SFM image reconstruction reducing tip artifacts

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SUMMARY

We describe procedures for image refinement aimed at partially reducing the topographic distortion induced by the finite size of the tip. The shape of the used tip can be reconstructed using a sample with high aspect-ratio features of known geometry. A macro allows to "erode" images of the investigated sample taken with the same tip. Examples of reconstructed images of nanostructures and of high aspect-ratio surface defects in semiconductor monocrystals are reported.

INTRODUCTION

Scanning Force Microscopy (SFM), frequently named also Atomic Force Microscopy (AFM) (1), is a technique whose working principle is similar to that used by phonographs to play the old polyvinyl audio discs (2), The detected signal in both cases is originated by the interactive force between the scanned surface (disc or sample) and a thin tip acting as a probe.

Normally the tip is attached to the end of a cantilever which works as force sensor, by converting the force into deflection. In the common SFM setup a feedback system keeps constant the tip-sample force, by suitably changing the vertical position of the sample (or of the tip) during the surface scan. The sample (or tip) displacements are produced by a piezo actuator, both on the raster-scanning (3) plane x,y and along the vertical axis z. The matrix I=z (x,y) of the z displacement as a function of the x,y position is stored in the computer memory as topographic map of the sample surface (SFM image of *constant force* (4) between tip and sample).

IMAGE DISTORTION DUE TO THE TIP GEOMETRY

Many effects may contribute to the distortion of the acquired image: scanner non-linearity, creep-effect, thermal drifts… but even if all these would be negligible the *real surface topog-*

raphy S(x,y) could be obtained only by using an infinitely sharp tip, (i.e. with an apex with zero curvature radius).

If P(x,y) is the function describing the tip surface, the recorded image I(x,y) is the locus of points produced by the "envelope" of S(x,y) and of the mirror reflection of P(x,y) with respect to the surface sample plane.

Among SFM microscopists this effect is often named "tip convolution effect"(5), that may produce strongly distorted images for samples with sharply corrugated surface and/or blunt tips. In particular the lateral size of nanoparticle dispersed onto a substrate results overestimated and the aperture of steep cracks on a flat sample results underestimated.

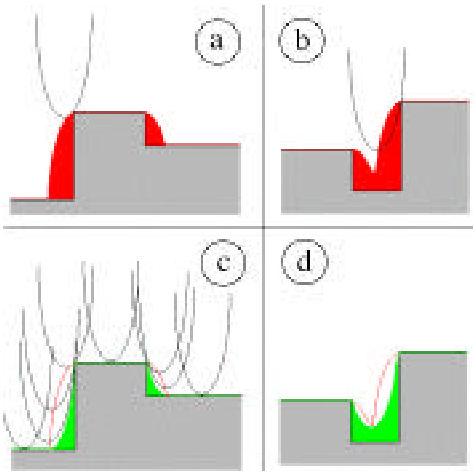

Fig 1 Sketch of the tip convolution effect. Dilated profiles of step-like (a) and and groove-like (b) reliefs due the finite tip radius. Erosion (c), (d) of the dilated profiles.

In Figs.1a,b we sketch in a vertical cross-section the essential features of the tip-induced image distortion. Here we assume a stationary sample, with a double vertical step S(x,y) and a scanning tip, with parabolic shape P(x,y). The resulting image I(x,y) is the surface traced by any single point of the tip during the scan, e.g. by the tip apex. The sample surface (bordering the gray areas) is mapped into the image surface (bordering the red areas): the two surfaces are different when the contact point between sample and tip differs from the tip apex.

A partial recovery of the information on the sample topography may be obtained by performing a suitable transformation of the image matrix I(x,y). The algorithm obviously depends on the shape of the tip used to produce that image, and only if we know the shape of the tip used to generate the SFM image we can reduce at best the distortion due to the finite size of the tip. Even in this case however there are some regions of the sample that never touch any tip point, and these regions cannot be reconstructed by any subsequent image elaboration, because the information on their structure was lost during image acquisition.

In the matrix I(x,y) each element is (6) the maximum of the function w(x,y) = S(a+x,b+y) - P(x,y), where (x,y)   P and (a+x,b+y)   S.

$$I(x,y) = \underset{\substack{(x',y')\ P \\ (x+x',\,y+y')\ S}}{Max} \left[S(x+x',\,y+y') - P(x',y') \right].$$

By inverting the previous algorithm we get from I(x) the “eroded” profile E(x,y)

$$E(x,y) = \underset{\substack{(x',y')\ P \\ (x+x',\,y+y')\ I}}{Min} \left[I(x+x',\,y+y') - P(x',y') \right]$$

which is the best approximation to S(x,y) we can obtain from I(x,y). The erosion effect is sketched in Figs. 1c,d: here thereconstructed topography is the surface bordering the green area.

EXAMPLES OF SURFACE RECONSTRUCTION

As an example of the image recovery that can be obtained with the described technique, Fig.2a shows a 3D view of SFM image of InAs nano-islands (7) on InP substrate. Fig.2b shows a line profile taken on the original image and on the image eroded by a parabolic tip with the 10nm nominal (8) curvature radius of the tip-apex. The erosion procedure partially reduces the overestimation of the island lateral size.

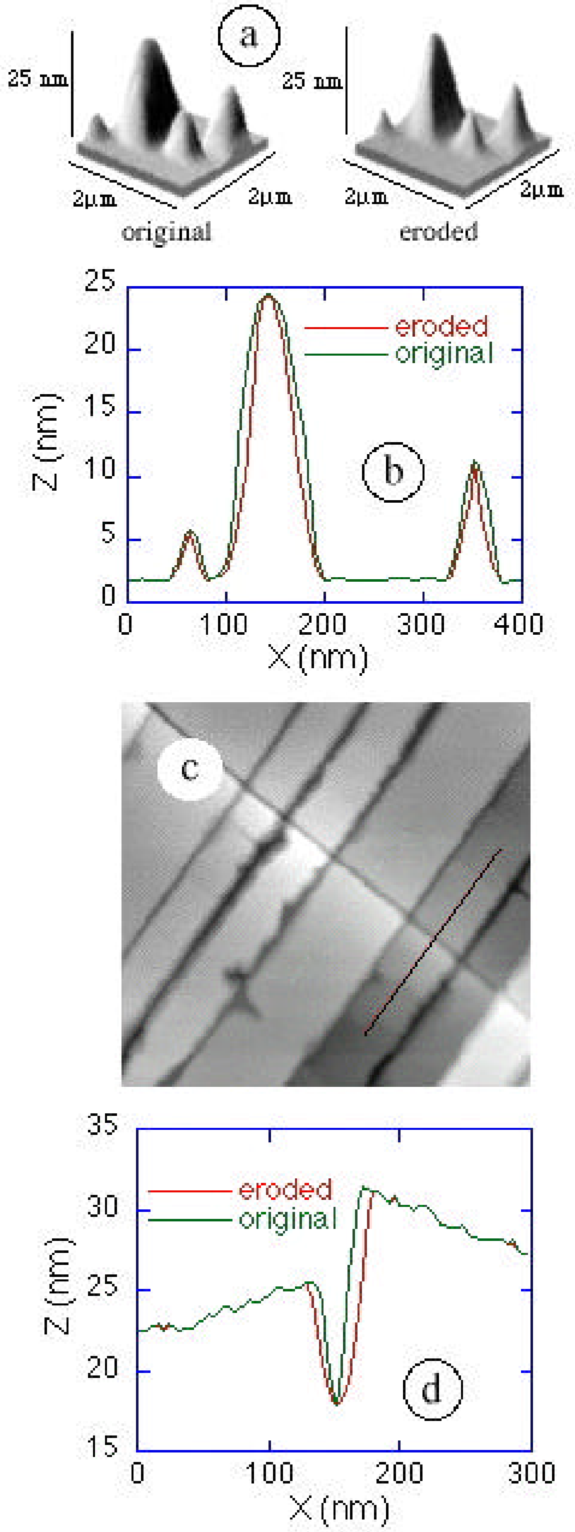

Fig 2. (a) Nano-islands of InAs grown onto InP monocrystal substrate by MOVPE (Park Sci. Intrum. AFM, contact-mode). (b) Line profiles of original and eroded images. (c) Film of $In_xGa_{1-x}As$/InP, x= 21% (Park Sci. Intrum. AFM, contact-mode). (d) Line profiles of original and eroded images

A second example is shown in Fig. 2c, where a sample with a tensile-strained layer of InGaAs onto InP substrate developed cracks whose aperture size had to be measured (9). Fig.2d shows the same line profile taken on the original and eroded images: here the erosion procedure partially reduces the underestimated aperture size of the crack.

SEARCH FOR THE REAL TIP SHAPE

In the erosion procedure we assumed for the tip a parabolic shape with a given radius of curvature r of the apex. But there is experimental evidence (from SEM images of new and used tips) that the tip may be weared out by image acquisition, specially when used in contact mode. Moreover when the sample surface has sharp reliefs some hundreds nm high, the parabolic shape cannot be assumed as reliable approximation. In this case the real tip shape must be reconstructed starting from images of samples of precisely known geometry taken with the same tip.

If we take an SFM image Is(x,y) of a reference sample (with sharp reliefs), whose surface topography Sr(x,y) is well known, we may use the inverted surface Sr'(-x,-y) to erode Is(x,y). The resulting surface Es(x,y) is a collection of reconstructed tip apexes.

The general procedure is resumed in Fig.3. If the reference sample has sharp reliefs with well known geometry, by eroding the SFM image with the reference sample surface we obtain the reconstructed tip shape. The result can be tested by using the reconstructed tip surface to erode again the SFM image and compare the result with the known sample geometry.

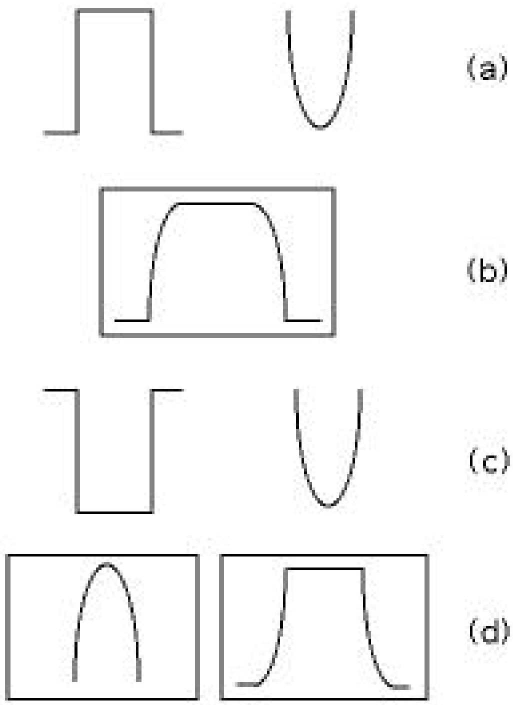

Fig. 3 Schematics of tip reconstruction by erosion with a reference sample or sample reconstruction by erosion with a known tip: (a) interacting objects: sample and tip. (b) SFM dilated image (c) Surfaces used for erosion: known tip or known sample. (d) Reconstructed sample or tip.

This process, however, is not a simple task because the shape of the reconstructed tip does strongly depend on the match between the real topography of the reference sample and its model described by the matrix Sr(x,y). It is worth noting that important mismatches may be due to any small rotation of the reference sample x-axis on the horizontal plane with respect to the model x-axis.

As an example we report here a tip reconstruction obtained using, as reference sample, a commercial grating (TGX01) produced by NT-MDT (10). This grating is made of a series of double pyramids whose nominal geometry is given by the manifacturer (Fig. 4).

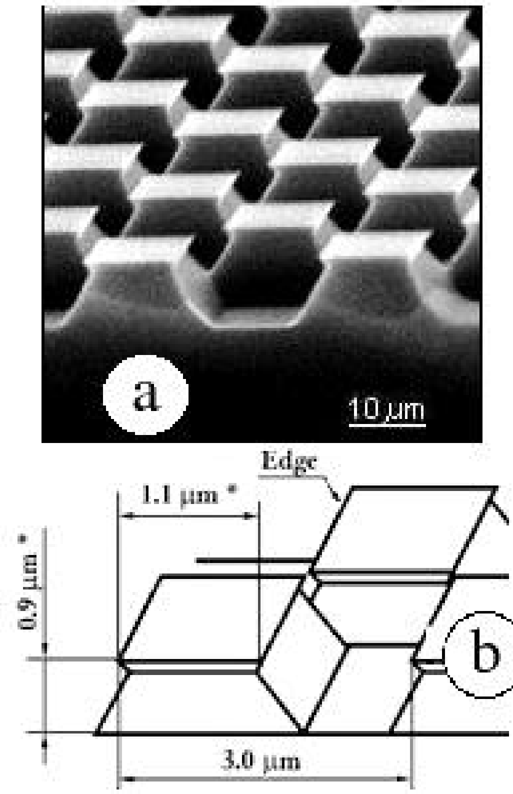

Fig. 4: TGX01 grating produced by NT-MDT with selective etching of Silicon. (a) SEM image of the grating. (b) nominal sizes of the structures

Fig. 5a shows the SFM image of TGX01 obtained in contact mode with an Ultralever™ Tip from Park Sci. Instrum., and Fig. 5b the reconstructed tip apex. The distortion in the reconstructed tip (the sharp lateral edges far from the apex). is due to a residual angle mismatching between the actual TGX01 geometry and the model used for erosion. This type of distortion may be reduced by repeating the erosion with different values of the tilt angle until a minimum is reached for the resulting tip volume. However a practical use of such iterative process requires a faster (compiled) version of our algorithm(11). We used an in fact an interpreted macro-procedure within the image processing application SXM (12).

SXM is public-domain software for Macintosh® Operating System, developed by Steve Barrett (13), that is based on NIH-Image (14). The last versions of SXM (from v.1.61) include a compiled macro named Tip Locus Effect that executes an image erosion with an user-defined curvature radius for parabolic tip. Also a line-profile erosion macro is provided.

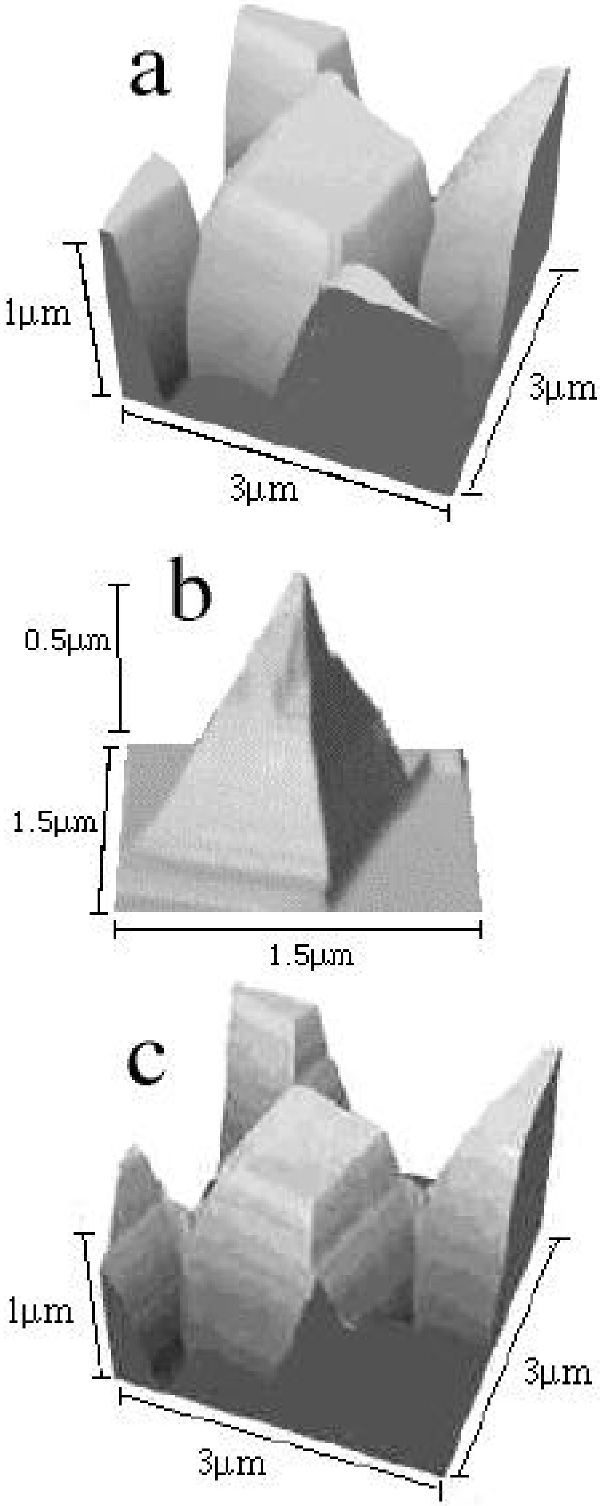

Fig. 5 (a) Original SFM image of TGX01 grating. (b) Reconstructed tip, obtained by erosion with the nominal TGX01 geometry. (c) Image eroded by the reconstructed tip.

(1) Atomic resolution is possible with SFM only through FFT spatial filtering of images taken on samples where the atoms are placed in regular arrays (monocrystals). Direct atomic resolution is instead possible with STM (Scanning Tunneling Microscope

(2) Mariani T. et al., Atomic force phonograph, *Microscopy and Analysis*, march, 31, 1996

(3) The maximum width of the raster scan is typically 100μm×100μm

(4) As feedback signal either the short range repulsive force (contact mode) or the long range attractive force (non contact mode) can be used.

(5) The term "convolution" is actually inappropriate because it wrongly suggests a procedure involving Fourier transform: a more appropriate term is "dilation", whose inverse operation ("erosion") is also frequently named "deconvolution".

(6) Villarrubia J.S., Algorithms for scanned probe microscope image simulation, surface reconstruction, and tip estimation, *J. Res. Natl. Inst. Stand. Technol*. **102**, 425 (1997).

(7) Berti M. et al., Experimental evidence of 2D-3D transition in the Stranski-Krastanow coherent growth, *J. Vac. Sc*. **B 15** , 1794 (1997)

(8) Park Scientific Intruments Ultralever Tips™ Datasheet.

(9) Drigo A.V. et al. , Strain relaxation under compressive or tensile stress" *Lattice mismatched films in The minerals, metals & materials society*, E.Fitzgerald Ed. (1999)

(10) NT-MDT (Molecular Devices and Tools for Nano Technology) http://www.siliconmdt.com/

(11) Barrett S. et al, The use of macros in AFM image analysis and image processing,, *Journal of Computer Assisted Microscopy*, in press.

(12) The latest version may be found in the web page http://reg.ssci.liv.ac.uk. SXM can directly import image files produced by many different devices (SFM, STM, SEM… by Park, Digital, Topometrix, Burleigh, Omicron …) and it does support the standard macro language of NIH-Image.

(13) Surface Science Research Centre, University of Liverpool, UK

(14) NIHimage is a general purpose free software for image handling and analysis Programs, documentation, macro archives, and related information for Macintosh or PC may be found in ftp://zippy.nih.gov/pub/nih-image.