 0.135; (Y): 0.101.

Fig.2. Retrieved image. Error δ=0.09 mV.

Fig.3. Retrieved image. Error δ=0.085 mV.

Fig.4. Retrieved image. Error δ=0.075 mV.

Fig.5. Initial image of a single atom.

Fig.6. Retrieved image. Error δ=0.09 mV.

Fig.7. Retrieved image. Error δ=0.085 mV.

Fig.8. Retrieved image. Error δ=0.075 mV.

Fig.9. Transfer function.

Fig.10. Initial image of the square surface region with a lateral size of 130 nm, obtained using scanning atomic-force microscopy.

Fig.11. Retrieved image.

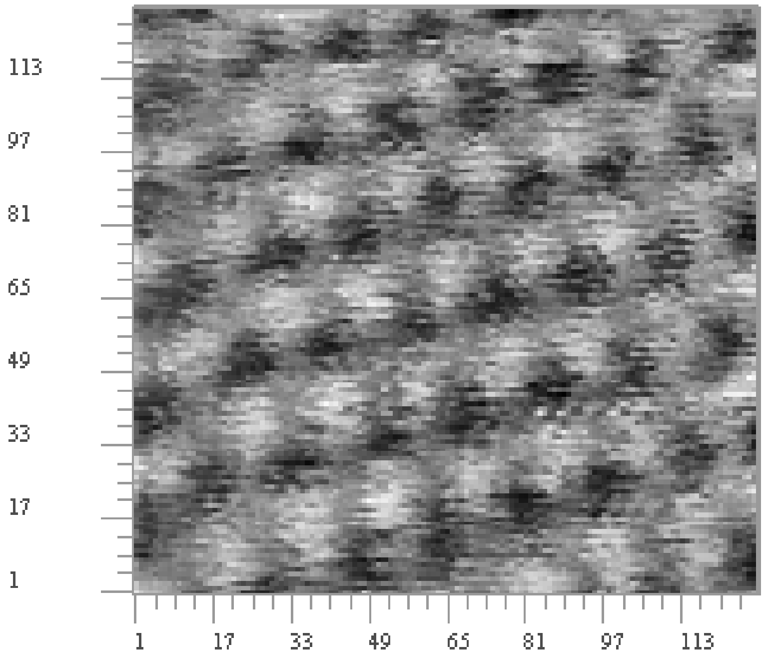


Fig.1.

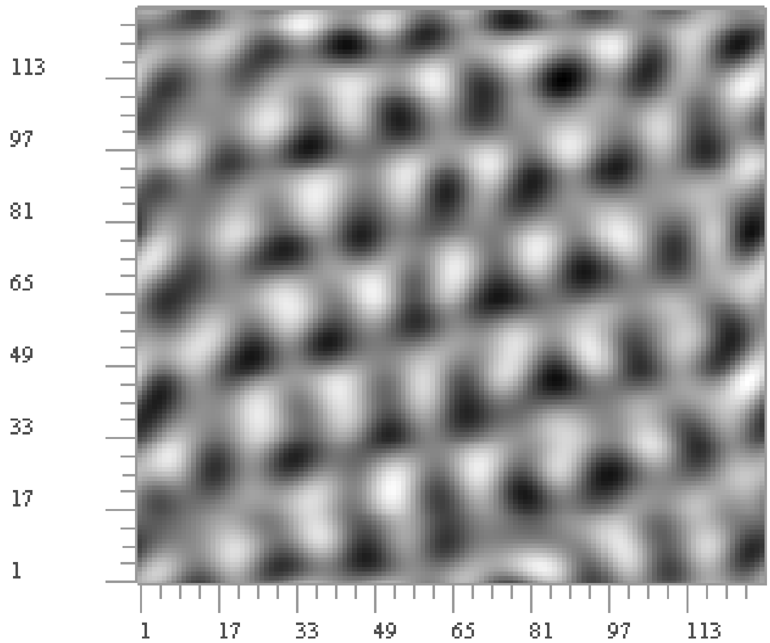


Fig.2.

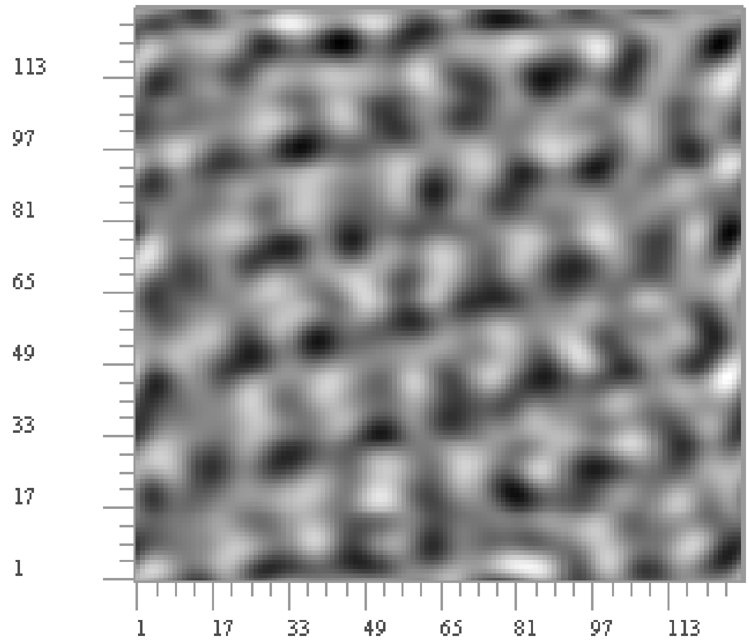


Fig.3.

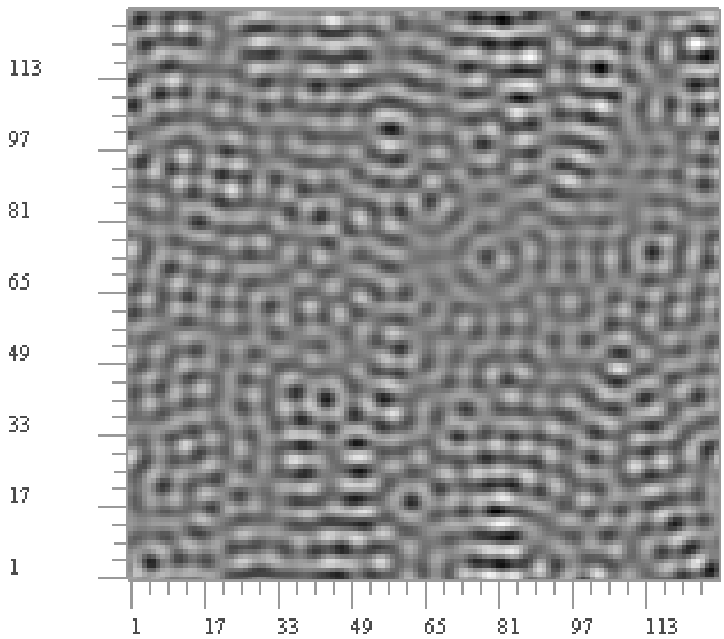


Fig.4.

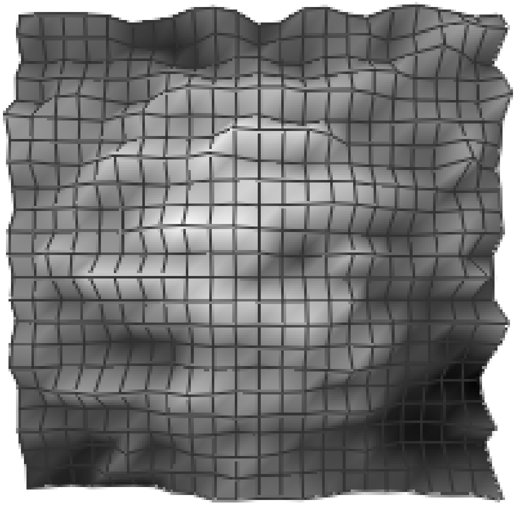


Fig.5.

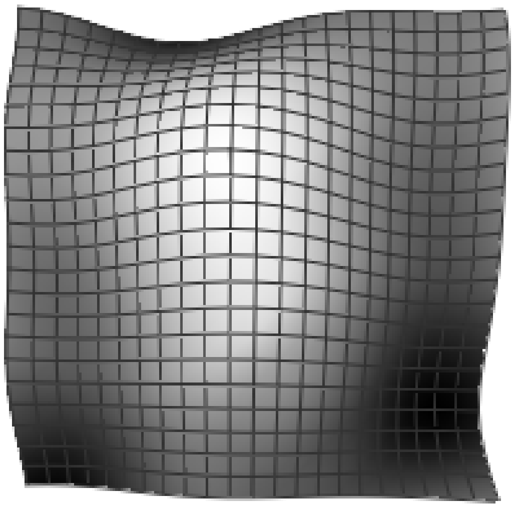


Fig.6.

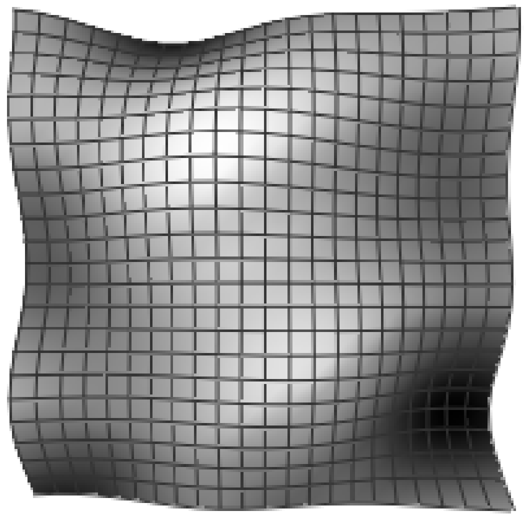


Fig.7.

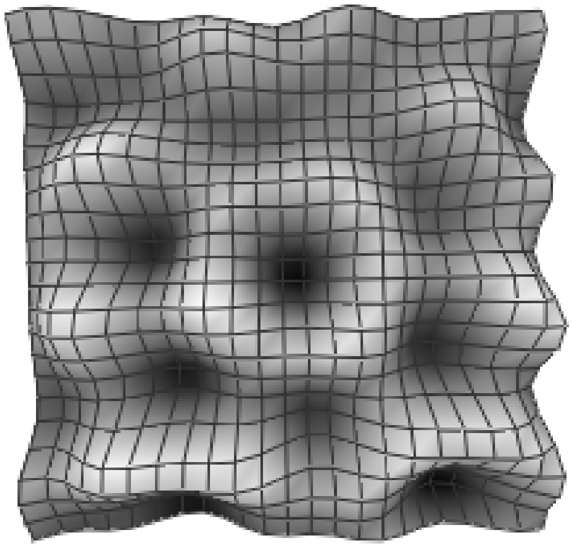
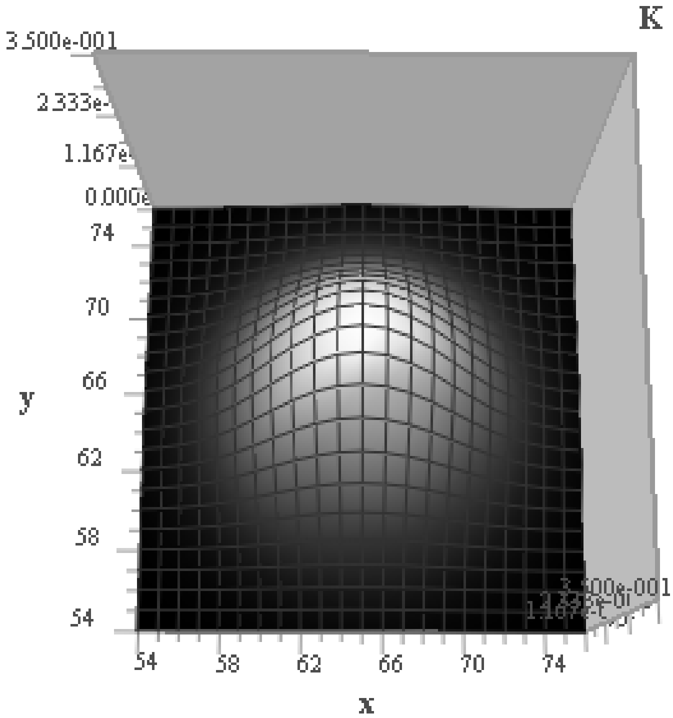


Fig.8.


K
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2.333e-
1.167e
0.000e
74
70
66
62
58
54
y
3.500e-001
1.167e-0
54
58
62
66
70
74
x

Fig.9.

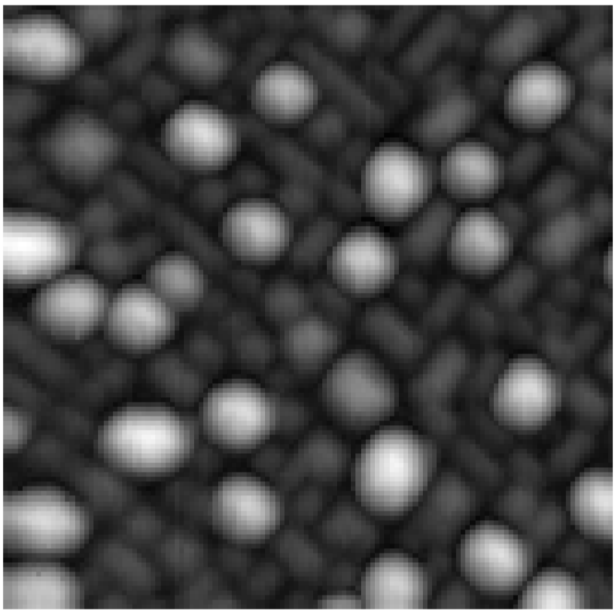

Fig.10.

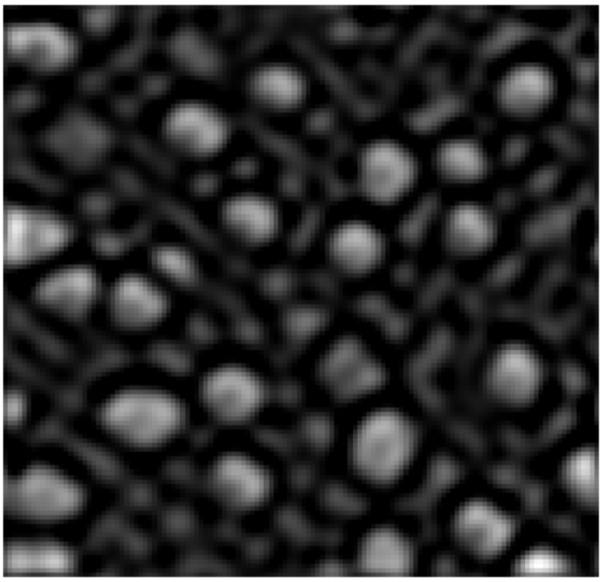

Fig.11.