Methods for Improving the Accuracy of Nanomeasurements Using a Scanning Probe Microscope

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Abstract. The article proposes a method of measurement using a Scanning Probe Microscope. Possibilities of direct measurements of microrelief of surfaces with high spatial expansion in the form of two-dimensional function Z (x, y) are described. The calculation of the main statistical parameters of the roughness ensemble is carried out. Methods for obtaining and restoring a digital image of the nanorelief of the surface of the measuring object are proposed. The main ways of further improvement of metrological works in the nanometer range with the use of a Scanning Probe Microscope are determined. In this paper, several data processing methods are presented, some experimental results are demonstrated. It is proved that the proposed method of measurement using a scanning probe microscope will greatly simplify the process of measuring objects in the nanometer range and increase the accuracy of measurements of the microrelief of surfaces with high spatial expansion. The implementation of the proposed methods of obtaining and restoring a digital image of the nanorelief of the surface of the measuring object will significantly reduce the number of anomalous deviations in the measurements and will increase the accuracy of the obtained digital image.

1. Introduction

In recent decades, the field of metrological support is characterized by the intensive development of fundamentally new methods of measuring surfaces with nanometer and atomic spatial expansion. Surface research with high spatial expansion is an important element in the development of new technologies in various fields of science and technology. Currently, there are many devices that provide images of the investigated surface with nanometer expansion [1-7]. Of particular note is a new direction in the study of the properties of the surface of a solid body with high spatial expansion - scanning probe microscopy (SPM).

2. Literature review and problem statement

In this regard, recently, methods for measuring nanorelief using SPM are widely used to study the various statistical characteristics of the surface of the samples at the nanometer level. A number of phenomenological characteristics are used to describe the geometric parameters of the surface of solids.

Measurement of geometric parameters of the nanoobject surface using SPM is represented as a two-dimensional function $Z = f(x, y)$, which allows you to calculate all the necessary statistical characteristics [8-11].

3. The aim and objectives of research

Given the development of scanning probe methods, digital signal processing is of great importance to ensure the reliability of the presentation of the information received. The aim of the proposed work is to develop new and improve existing methods of obtaining and restoring a digital image of the nanorelief of the surface of the measuring object will significantly reduce the number of anomalous deviations in the measurements and will increase the accuracy of the obtained digital image.

4. Theoretical bases and method

When moving the probe of the scanning microscope along the surface of the sample there is a change in the parameter of interaction P, due to the relief of the surface [12-13]. The operating system handles these changes as follows: when moving the probe in the plane *Z*, *Y*, the signal on the actuator becomes proportional to the surface relief. The obtained values are registered in the form of a discrete two-dimensional function *Z* (*x*, *y*) and a digital image of the surface is built with the help of software. Typically, SPM frames are square matrices of size $N \times N$ (mainly 256 × 256 and 512 × 512) elements. An important principle of obtaining a reliable digital image from the SPM is the principle of scanning, ie obtaining not averaged information about the object of study, and discrete movement of the probe and reading information at each point. The effective determination of the roughness of the terrain according to SPM is calculated using the first central moment as follows:

$$\varpi = \frac{1}{N}\sqrt{\sum_{ij}\left(Z_{ij} - \overline{Z}\right)^2}\,, \tag{1}$$

where: Z_{ij} - the value of the height of the relief at a point with coordinates *i* and *j*, $\overline{Z}$ - the average value of the height of the relief on the SPM frame.

By means of the second central moment the two-dimensional rms deviation of heights of a relief is calculated, namely

$$\varpi_2 = \left[\left(\frac{1}{N}\right)^2 \sum_{ij}\left(Z_{ij} - \overline{Z}\right)^2\right]^{\frac{1}{2}}. \tag{2}$$

The spectral power density is determined as

$$S_{\alpha\beta} = \left|F_{\alpha\beta}\right|^2, \tag{3}$$

where: $F_{\alpha\beta}$ - Fourier image of the function Z_{ij}.

The correlation function of the surface was calculated as the inverse Fourier transform from the power spectral density

$$k_{ij} = \sum_{\alpha\beta} S_{\alpha\beta} \exp\left[2\left(\frac{a \times i}{N} + \frac{\beta \times j}{N}\right)\pi\right]. \tag{4}$$

The roughness correlation radius can be defined as the distance at which the correlation function decreases *e* times. On the basis of the nanorelief of the surface obtained with the help of an atomic force microscope, it is possible to build a mathematical model of the surface of the object of measurement and with the help of special software to obtain its digital image. There are various ways to restore (deconvolution) the digital surface of the sample. One of the most common methods is Fourier filtering. The Fourier transform (FF) is based on an extremely simple, but extremely fruitful idea - almost any periodic function can be represented by the sum of individual harmonic components (sinusoids and cosines with different amplitudes A, periods T and, therefore, frequencies ω). In Figure 1 shows a profile before filtering.

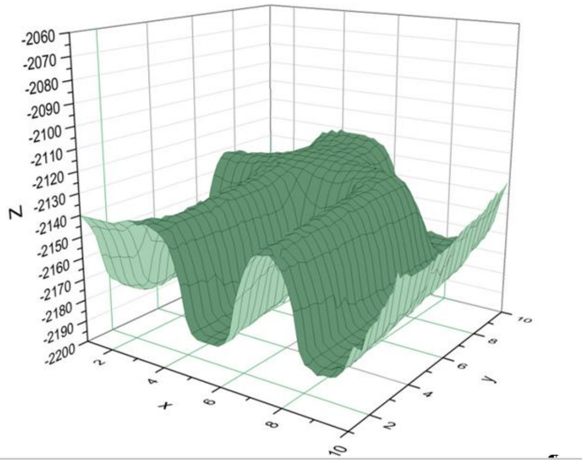

Figure 1. Sample profile without any processing.

The indisputable advantage of PF is its flexibility - the transformation can be used both for continuous functions of time and for discrete ones. Fast Fourier Transform (FFT) is a fast discrete Fourier transform algorithm. In Figure 2 shows an example of filtering by a threshold FFT filter of the amplitude-frequency characteristic of one of the resonators used in a microwave microscope [4].

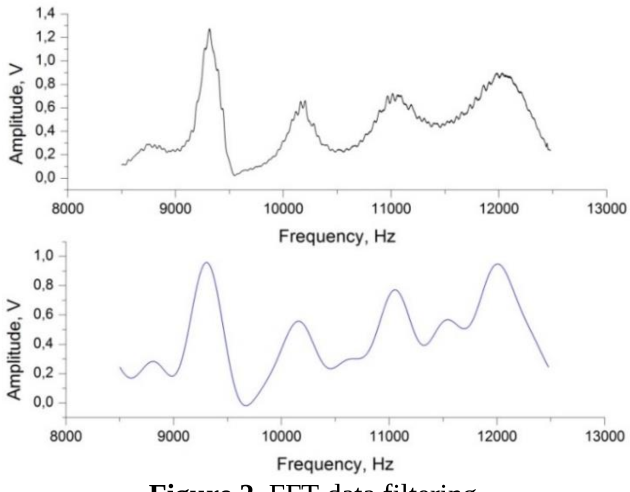

Figure 2. FFT data filtering.

Approximation allows one to study the numerical characteristics and qualitative properties of an object, reducing the problem to the study of simpler or more convenient objects (for example, those whose characteristics are easily calculated or whose properties are already known). The approximation consists in the fact that using the available information on f (x), we can consider another function φ (h) close in some sense to f (x), which allows one to perform the corresponding operations on it and obtain an estimate of the error of such a replacement. An image reconstruction method is proposed, which consists in repeated numerical scanning of the obtained SPM image inverted relative to the horizontal and vertical axes of the probe. Provided that the probe can receive measurement information from all points of the surface, it is possible to completely restore the surface of the test sample. If the probe cannot reach some parts of the surface (for example, if the sample has walls with a negative slope), then there is only a partial restoration of the surface.

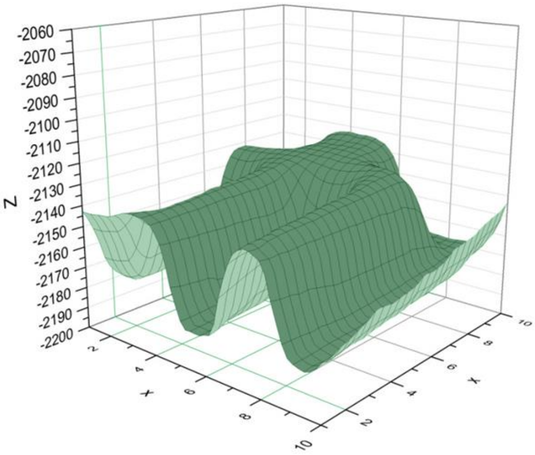

Figure 3. Polynomial approximation.

This method of image recovery is based on the use of some model ideas about the shape of the probe (pyramid, cone, etc.), but more accurate results are obtained using the real shape of the SCM probes in the process of deconvolution.

5. Example of error prediction

The actual shape of the SCM probe can be determined, for example, by scanning electron microscopy or from experiments on scanning test structures with a well-known terrain.

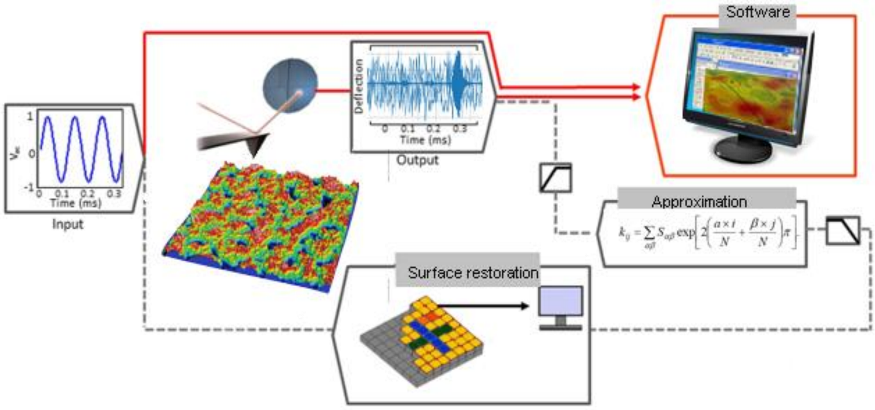

Figure 4. Method of restoring images of the nanoobject surface.

There is also a certain class of methods of so-called "blind" deconvolution. The main difference between such methods is that the information about the shape of the probe is obtained directly from the MRM image of the studied samples. In other words, the methods of "blind" deconvolution do not require special experiments to determine the shape of the probe or the use of any model ideas about it. In addition, the distance between the probe and the sample often changes indefinitely during scanning. This is due to micromovements in the structural elements of the measuring head of the microscope or due to changes in the state of the working part of the probe (for example, capture by the tip of the probe nanoparticles from the surface of the sample). As a result, stairs appear on the SPM image (Figure 5). A method of correcting such defects using the procedure of alignment of relief measurements in rows.

Each scan line contains the average elevation value

$$Z_j = \frac{1}{N} \sum_i Z_{ij} , \tag{5}$$

where N is the number of measurement points in the row.

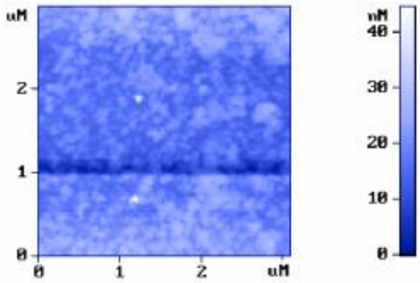

Figure 5. Stairs on the SPM image.

In Figure 6, the result of line alignment of a real surface image obtained using an atomic force microscope (AFM), which contains a stepwise change in brightness, is presented.

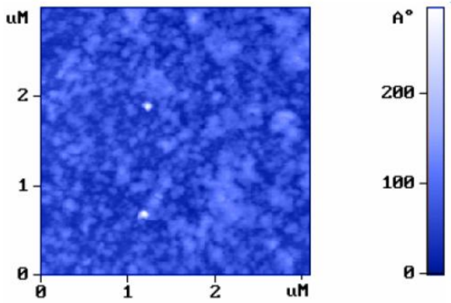

Figure 6. The result of line alignment of a real surface.

Then the corresponding averages are subtracted from the values in each row of the measurement set

$$Z_{ij}^{o} = Z_{ij} - Z_{j}\,. \tag{6}$$

In the new set, the average value in each line is zero. Therefore, it does not contain steps associated with abrupt changes in the average value in the rows. The resulting differences between the lines are proposed to remove the signal by filtering the columns of the frame.

6. Discussion the research results

However, the presented method of filtration has an obvious disadvantage. The presence of a large object on the surface ("protrusion" or "recess") necessarily leads to a non-standard average value of measurements. Therefore, it is proposed to calculate the sum of measurements not on all rows for each column, but only on a few previous rows. Satisfactory results are obtained by changing the brightness of the current line, based on the average measurement of the 4 previous lines

$$\begin{cases} Z_{ij}^{'} = Z_{ij} - Z_{j}, \\ Z_{j} = \dfrac{1}{4}\sum\limits_{k=i-4}^{i} Z_{ij}. \end{cases} \tag{7}$$

where $M = N - 2n$, N is the number of points in the scan line. After that, a graph of dependence was built

$$\ln\left[\left(\frac{N}{n}\right)^{3} V_n\right] \text{ from } \ln\left[\frac{N}{n}\right] \text{ for } n=1,2,\ldots\, n_{\max}$$

The tangent of the angle of inclination of this graph to the abscissa gives the value of the fractal dimension D_{SPM}. According to the known fractal dimension, the Hirst coefficient was calculated

$$h_{\mathrm{SPM}} = 3\text{-}D_{\mathrm{SPM}}.$$

Studies of scanning probe microscope images show that for correct averaging of measured values it is recommended to take an odd number of rows, as deviations from the average level of measurements in a row, as shown by comparison of adjacent rows, usually alternate through one. In the further processing of such measurements should take into account the fact that the line spacing does not completely avoid the specified alternation of brightness, but only reduces it.

Conclusions

Scanning probe microscopy is a promising area in the field of microelectronics and nanotechnology. Given the development of scanning probe methods, digital signal processing is of great importance to ensure the reliability of the presentation of the information received. In this paper, several data processing methods are presented, some experimental results are demonstrated. It is proved that the proposed method of measurement using a scanning probe microscope will greatly simplify the process of measuring objects in the nanometer range and increase the accuracy of measurements of the microrelief of surfaces with high spatial expansion. The implementation of the proposed methods of obtaining and restoring a digital image of the nanorelief of the surface of the measuring object will significantly reduce the number of anomalous deviations in the measurements and will increase the accuracy of the obtained digital image. This opens the possibility of further research, the purpose of which is to develop new unified methods and means of metrological support when working with nanomaterials and to create a standard nanometer of Ukraine.

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