EUROPHYSICS LETTERS 10 April 1994

Europhys. Lett., 26 (2), pp. 103-107 (1994)

Atomic Force Microscopy and Real Atomic Resolution. Simple Computer Simulations.

V. KOUTSOS, E. MANIAS, G. TEN BRINKE and G. HADZIIOANNOU

Polymer Science Laboratory and Materials Science Centre
Department of Chemistry, University of Groningen
Nijenborgh 4, 9747 AG Groningen, The Netherlands

(received 16 November 1993; accepted in final form 11 February 1994)

PACS. 61.16D – Electron microscopy determinations (inc. scanning tunnelling microscopy methods).
PACS. 68.20 – Solid surface structure.

Abstract. – Using a simple computer simulation for AFM imaging in the contact mode, pictures with true and false atomic resolution are demonstrated. The surface probed consists of two f.c.c. (111) planes and an atomic vacancy is introduced in the upper layer. Changing the size of the effective tip and its registry with respect to the atoms of the crystal probed, images with completely different qualitative features are obtained. If the effective tip is a single atom the vacancy is clearly imaged. However, if the tip consists of several atoms and is in registry with the sample, a virtual atom appears instead of the vacancy and the crystal lattice is perfectly reproduced. If the tip is out of registry with respect to the sample, artifacts having the size of the effective tip are reported.

Even though Atomic Force Microscopy (AFM) [1,2] has been successful in imaging surfaces with atomic resolution, it is still doubtful whether true atomic resolution is really obtained. Most images reported show perfect crystal lattices or defects much larger than atomic-scale defects. On the other hand, the situation in Scanning Tunnelling Microscopy (STM) is quite different and images with point defects are routinely obtained [3]. This is usually attributed to the fact that the tunnelling current is laterally localized in an area of few Angstroms in diameter, while in force microscopy the effective part of the probing tip is laterally much larger. Thus the atomic resolution is not obtained by a point interaction but by a superposition of several interactions between the atoms in the tip and the sample.

This assumption is justifiable if one considers that even in the case of a diamond tip and a diamond sample, using typical loads, the tip-sample contact area is larger than a single-atom one [4,5]. The two surfaces (tip and sample) are generally deformed when they are in contact [6]. For softer materials this tendency for larger contact areas under load is even more prevalent [4]. For materials with layered structures (*e.g.* pyrolytic graphite) the assumption that the tip drags a flake of the material as it scans the surface has proved to be very fruitful [7,8] and provides results in agreement with the experiments. Especially for the layered materials the same considerations of flakelike tips (or multiple-atom tips) can also be applied to the STM imaging mechanism [7,9,10]. However, the usual case in STM pictures is

the imaging of single-point defects in a variety of materials. This fact excludes the possibility of laterally large effective tips as has been shown [11].

Thus, there are two physical mechanisms that make the tip-sample contact area become of some considerable size: *a*) loads (even the lowest ones) result in a flat contact area of considerable size, *b*) especially for layered materials the tip drags a flake of the sample probed and this flake is the effective tip. The main difference of the two cases is that while in the first case the material of the tip is in general different from the material of the sample, in the second case the effective flakelike tip is of the same material.

In this study simple computer simulations are performed imaging a point defect in the perspective of demonstrating situations in which the periodicity of the lattice is reproduced without probing the atomistic details of the sample (false atomic resolution) or, alternatively, cases in which individual atoms and defects are imaged (true atomic resolution).

The sample used is an f.c.c. surface consisting of two (111) planes. The forces between the tip and the surface are calculated by adding the pair interactions between the tip atoms and each atom in the sample which are modelled by a pairwise Lennard-Jones potential:

$$U_w(r) = 4\varepsilon_w\left(\left(\frac{\sigma_w}{r}\right)^{12} - \left(\frac{\sigma_w}{r}\right)^{6}\right). \tag{1}$$

The point-defect used is a vacancy in the upper layer of the f.c.c. lattice. Thermal motion and surface relaxation are not implemented since they do not substantially affect the images obtained when introduced. Furthermore the point defect could also be a contaminant atom and in this case the relaxation of the surface would be quite different. The present study is of qualitative nature and not material specific and we are only interested in the general features of the images. Two modes of AFM operation are simulated: constant height and constant force (in the contact regime). In both cases the images obtained have the same qualitative features.

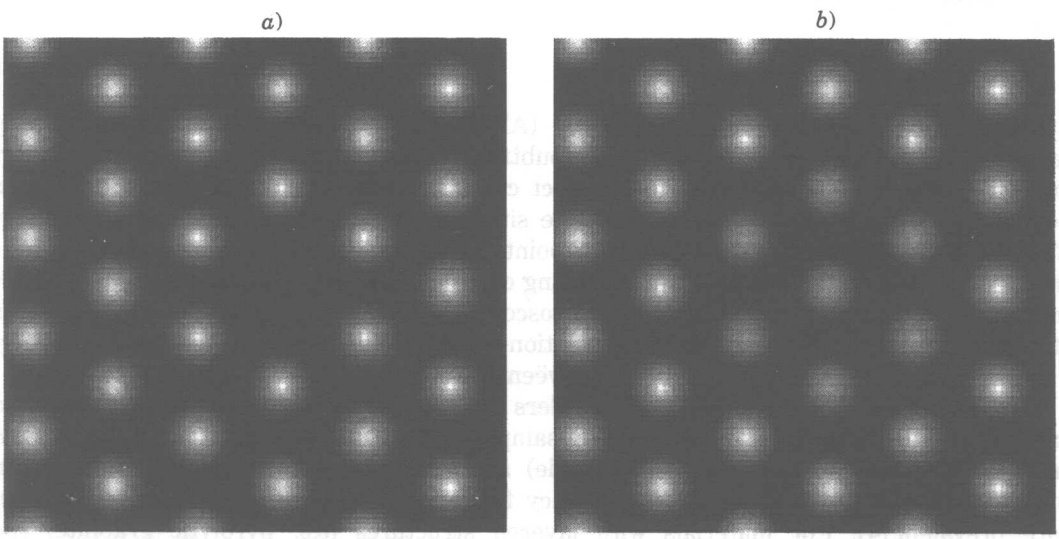

Fig. 1. – AFM images of an f.c.c. lattice with an atomic vacancy. *a*) When the scanning is carried out with a single-atom tip the vacancy is clearly imaged. *b*) When the same surface is scanned by a 7-atom flakelike tip, having its atoms in registry with the atoms of the lattice, the vacancy disappears and an imaginary atom is imaged instead.

A number of different pyramidlike tips ending in one atom have been used revealing, as expected due to the steepness of the LJ potential in the repulsive regime, that it is sufficient to consider only the end atom of the tip. Consequently in further simulations only one close-packed layer of atoms is used as a flakelike tip. The lattice constants of the tip are taken to be identical to those of the sample.

Using a single-atom tip every individual site in the surface is imaged (fig. 1*a*)). Thus a monoatomic probe is apparently capable of imaging with true atomic resolution. On the other hand, using even a rather small flakelike tip consisting of 7 atoms and in registry with the sample, an imaginary atom is present in the position of the vacancy as can be clearly seen in fig. 1*b*). The vacancy has disappeared due to the coherent superposition of the forces between all the tip atoms and each one in the sample. The crystal lattice seems to be perfect although this is not really the case (false atomic resolution). In addition, it is worth mentioning that the flakelike tip is depicted in the picture by the seven atoms of the sample (the imaginary one and those surrounding it) being more vaguely imaged. Thus a fingerprint of the tip can be observed on the scanning image. If the tip is rotated and consequently the tip atoms are placed out of registry with respect to the surface atoms, the image will be distorted due to the incoherent superposition of the interactions. In fig. 2*a*) the 7-atom tip is rotated by 14° and the lattice still looks pretty regular. However, in fig. 2*b*) the tip is rotated by 22.5° and the distortion around the point vacancy is much stronger, giving the impression of an extended defect. Further away from the distortion, areas with a periodical pattern are observed in agreement with experimental and simulation findings [8, 2]. In order to further emphasize the effect of the tip size a series of simulations is performed using a 31-atom tip. Since the tip now consists of more atoms, the forces are considerably larger and the crystal lattice looks completely regular when the tip is in registry as is evident in fig. 3*b*). In fig. 3*a*) the same area of the sample is scanned by a single-atom tip for comparison. When the tip is out of registry the distortion becomes much larger revealing the size of the effective tip. As is shown in fig. 4*a*) a rotation of 14° has a relatively weak effect but by rotating the tip 8.5° more a strong distortion is created (fig. 4*b*)). This kind of distortions could be interpreted wrongly

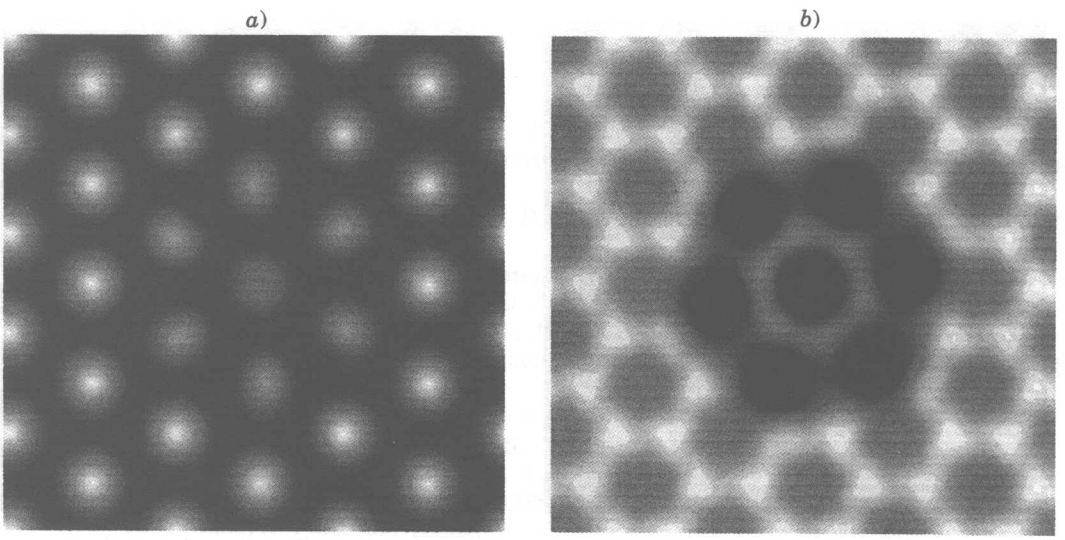

Fig. 2. – AFM images scanned by the 7-atom flakelike tip out of registry. The distortion of the images due to incoherent superposition is of the scale of the dimensions of the flake. In *a*) the orientation angle is 14° resulting in a relatively weak distortion. In *b*) the orientation angle is 22.5° and a strong artifact is created.

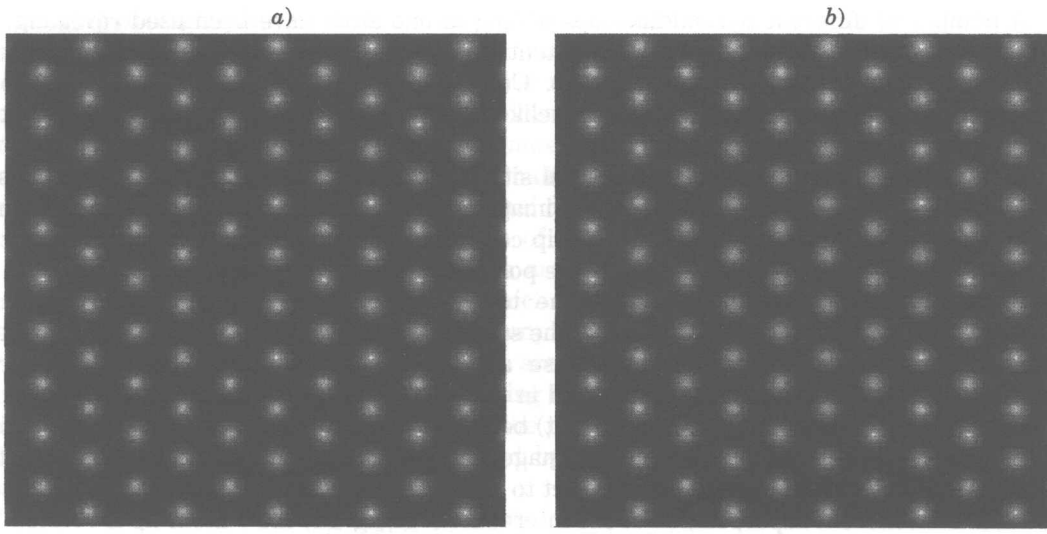

Fig. 3. – The scanning covers a larger area of the sample. *a*) The scanning has been performed using a single-atom tip. *b*) A 31-atom flakelike tip is used in registry with the sample resulting in an image with a perfect periodicity and the vacancy has disappeared.

as contamination layers on the sample probed. However, it is a tip artifact produced by the single vacancy in the lattice.

The model system that has been considered is closer to layered materials since the flake tips used have the same lattice constants as the sample probed. Nevertheless, as has been

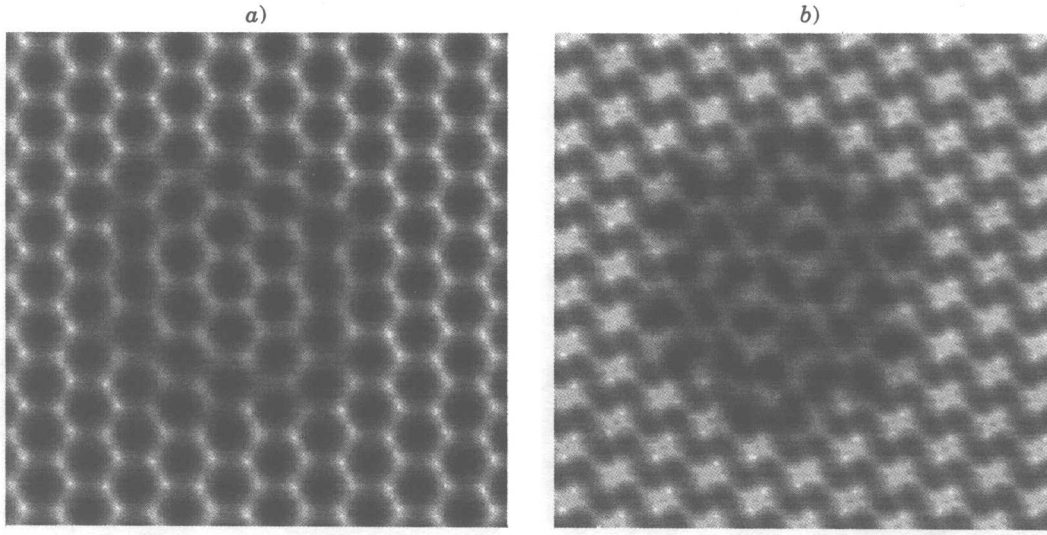

Fig. 4. – AFM images using the 31-atom flakelike tip out of registry. The distortion of the images is again of the scale of the dimensions of the flake. *a*) The orientation angle is 14° and the distortion is relatively weak. *b*) The orientation angle is 22.5°. Due to the incoherent convolution a strong artifact is created. This kind of tip artifacts can be mistaken for contamination.

stated even for hard materials the contact area is deformed and flattened, thus the situation can be treated as if the contact area were a flake. The «flake» regarded now has in general different lattice constants making the situation more complicated and material specific (as far as the lattice constants are concerned). However, for the sample of one vacancy regarded here, the qualitative features of the images remain the same and furthermore the artifacts generated are expected in general to be more intense.

As can be clearly deduced from the simple demonstration above, true atomic resolution can be obtained if the effective tip is a single atom. An elegant experimental demonstration of this fact has appeared recently [12]. Furthermore, one should be very careful in interpreting AFM images since even a one point-defect can generate tip artifacts of the size of the effective tip on the nanometer scale. This effect has been actually observed on larger scales not due to vacancies but due to sharp points (protrusions) in a lattice [13]. Figure 1*b*) and 3*b*) demonstrate clearly why point-defects in layered materials are not observed. The tip carries a piece (sliding plane) of the material in registry with the surface and the image is obtained due to coherent superposition of forces between the atoms in the sliding plane and the sample atoms. Thus, an imaginary atom appears in the vacancy and the periodicity of the layered crystal is reproduced fully but falsely.

If the sliding plane is out of registry with respect to the sample, a single point-defect is capable of generating tip artifacts having the size of the effective tip and giving the impression of rather large contaminated areas. Outside the artifact generated by the vacancy the atoms look more elongated and even multiple. This is due to the registry mismatch. The images are distorted as if they were generated by a multiple tip.

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VK would like to thank Dr. J. VRIJMOETH for helpful discussions and valuable comments. This work was supported by the Netherlands Foundation for Fundamental Research on Matter (FOM), the Netherlands Organization of Technology (SON-STW) and the Netherlands Organization for Scientific Research (NWO).

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