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Uncertainty of atomic force microscopy measurements

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We consider the problem of uncertainty in geometrically linear measurements in scanning probe microscopy (SPM) represented by atomic force microscopy (AFM). The uncertainties under consideration are associated both with quantum phenomena in the space cantilever tip–sample surfaces and with effects of dynamic behavior of electronic and optic measurement and control systems. In our experiment, we have analyzed uncertainty of calibrated atomic force microscopy (C-AFM) measurement in two dimensions. Uncertainty of measurements has been estimated according to GUM procedure.

Keywords: uncertainty of measurement, atomic force microscopy (AFM).

1. Introduction

Quantum phenomena are natural consequences of the measurement resolution limits of the theoretically perfect scanning probe microscopy (SPM) systems working in the physical 3D space [1, 2]. On the other hand, this physical phenomenon may be expressed as mathematical model based on deterministic chaotic theory. In real SPM measurements, the final effect is some kind of "mixture" of the quantum and chaotic phenomena [3]. Quantum phenomena are associated with cantilever tip–sample surface interactions. Chaotic phenomena are related to effects in dynamic behavior of measurement and control systems of a microscope. From technical point of view it may be stated that uncertainty effects are associated instantaneously both with fundamental (quantum) physical limits, deterministic chaos and several kinds of instabilities and technical faults in SPM system. Deterministic theory of chaos may express influence of the measuring tool (several kinds of noises, deterministic chaos in measurement and control system).

Classical and quantum chaos from continuous quantum measurements has been analysed by MENSKY [4]. Characteristic features of the SPM system treated as a chaotic

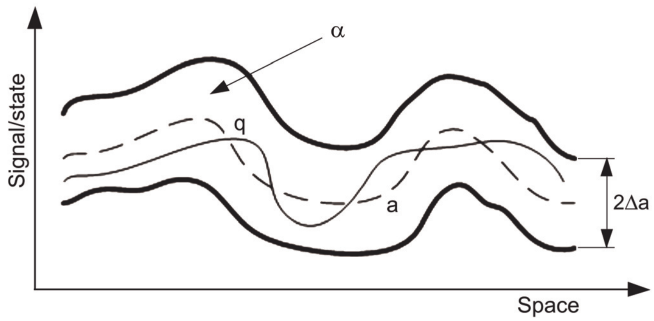

Fig. 1. The output of the SPM measurements presented by a corridor $2\Delta a$ (doublet measurement error).

system are naturally formulated in terms of trajectories as a result of control and measurement process. In quantum mechanics, the language of wave functions is usually applied. The difference in languages is unavoidable. Mensky states *...the problem of quantum chaos is conventionally formulated as investigation of characteristic features of quantum systems obtained by quantisation of chaotic classical systems*. Of course, this problem may be treated from another point of view as deterministic chaos. As a results of his considerations, Mensky presents (theoretically) the results of the measurement process as a corridor α having the width $2\Delta a$ (*i.e.*, the doublet measurement error), see Fig. 1.

The random result of measurements q at any moment of time may differ from a, but not more than by Δa. In any case, adequate representation of the SPM measurements is not average trajectory a but a corridor (uncertainty) α of the width $2\Delta a$ centred around a (see Fig. 1).

The width of corridor $2\Delta a$ may be treated as uncertainty and indeterminacy of general SPM measurements. The expression of uncertainty in measurements is stated by international standard organisations like, for instance, NIST, ISO, IEC [5–7]. The idea of uncertainty of measurements was defined in 1992 by International Organization for Standardization (ISO) in *Guide to the expression of uncertainty in measurement*, abbreviated to GUM [6]. The ISO GUM is not a standard in precise sense. However, it is a basis for standards in metrological subject. NIST Technical Note 1297 (similar to GUM) [5] includes classification of components of uncertainty which are very important for SPM measurements. In the first point, it states: *In general, the result of a measurement is only approximation or estimate of the value of the specific subject to measurement, that is, the* ***measurand*** *(a sample), and thus the result is complete only when accompanied by a quantitative statement of uncertainty*.

In the next point, the Note states: *The uncertainty of the result of a measurement generally consists of several components which may be grouped into two categories according to the method used to estimate their numerical values [8]:*

A. those which are evaluated by statistical methods,

B. those which are evaluated by other means.

In the third point, the Note states: *There is not always a simple correspondence between the classification of uncertainty components into categories A and B and the commonly used classification of uncertainty components as "random" and "systematic"*. This last point is very important in SPM characterization of nanosystems. The near atomic resolution of many SPM measurements precludes only application of A-method for the sake of quantum effects between cantilever tip and sample surface.

Uncertainty components in A-method are represented by statistically estimated standard deviation termed *standard uncertainty* with symbol u_i, and equal to the positive square root of the estimated variance u_i^2 [5, 6] (u_i represents each component of uncertainty that contributes to measurement result).

Uncertainty components in B-method are represented by quantity u_j which may be considered as an approximation to the corresponding standard deviation (positive square of u_j^2), which is obtained from an assumed probability distribution based on all available information on SPM measurement process [5, 6, 9]. Thus, mathematical model of B-type uncertainty may be expressed like positive square root of variance of all u_j considered and square root of covariance between them. In the SPM process the sample is modeled by the relationship between the measured quantities $\mathbf{x} = \{x_j\}$. The standard uncertainty $u(y)$ is then:

$$u^2(y) = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j) \tag{1}$$

where $\partial f / \partial x_i$ and $\partial f / \partial x_j$ are sensitivity coefficients, and $u(x_i, x_j)$ is the covariance of x_i and x_j, and $u(x_i, x_i) = u^2(x_i)$ is the variance of x_i. The GUM recommends that the uncertainty of measurement result y should be expressed as a typically 95% confidence interval. The half-width of this interval is the expanded standard uncertainty $U(y)$ obtained as a product of $u(y)$ and coverage factor k.

If the result of every measurement, according to GUM procedures, is random variable these results may be expressed as a fuzzy set. This interesting approach is presented by Mauris *et al.* [10].

2. Uncertainty in characterization of nanostructures

The critical dimension (CD) of micro- and nanostructures, significant in characterization of nanostructures, may be measured in several ways. The comparison of the scanning electron microscopy (SEM), optical transmission microscopy and scanning force microscopy (SFM) is presented by Frase *et al*. [11]. Applying the Monte Carlo simulation and new algorithm for CD evaluation from SEM images allows us to characterize maximum deviation between the modeled and simulated CD less than 3 nm. Agetagawa *et al.* [12] present a calibration instrument for optical encoders obtained by combining regular crystalline surfaces, scanning tunneling microscope (STM) and phase modulation homodyne interferometer

PMHI [12]. The authors of this article *believe that their results show that the proposed instrument has the capability of calibrating optical encoders with an uncertainty of 10 pm order*.

The National Physical Laboratory (UK) together with other institutes for measurements has constructed a metrological atomic force microscope (MAFM), which delivers traceable calibration of AFM measurements [13, 14]. MARINELLO *et al*. [15] present a method for accurate imaging of the three-dimensional surface topographies by vertical drift correction. Their method may be applicable to the whole family of SPM.

3. Components of uncertainty in linear AFM measurements

We have made an attempt to determine crucial component of uncertainty in the case of linear AFM measurement. An example of application is determination of essential components of uncertainty, presented in Fig. 2 [16]. C-AFM used in our measurements is a system in which a cantilever tip moves along orthogonal axes. The position of the cantilever tip is deduced from the voltage input to the scanning piezoelectric actuator and additionally is characterized by distance sensors with optical interferometric analysis. In another system of MAFM, this position is measured by a capacitive distance sensor [17].

In our experiment, we have analyzed uncertainty of C-AFM measurement in two-dimensional way in the chromium mask (produced by Leica) surface: x – along the sample and z – along step height. The nominal dimension of the measured step is 400 nm×100 nm. Similar analysis has been performed by MISUMI *et al*. [18, 19], BIENIAS *et al*. [20] and MELI *et al*. [21]. GARNAES *et al*. [22] have analyzed the problem of step heights and roughness measurements with atomic force microscopes with distance sensors. Their result of the uncertainty inference for step heights of about 200 nm is 0.5% (1 nm) and for step heights below 50 nm the standard uncertainty is 0.5 nm.

A complete specification of the microscope (C-AFM) and algorithm for the measurement of the sample is presented in [16]. The qualitative result of x, y, z measurements of the surface topography of the measured part of the sample (selected line of the mask) is shown in Fig. 2. A scheme of the vertical cross-section and cantilever trajectory in x and z directions in relation to the tip of the cantilever and results of quantitative measurements is presented in Fig. 3.

The inference of uncertainty of measurement results is the next problem linked with the hypothesis on the set of factors influencing precision of the C-AFM measurement process and next with analysis of those factors. Unfortunately, a detailed analysis of each of the factors influencing uncertainty of measurements is associated with many additional assumptions, experiments, inferences and computations. This task was accomplished by Marendziak, who presented it in his thesis [16]. Our main results of the analysis are the following. The set of factors consists of 11 main items associated with uncertainty in: optical interferometric process, nonlinearity of piezoelectric actuator, inaccuracy of inference of laser wavelength, impact of instability of the temperature and humidity, thermal instability of the sample size, incorrect position of the optical fibre, *etc*. For those 11 factors error distribution has been assumed as uniform, triangular (or pseudotriangular) and Gaussian (normal). Eventually, the estimated total uncertainty of linear C-AFM measurement is in our case 81 nm. For the measurements focused on selected detail of the investigated mask the result for x direction was 399 nm ± (9 nm, 18 nm, 27 nm) and for

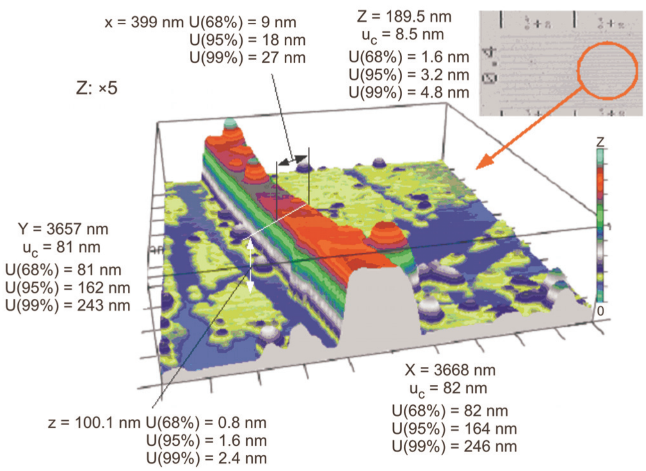

Fig. 2. The result of the C-AFM measurement of the sample topography [16].

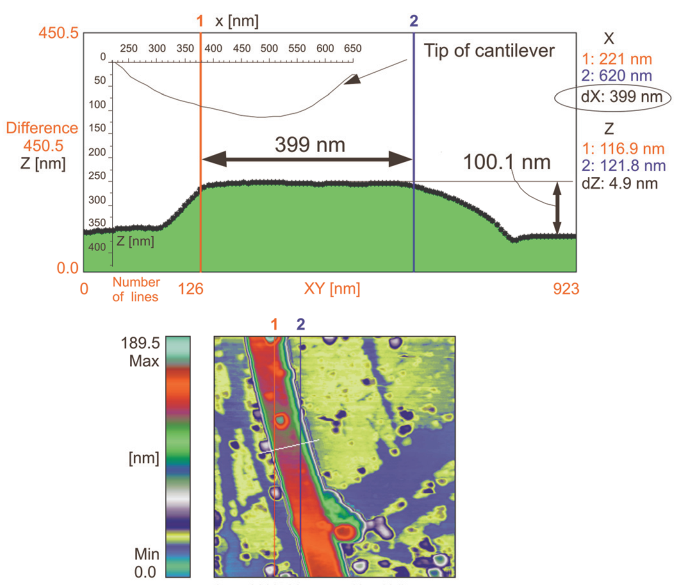

Fig. 3. Scheme of the measured profile [16].

z direction 100.1 nm ± (0.8 nm, 1.6 nm, 2.4 nm). The uncertainty estimations in brackets correspond to the coverage factors 1, 2, 3, which are related with probabilities of 68%, 95% and 99%, respectively [6].

4. Conclusions

The authors presented and discussed the problem of estimating the uncertainty of linear AFM measurements. The phenomenon of uncertainty in SPM measurements is related to both analysis of quantum phenomena appearing between the cantilever tip and sample surface, and additionally, to the dynamics of the measurement and control systems. The measurement result presented in Fig. 3 in comparison with nominal dimensions of the measured sample and results presented by other authors, led to the conclusion that our estimation of uncertainty is probably excessively pessimistic. This result of our estimation of uncertainty of linear C-AFM measurements is associated with determination of the factors influencing the uncertainty in relation (1). Estimation of the sensitivity factor $\partial f/\partial x_i$ and sometimes variance and covariance of x_i, x_j, include arbitrary part which is difficult to experimentally verify.

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