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Correction of nonlinear lateral distortions of scanning probe microscopy images

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ABSTRACT

A methodology for the correction of scanning probe microscopy image distortions is demonstrated. It is based on the determination of displacement vectors from the measurement of a calibration sample. By moving the pixels of the distorted scanning probe microscopy image along the displacement vectors an almost complete correction of the nonlinear, time independent distortions is achieved.

1. Introduction

The inverse piezoelectric effect is commonly utilized to position the tip or the cantilever with atomic precision in scanning probe microscopes (SPMs) [1]. Although the properties of modern piezoelectric materials are well known, their application in SPMs requires a calibration of their lateral and vertical positioning, which is usually achieved by acquiring images of atomic lattices and comparing them with the perfect periodical arrangement of the atoms of a crystalline surface. Hence, the calibration is optimized for a nanometer scan range. However, sometimes the measurement requires scanning parameters that exceed the designated linear range of the calibration. Then, nonlinear effects of the piezoceramic actuators, like hysteresis creep, drift, and a nonlinear dependence of the displacement on the applied voltage often result in image distortions. These effects are inherently connected with most scanning tubes [2] used in modern SPMs.

In order to overcome nonlinear piezoelectric effects, various attempts have been made. Most of them follow two different strategies: on the one hand, the different nonlinear effects of the piezoceramic are described theoretically, for example using a Preisach model [3]. Based on such a model, nonlinearities can be corrected while or after measurement. However, it is very difficult to include all types of nonlinearities in the model. On the other hand, optical [4–9] and capacitive [10,11] tracking systems (or a combination of both [12]) are used to determine the displacement of the piezoceramic during the actual scanning and data acquisition process. These tracking systems allow the acquisition of SPM images with high accuracy, but as a drawback, additional equipment within the scanning probe microscope is needed. Hence, it is very difficult to install such systems in existing SPMs.

A totally different approach applies a Fourier transform on distorted atomic scale images [13]. Due to the periodicity of the atomic lattice, distortions can be identified and corrected in the Fourier space. This method, commonly used in transmission electron microscopy, is only applicable for relatively small distortions.

In this paper we present a simple and fast method for correcting nonlinear, but reproducible image distortions after the measurement. We used a calibration sample, which exhibits periodic surface features with precisely defined distances. For each set of scanning parameters that produce nonlinear distortions, an image of the calibration sample is measured and used to build a displacement tensor. Once a displacement tensor is found for a certain set of scanning parameters, all images that are measured using this set of parameters can be corrected. The advantages of this method are that no additional equipment, except a sample with a periodic pattern, is needed to perform the calibration and that nonlinearities that are not time dependent can be corrected even without knowing their exact origin or quantitative physical description. In addition this method allows us to correct very large nonlinear distortions and to control the aging of the piezotube.

2. Experimental setup and calibration sample

The calibration is illustrated for data acquired using an Omicron VT-STM. The calibration sample is based on a $SrTiO_3$ (Nb doped)

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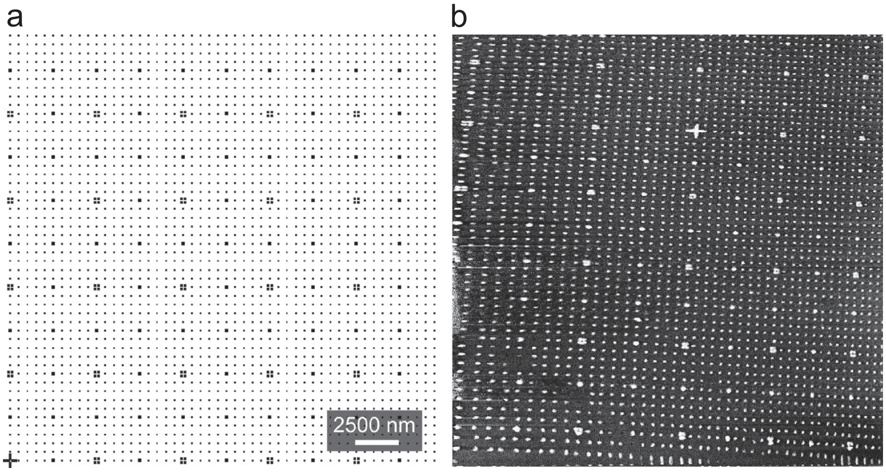

Fig. 1. (a) Schematic view of the dot pattern grown on the $SrTiO_3$ calibration sample. Every fifth and tenth TiO_2 dot is enhanced in size or represented by four closely grouped dots to provide an easy to recognize scale. (b) STM image of the calibration sample. The dot pitch is 500 nm on the entire sample. Note the distinct distortion of the normally regular dot array.

single crystal substrate, which was selected due to its resistance to oxidation or degradation up to very high temperatures, its flatness, and its hardness. The sample was patterned by electron beam lithography. An array of Ti dots with a height of 10 nm and a pitch of 500 nm in both horizontal (x) and vertical (y) directions was deposited using the lift-off technique. The Ti dots were then oxidized to TiO_2 dots. Every fifth and tenth dot is enhanced in size or represented by four closely grouped dots to provide an easy to recognize scale [see Fig. 1(a)]. Ti was chosen as a material for the dots, because Nb-doped $SrTiO_3$, TiO_2 and Ti form electrically conducting contacts with each other.

The electron beam writer (Vistec EBPG 5000plus, positioning accuracy: 5 nm on a 320 × 320 μm^2 main field) exhibits very high accuracy of the written pattern. Hence, the error of the dot pitch of $\sim 1\%$ is much smaller than the distortion created by piezo nonlinearities and thus is neglected in the following.

3. Measurement of the distortion

Although the used Omicron VT-STMs exhibit an accurate calibration for atomic scale images, some distortions appear when extending the scan area toward the micrometer range. Fig. 1(b) shows a 15 × 15 μm^2 STM image of the calibration sample. Although the dot pitch is 500 nm on the entire sample, the distance between two neighboring dots appears to be larger in the lower left part of the image as compared with the upper right side. The apparent horizontal dot separation in the lower left part of the image is almost reaching twice the apparent dot separation in the upper right part. Also the vertical dot separation is multiplied by a factor of about 1.25 at the lower left side, compared to the upper right.

This distortion does not depend on the scan speed or the movement of the piezotube performed before scanning the image. On the other hand, the size of the scan area and the rotation angle of the scan area do significantly affect the distortions. As an example, Fig. 2 illustrates the distortion of the dot grid as a function of the rotation angle of the scan area. Note the curvature of the rows which depends on the scanning angle. We were able to reproduce this behavior on a 14-year-old Omicron VT-STM as well as on a new one (2010). From these facts we conclude that the commonly known piezocreep and hysteresis as well as piezoelectric aging cannot be the explanation for this distortion alone. There may be some piezocreep or hysteresis resulting from the large deflection of the piezoelectric while scanning micrometer sized images, but due to the very good reproducibility, the most likely explanations for this phenomenon are an inaccurate calibration or linearization of the measurement software at large sized images, a cross coupling between the vertical and horizontal scanning direction, and capacitive coupling of wires and connectors within the STM.

However, sometimes such extreme scanning parameters are needed without changing the internal calibration of a piezoscanner in the SPM measurement software. A good example of the need of acquiring small and large STM images without the possibility to change the software calibration is the imaging of thin films by cross-sectional scanning tunneling microscopy [14–18]. In this case, large areas have to be scanned in order to identify the cross-section of the thin films, followed by nanometer sized images yielding high resolution images of this region.

4. The calibration and rectification algorithm

In a first step, a third order tensor with $m \times n \times 2$ components needs to be created. For the sake of an intuitive understanding and a better distinguishability the third order tensor can be separated into a second order tensor $\underline{\underline{\boldsymbol{P}}}$ where each component is a two-dimensional (2D) vector. This approach is used throughout the following description of the mathematical algorithm.

The second order tensor represents an $m \times n$ grid, which is overlaid with the STM image of the calibration sample. The points of this grid represent the equidistant (undistorted) TiO_2 dots on the calibration sample. Hence, m is the number of dots per column and n is the number of dots per row. Due to the distortion, these numbers are not equal for each column or each row of dots on the STM image. For our purpose, the number of dots per column or row with the fewest dots is usually sufficient. If all points visible at the STM image should be taken into account, the tensors may have some 'empty' components. The dot pitch of the overlaid grid d_x (and d_y) is given by the physical dot pitch $d_{dotpitch,x}$ (and $d_{dotpitch,y}$) of the calibration sample converted into units of pixels:

$$d_x = d_{dotpitch,x} \cdot R_x$$
$$d_y = d_{dotpitch,y} \cdot R_y \qquad (1)$$

where the resolution factor R_x (R_y) is defined by

$$R_x = \frac{N_{\mathrm{pixel},x}}{\Delta x_{\mathrm{nominal}}}. \qquad (2)$$

$N_{\mathrm{pixel},x}$ is the number of pixels of the STM image in the x direction and $\Delta x_{\mathrm{nominal}}$ represents the nominal scan width in the x direction. R_y follows by analogy.