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THREE-DIMENSIONAL PROBE AND SURFACE RECONSTRUCTION FOR ATOMIC FORCE MICROSCOPY USING A DECONVOLUTION ALGORITHM

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Abstract

Atomic force microscope (AFM) images often contain distortions caused by the convolution of the tip and sample surface. The offered numerical deconvolution, with the use of an inverted tip located at a constant height from the surface, noticeably differs from methods previously published and is essentially simple for a concrete practical realization. Nanometer-sized spheres were successfully used to extract the shape of the AFM square pyramidal tip by means of this algorithm. Once a deconvolution procedure was used with the reconstructed AFM tip shape, truer structures of the spherical 90 nm sized particles were obtained.

Key Words: Scanning probe microscopy, dimensional metrology, surface reconstruction, convolution, deconvolution, calibration grids, nanoparticles.

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Introduction

Three-dimensional microscopic metrology is one of the main problems in semiconductor manufacturing. The importance of the microscopic measurements has grown as technology has reached submicrometer and nanometer dimensions. Until recently, a scanning electron microscope (SEM) was usually used as a measuring instrument. Unfortunately, some limitations exist which degrade the accuracy of SEM measurements [6]. A scanning tunnelling microscope (STM) has a number of advantages over a SEM. However, the usage of STM for microscopic measurements in semiconductor manufacturing is significantly limited because it is impossible to directly observe images of nonconducting surfaces and because of STM image distortions, caused by an absorbed film or inhomogeneous contributions of electronic properties along the surface [2].

With the invention of an atomic force microscope (AFM) or a scanning force microscope (SFM), it has become possible to overcome most of the problems mentioned above [13]. However, in AFM metrology, there is the well-known problem of obtaining a true surface image, since AFM image is distorted by the effect of a convolution of the tip and the actual surface (convolution effect) because the obtained images reflect a cantilever deflection at a tip-sample contact interaction. This deflection does not always coincide with an actual relief height because different segments of the tip may come into contact with the investigated surface. Such image distortions are increased as soon as the AFM tip becomes comparable in size with the surface structures [6]. That is why during AFM experiments it is necessary to know precisely the shape of the tip used in order to remove distortions of the surface image caused by the tip, applying the deconvolution procedure.

Currently, there are many publications devoted to this problem [4, 5, 7-12, 14, 15, 17-21]. Each of the published methods has some advantages and shortages. The main disadvantage of all surface reconstruction methods is that it is impossible to define an actual contour of those surface areas which the microscope tip does not contact during scanning due to its final size (i.e., the tip does not penetrate into such an area). Using some methods [8, 11, 17], these areas, called "black holes," can be detected, but a relief height in “black holes” can not be determined.

Simplicity and relative speed of the deconvolution algorithm are criteria for its worth. It is also important how close the deconvoluted surface image is to the true topography. Moreover, the algorithm should be applicable to any shaped tips and surfaces, and their AFM images.

The basis for most surface reconstruction methods is the search for coordinates of an actual point of contact between the tip and the investigated surface. In references [8, 14, 19], in-depth mathematical descriptions of such an approach are given. However, in these papers, the deconvolution problem is solved by complicated mathematical evaluations based either on the Legrande transformation [8], or a calculation of the system of partial differential equations via numerical methods.

Another approach to the problem of surface reconstruction was offered by Keller and Franke [9] and widely tested by Markiewcz and Goh [10, 11, 12]. Its essence is in the construction of a set of curves describing the tip shapes and positions during scanning over the investigated sample, with the consequent envelope search of this curves set. The obtained envelope is the reconstructed surface that is confirmed by the experimental investigations of test samples. However, in our opinion, some difficulties with the digitization of the outcomes are possible after the application of the given algorithm.

In all the algorithms mentioned above, a tip shape for surface reconstruction from the AFM image should be known. The deconvolution procedure of the AFM images of the test samples with the known topography is carried out for the determination of the shape of the used tip. For example, the method of the envelope reconstruction [9] may be used for such tip reconstruction. For this purpose, the set of the inverted surfaces of the test sample is placed in all points of the AFM image profile. The envelope of this set is defined as the inverted image of the tip. To simplify the extraction of the tip shape, test samples with a relatively simple relief were applied, for example, a grid structure [7] or separately located spherical submicron particles [19]. The sharp and pin-like structures on a rather smooth surface were used as samples for visualization of the AFM tips [1, 15]. With the help of this method, it is possible to image and control the tip “quasi *in situ*.”

In 1994, the original method of “blind” surface reconstruction was offered [20]. A peculiarity of this method is that it is not necessary to have information of the used tip shape. The reconstructed surface and the microscope tip shape is obtained as a result of a series of consistent iterations. However, this method has the drawback that the sequence of approximated images must have a limit. Furthermore, the tip shape and the surface profile obtained after long and difficult evaluations are defined as only morphological approximations. Nevertheless, “blind” surface reconstruction method is applied in practice [5, 21].

In this paper, the method of computer deconvolution for the AFM tip shape reconstruction and also for further improvement of the AFM image of the investigated surfaces is explored. The offered numerical deconvolution method, with the use of the inverted tip located at a constant height from the surface (the method “of constant height”), noticeably differs from the methods mentioned above, and is significantly simple for a concrete practical realization. The algorithm was invented by us in 1991 [3] and is briefly described in reference [2].

Methods

The basis for our deconvolution method is the search for coordinates of actual contact points of the tip and the surface during the scanning process. Figure 1a illustrates the process of the two-dimensional simulation of the image obtained in an atomic force microscope operating in the contact mode. The tip determined by the function $T(x)$ with the top at the point $x = 0$ {i.e., $T(0) = 0$} is located over the surface at a constant height C_0. Then horizontal step by step displacements of the tip along the surface are performed so that its height C_0 always remains constant (principle “of constant height”). The height C_0 is selected arbitrarily, except that it must ensure that the tip is always higher than the surface profile [16]. The tip with the top on the point x_0 is defined as:

$$T'(x,x_0) = T(x-x_0)+C_0 \qquad (1)$$

After each displacement, the minimal distance along the z-axis from the tip profile $T'(x,x_0)$ up to the sample surface $S(x)$ is determined by the exhaustive search

$$h(x_0) = \min_x\{T'(x,x_0)-S(x)\} \qquad (2)$$

Then the tip is moved down to the surface on this distance, i.e., it is brought into contact with the surface. Its equation is the following

$$T''(x,x_0) = T(x-x_0)+C_0-h(x_0) \qquad (3)$$

This procedure is similar to an actual scanning process. As a result of such displacements, the top of the tip (or any other fixed tip point) will trace out the trajectory corresponding to the observable AFM image

$$I(x_0) = C_0-h(x_0) \qquad (4)$$

It is possible to obtain the surface $Z(x)$ carrying out the similar procedure with the obtained image $I(x)$ (Fig. 1b) using the inverted tip $T_{inv}(x) = -T(-x)$ located at a constant distance, but already under the image profile $I(x)$. $Z(x)$ coincides with the actual surface except the points which the tip did not touch during scanning ("black holes" areas). The inverted tip profile application for the deconvolution is the main idea of the deconvolution procedure in our method.

Figure 2 shows the process of convolution/ deconvolution for the two-dimensional case. As the tip contacts with the surface at the point x^*, the following equations describing a tangency of the two curves (Fig. 2a) are true for the convolution process

$$\frac{\delta S(x)}{\delta x}\Bigg|_{x=x^*} = \frac{\delta T''(x)}{\delta x}\Bigg|_{x=x^*} = \frac{\delta T(x)}{\delta x}\Bigg|_{x=x^*} \quad (5)$$

$$S(x)\Big|_{x=x^*} = T(x - x_0)\Big|_{x=x^*} + I(x_0) \quad (6)$$

The corresponding equations for the deconvolution process (Fig. 2b) are

$$\frac{\delta I(x)}{\delta x}\Bigg|_{x=\bar{x}^*} = \frac{\delta T_{inv}''(x)}{\delta x}\Bigg|_{x=\bar{x}^*} = \frac{\delta T_{inv}(x)}{\delta x}\Bigg|_{x=\bar{x}^*} \quad (7)$$

$$I(x)\Big|_{x=\bar{x}^*} = T_{inv}(x - \bar{x}_0)\Big|_{x=\bar{x}^*} + Z(\bar{x}_0) \quad (8)$$

The use of eq. (8) and the condition of the tip inversion lead to

$$Z(\bar{x}_0) = T(\bar{x}_0 - x)\Big|_{x=\bar{x}^*} + I(x)\Big|_{x=\bar{x}^*} \quad (9)$$

In other words, the deconvolution algorithm is a convolution of the AFM image $I(x)$ and the inverted tip $T_{inv}(x)$. On the basis of the equations given above and Figure 2, it can be expected that we should obtain the surface $Z(x)$ coinciding with the actual sample surface after the second procedure of the convolution, i.e., $Z(x) = S(x)$. Therefore, the process of the secondary convolution with the inverted tip is identical to the deconvolution procedure.

The proof of the equality $Z(x) = S(x)$ is obvious from Figure 2c, where C is the inversion center. Equations 6 and 9 are equivalent, if conditions $\bar{x}_0 = x^*$ and $x_0 = \bar{x}^*$ are simultaneously fulfilled. These conditions are met by virtue of the inversion properties. In fact, if we place the top (maximum) of the inverted tip curve $T_{inv}''(x)$ at the point x^* and thus execute the condition $\bar{x}_0 = x^*$, the inverted tip curve

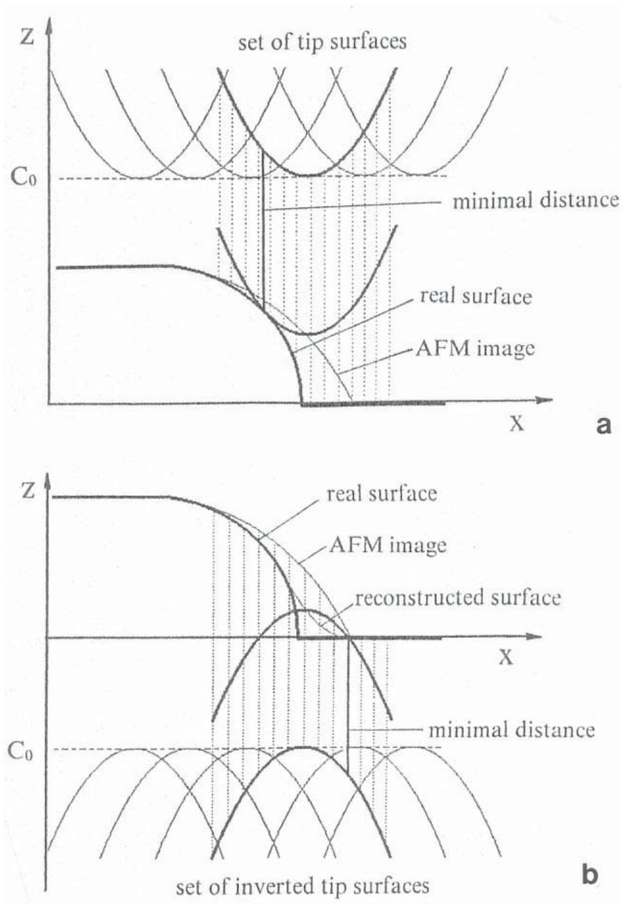

Figure 1. Two-dimensional simulation scheme of obtaining the AFM image (**a**) and reconstructed surface (**b**) with the known tip shape function using the method "of constant height." C_0 denotes the constant height.

$T_{inv}''(x)$ will intersect the initial tip curve $T''(x)$ in its top x_0. By virtue of properties of inversion, the coordinate of this point coincides with the coordinate of the contact point of the inverted tip and the AFM image $I(x)$ and that is why $x_0 = \bar{x}^*$. These conditions will be true at all contact points of the inverted tip and the surface image. Therefore, the eqs. (6) and (9) are equivalent and $Z(x) = S(x)$. It is apparent that this is correct for three-dimensional deconvolution, too, as we have shown using numerical simulation.

It is necessary to note that the reconstructed image will completely coincide with the actual contour of the surface only if the AFM tip touches all points of the investigated surface during scanning. However, according to our computer simulation and experimental investigations, even if this condition is not fulfilled, the reconstructed image is still much

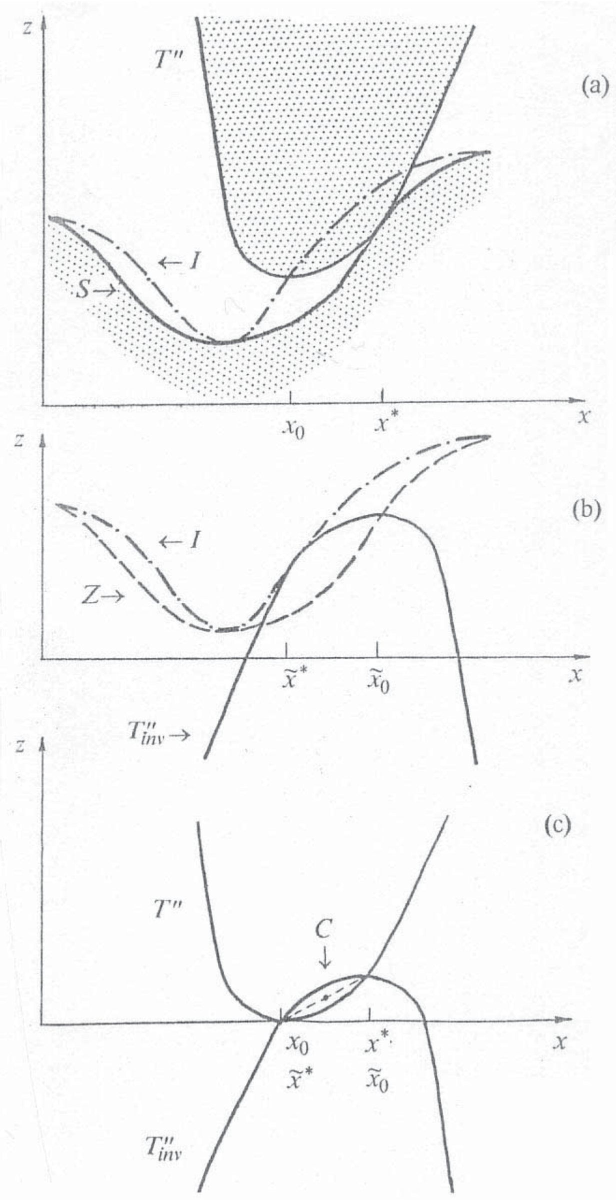

Figure 2. Two-dimensional simulation of the tip-sample convolution (**a**) and deconvolution (**b**) process. (**c**) Presentation of the intersection of the inverted and initial tips. *T*''= tip surface; *S* = true surface; *I* = image surface; *Z* = reconstructed surface; T_{inv}'' = inverted tip surface; C = inversion center.

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closer to the actual surface. The effectiveness of the image reconstruction depends on the ratio of the number of the surface points which have been in contact with the tip during scanning to the number of surface points which have not

(Figures 3 and 4 on facing page)

Figure 3. Three-dimensional computer simulation of the absolutely true surface reconstruction through deconvolution. (**a**) Initial true surface; (**b**) tip surface; (**c**) AFM image surface; and (**d**) reconstructed surface.

Figure 4. Three-dimensional computer simulation of the square protrusion partly reconstruction. (**a**) Initial true surface; (**b**) tip surface; (**c**) AFM image surface; and (**d**) reconstructed surface.

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been in contact with the tip.

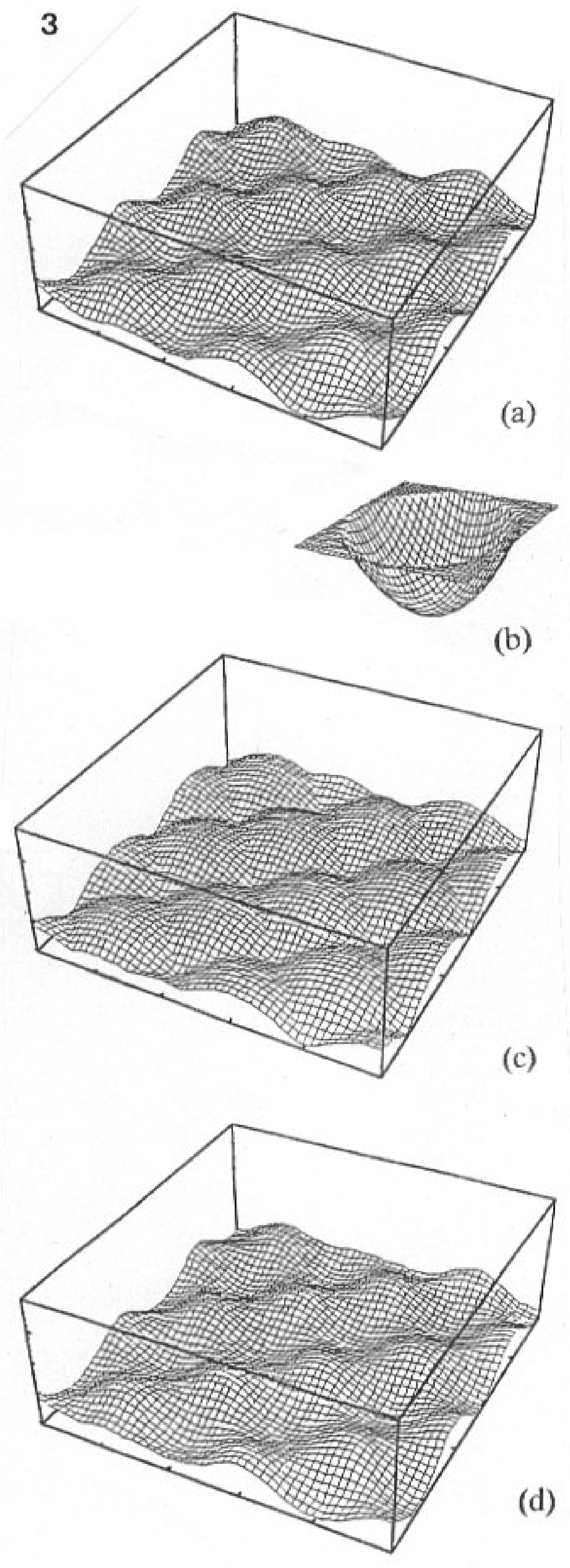
Figure 3 illustrates the computer simulation of full reconstruction of the true surface image. For other surface structures, where the AFM tip does not contact the all surface points (Fig. 4), only partial reconstruction is observed. We are sure that further improvements of the offered deconvolution method will allow delineation of the "black holes" areas on the partially reconstructed images.

From the equations mentioned above, it follows that using a test sample with the known surface geometric parameters, it is possible to reconstruct the used tip shape from the AFM image by applying the similar deconvolution algorithm, where a role of the tip will be played by the actual surface. Figure 5 illustrates the computer simulation of such tip shape reconstruction using the test sample as a hemisphere of the known size located on the surface. The example shows that the calibrated spherical fine particles are a good test sample for the three-dimensional AFM tip apex reconstruction.

Experimental Realizations of the Probe and Surface Reconstruction using the Numerical Deconvolution Algorithm

The experimental AFM images were obtained in contact mode with the commercial scanning probe microscope P4-SPM (Nanotechnology-MDT, Zelenograd, Russia). The reflection of a laser beam from the rear side of cantilever was used to detect the small interaction between the tip and the surface. An amplified differential signal from a four section photo diode allows definition of the angular deflection of cantilever with an accuracy of up to 0.1", which provides the resolution of 0.1 nm. The scanning was carried out when the feedback is switched on, and in this case, the typical operating force was about 10 nN. The probe tips manufactured by Park Scientific Instruments (Sunnyvale, CA) were made of silicon nitride and had a square pyramidal shape. The typical radius of curvature of a standard tip was 50 nm, with a 70° cone angle.

The nanometer-sized latex spheres deposited on the silicon and mica substrate were used to test our deconvolution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(a)
(b)
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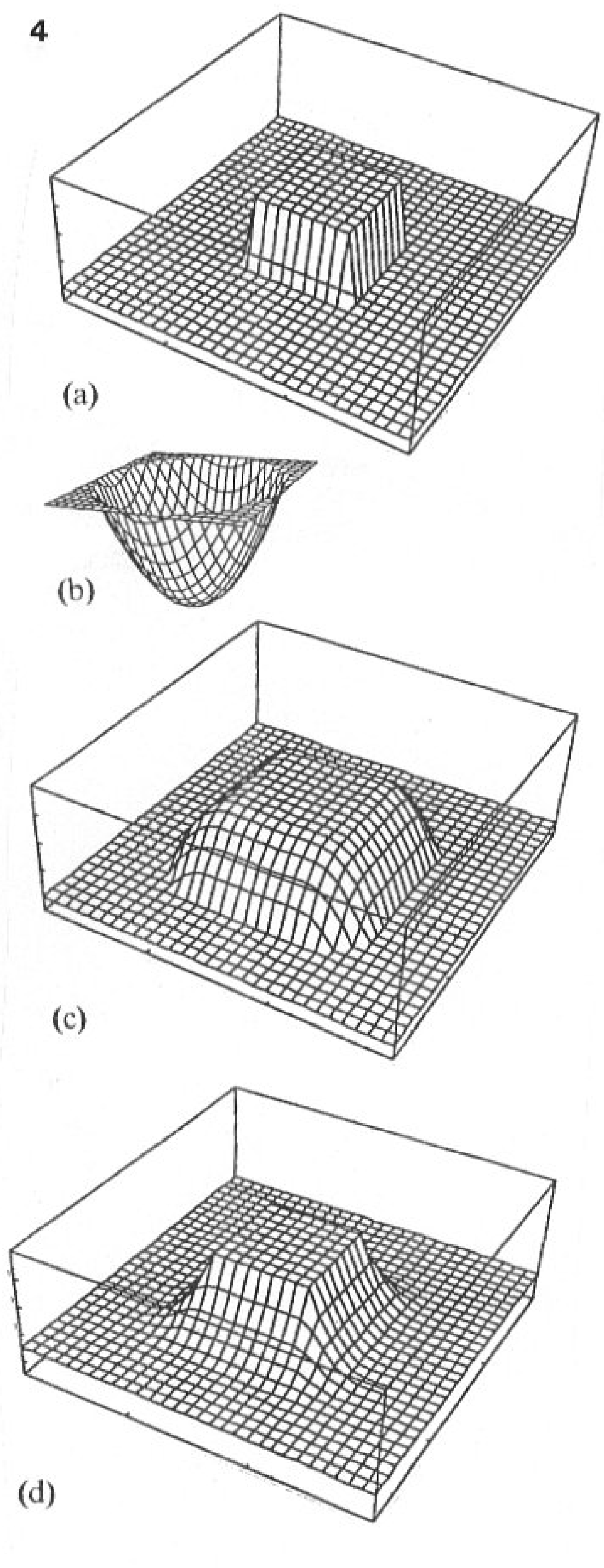
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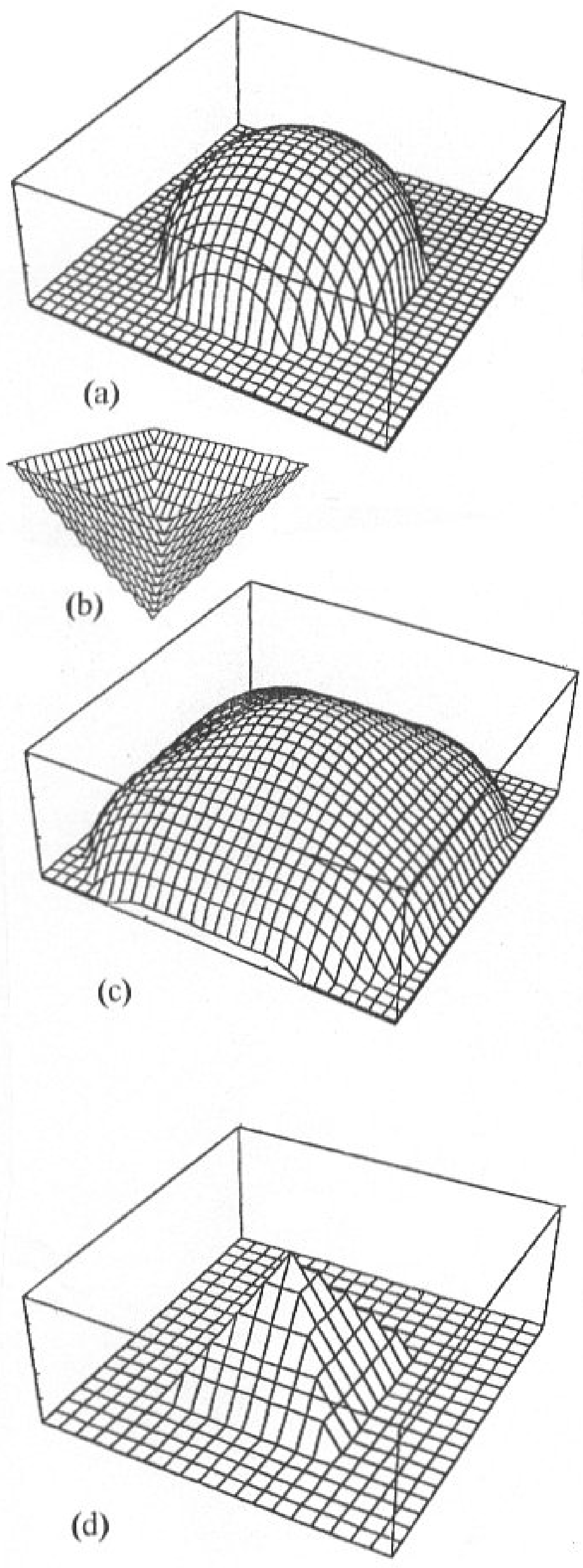

Figure 5 (*at left*). Three-dimensional computer simulation of the extraction of the pyramidal probe shape from the AFM image of the sphere protrusion using deconvolution process. (**a**) Initial true half sphere image; (**b**) tip image; (**c**) AFM half sphere image distorted by the tip convolution effect; and (**d**) extracted AFM probe shape.

algorithm and compare the experimental and computer simulated AFM images before and after the deconvolution procedure. A 20 nm gold coating was used to stabilize fine particles on the surface.

Figure 6c shows the AFM images of the three identical 200 nm latex spheres on the mica surface. The image distortion caused by the pyramidal tip convolution effect is evident. The tip reconstructed with the deconvolution procedure of one of these sphere is shown in Figure 6a. Measured curvature radius of the reconstructed tip apex is near 50 nm - a typical tip radius for such cantilevers. For comparison, the SEM image of the same tip is presented in Figure 6b. The attempt was made to extract a truer ball image from the convoluted experimental AFM data. But for the 200 nm sized latex spheres, well defined reconstruction of the sphere image was not observed.

A significantly better result was achieved with the deconvolution procedure of the AFM image of the 90 nm latex spherical particle on the flat silicon surface (Fig. 7). The cause of this phenomenon becomes clear after carrying out the two-dimensional computer simulation of the convolution and deconvolution for the tip and sample with suitable geometry. Figure 8 shows a computer simulation of the AFM imaging process of 90 and 200 nm sized particles with 50 nm radius tip apex. The convolution of such tip leads to the greater image distortion for 90 nm particles than for 200 nm particles because the apex radius is compared with the radius of the smaller particle. Correspondingly, the reconstruction with the deconvolution is more efficient for the 90 nm than for 200 nm particle. Unfortunately, the pyramidal AFM probes are not appropriate for the truer deconvolution of the surface structure with the undercut side walls (including the spherical particles on the flat surface) because only a very small part of such surfaces is in contact with the pyramidal tip during scanning. As it is mentioned above, the percentage of surface points that have been in contact with the tip determines the true reconstruction quality. The adequate reconstruction of the tip shape from the AFM image of the nanoparticles is a suitable example confirming this rule, since all points of the tip apex have been in contact with the spherical particle during scanning. Obviously, the tip with a special geometry presented in Figure 9 is the best for the three-dimensional reconstruction of the surface by means of the AFM image deconvolution.

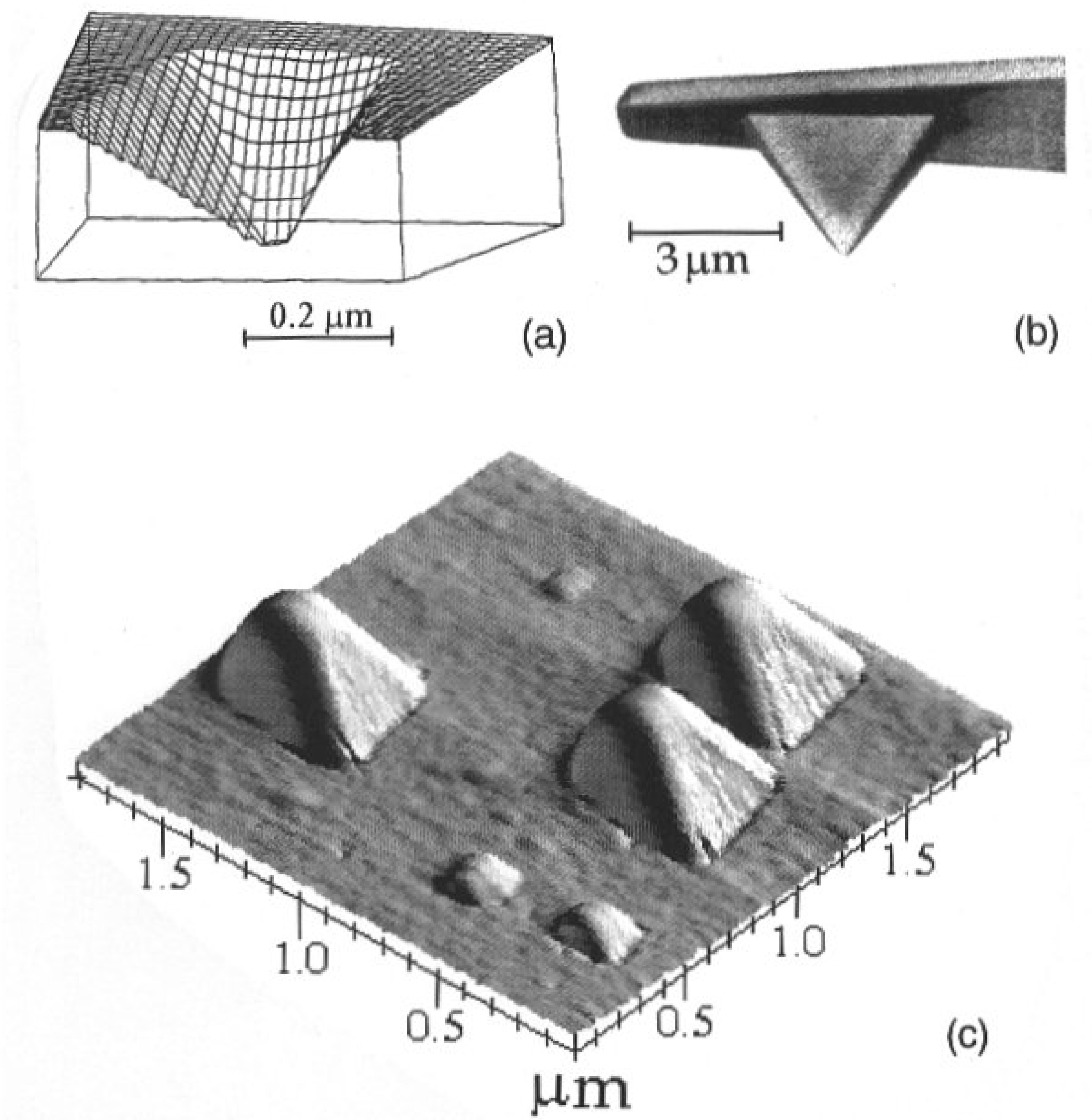

Figure 6. Deconvoluted image of the square pyramidal tip (**a**) obtained by processing of the experimental AFM image of one of three 200 nm latex spheres (**c**) deposited on the mica surface. (**b**) Used square pyramidal tip image obtained by SEM.

The cali-brated nanometer-sized ball as a tip apex permits to contact with the greatest quantity of surface points during scanning. That is why the surface reconstruction is best in this case.

Conclusions

In summary, we have presented a deconvolution algorithm that can be used for reconstructing a more accurate surface image from atomic force microscopy. The offered numerical deconvolution method, with the inverted tip located at a constant height from the AFM image profile, is relatively simple for concrete practical realization. Furthermore, the AFM image deconvolution using the inverted tip with the nanometer-sized ball apex results, in principle, in a more accurate image of the surface with undercut side walls.

Nanometer-sized spherical particles deposited on the flat surface were successfully used to extract the shape of the AFM probe with the help of this method. The extracted shapes of the AFM tips were coincident with those obtained by

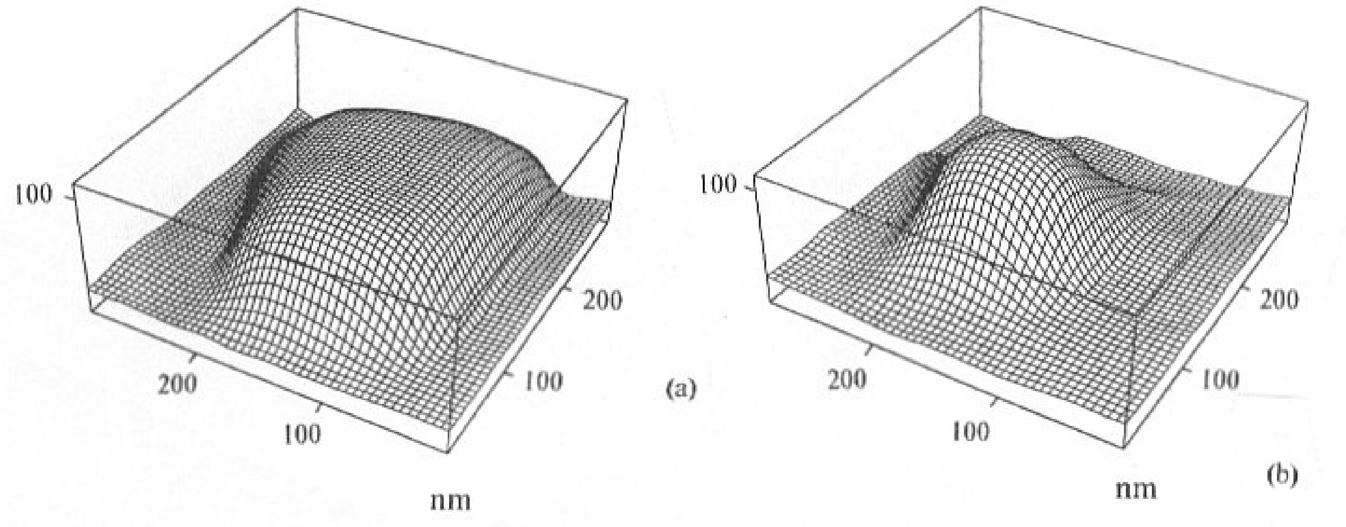

Figure 7. A truer image of the 90 nm latex sphere (**b**) obtained by deconvolution of the experimental AFM image of this particle (**a**) distorted by tip convolution effect.

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scanning electron microscopy. Using the extracted shape of the AFM tip, a more precise structure of the spherical 90 nm sized particles was deduced with the deconvolution procedure.

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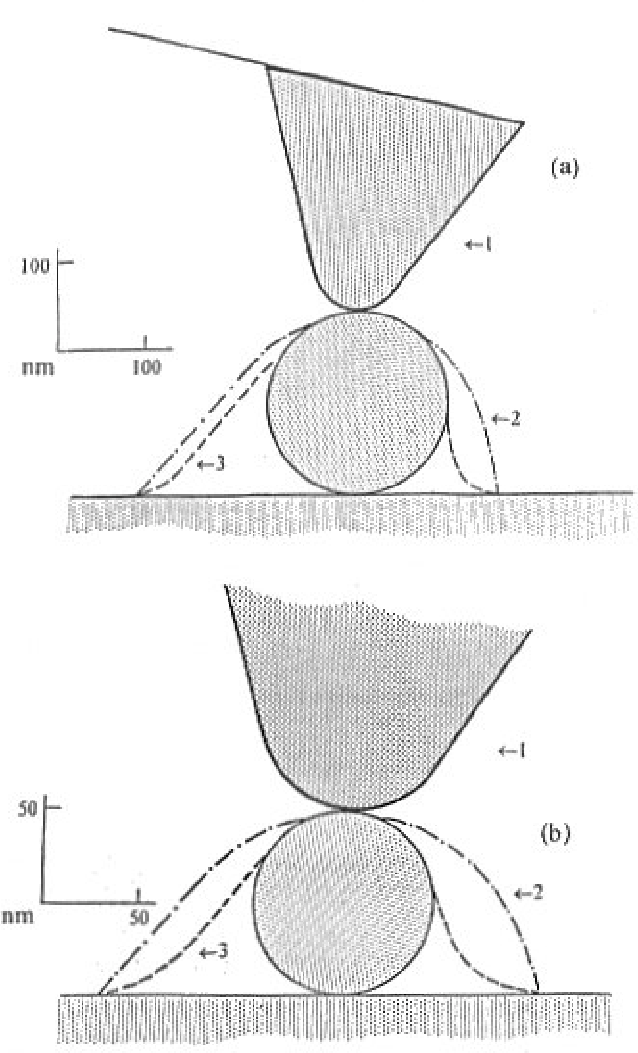

Figure 8. Two-dimensional simulation illustrates the tip-sample convolution/deconvolution degree for the same tip with 50 nm radius and two different balls with a 100 nm (**a**) and a 45 nm (**b**) radius. 1 = the tip; 2 = the convoluted profiles; and 3 = deconvoluted profiles.

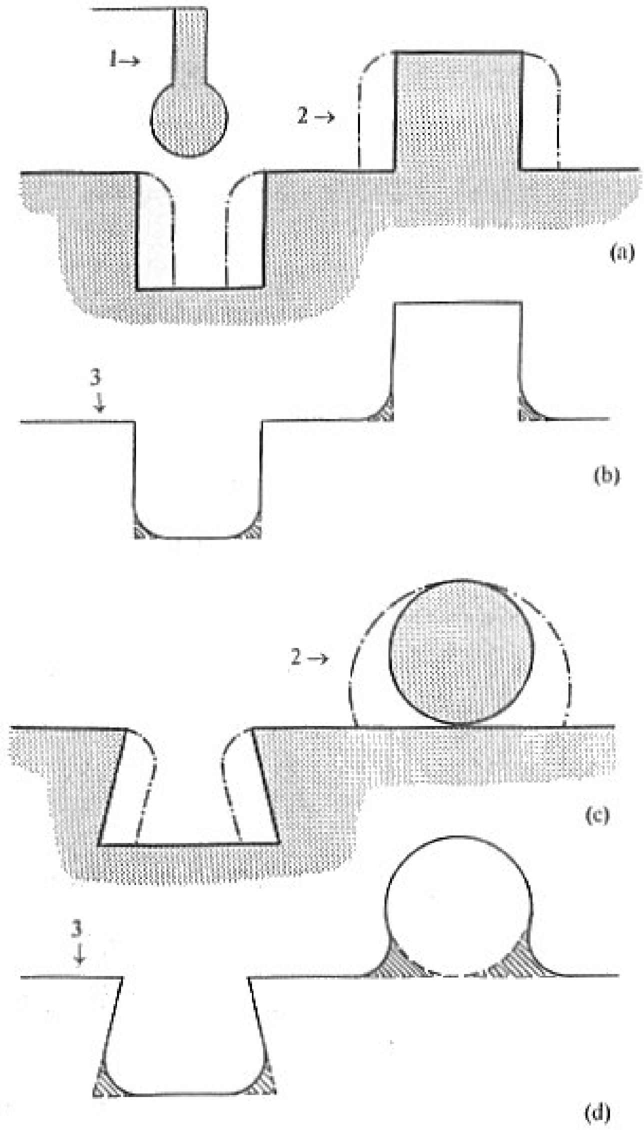

Figure 9. Two-dimensional tip-sample convolution/ deconvolution simulation illustrates the applications of the special AFM ball-probe (1) for the best surface reconstruction. (2) shows the convoluted surface profiles (dashed line); and (3) shows the deconvoluted surface profiles (solid curve). In (**a**), an area with a square hole and a square protrusion is examined as sample surface. In (**c**), sample surface is a composition of a conic hole and a spherical particle with the undercut side walls. In (**b**) and (**d**), the results of deconvolution of the corresponding surface images are presented; shaded sections at (**b**) and (**d**) are the differences between the true and decon-voluted surface profiles.

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Discussion with Reviewers

Reviewer I: Concerning the ability to measure undercut features, what are the limitations for the tip/sample structure for the kind of measurement?

Reviewer II: Do the athors know how robust the image reconstruction process is, i.e., under which conditions will it fail? Do the athors know how accurate the image reconstruction is (statistical deviation in nanometers from the true surface as independently verified by other technologies)?

Authors: Regarding limitations of our method, the essential restrictions on functionability of the given algorithm are not present, i.e., it can work with any shapes of surfaces and tips; it is an important advantage over some other techniques. However, our method allows one to determine the tip shape and actual topography of the sample, only accurate within tangency, i.e., those places of the surface, which the tip does not touch during scanning, will stay as "black holes" after the deconvolution procedure. In other points of the surface, the reconstruction will be fully accurate within experimental errors. This restriction is essential not only for given algorithm, but is a common property of all surface reconstruction techniques.

Reviewer I: It should be possible using this method to determine when either or both of the conditions (single tip point touching all surface points) are not met, thus giving some measure of the dependability of the calculation. Can this be quantified from derived tip shape and its reconstruction?

Authors: A tip does not touch the surface in the "black holes" areas and a real height of relief in these areas is not more than obtained after the deconvolution. The analysis of spatial distribution of magnitudes of derivatives of the reconstructed surface gives a possibility to mark such "black holes". We intend to publish this technique separately later and this problem is not discussed in the present paper.

Reviewer II: This paper attempts to present a new AFM image reconsruction algorithm. The computer simulations and actual deconvolutions ("image reconstructions") are very convincing, but unfortunately not new.

Reviewer III: The algorithm proposed by the authors has no difference from that originally proposed by Keller [8], which is discussed and cited in numerous other sourcers.

Authors: The basis of this deconvolution method is a search of the actual tip and surface contact points during scanning. We give a brief mathematical proof of such an approach. The more exact and full mathematical review of this principle of search of actual contact points has been given by Miller *et al.* [14]. However, these authors have solved a system of the differential equations in order to reconstruct the tip and surface shapes. In our case, the search of actual contact points happens in a much easier way by applying the special procedure. The technique offered by us is simple for a practical realization and operates in a rather short time. We use an inversion principle, as is done by Miller *et al.* [9]. However, in this paper, the inverted surface profile has been used for the extraction of the inverted tip shape with the envelope method which differs greatly from the presented method. In our algorithm, the inverted tip has been used for the truer surface reconstruction with the help of method of "constant height". The effective estimations of these two algorithms count in favour of our approach, since the envelope search, in our opinion, happens to be more complicated than the search of a minimum distance. Some difficulties with digitization of deconvolution results in computer experiments are possible in the envelope method, as well. All other difficulties and the shortcomings of "constant height" method and envelope method are the same. Our method was invented in 1991 [3]. Later, this method was also briefly reviewed by Bukharaev [2]. Originally, the method was supposed to be used for reconstruction of STM images, however, this method has appeared to be more suitable for reconstruction of AFM images and the tip apex shape of cantilever.