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Modeling of the Substrate Topography upon Nanosized Profiling by Focused Ion Beams

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Abstract—This paper presents the results of a mathematical model developed for calculating two-dimensional topography of the substrate surface when etching by a focused ion beam (FIB). A simulation of the two-dimensional relief of the substrate when irradiated by the FIB was carried out. An algorithm and software were developed making it possible to forecast the parameters of the surface relief depending on the characteristics of the ion beam and scanning system. The algorithm takes into account the redeposition of the sputtered material. The adequacy of the model is confirmed by a comparison with the results of experimental investigations.

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INTRODUCTION

The problem of creating a promising element base for nanoelectronics and the technology of nanosystems is related to the use and improvement of modern methods and techniques of handling nanoscale solid-state structures. One of the most promising methods for the submicron surface profiling of solids to create micro- and nanoscale structures is the method of focused ion beams (FIBs) [1].

In contrast to other methods of submicron profiling, the FIB technique has several advantages: high resolution, the high-speed formation of topological patterns without the need for specialized resists and masks, the ability to handle a wide range of materials and solid-state structures, and the locality and selectivity of the etching process. These advantages are achieved due to the possibility of varying the parameters of the process within a wide range [2]. Using multibeam FIB systems allows one to form the arrays of structures on the entire surface of the substrate, making it possible to use this method in the mass production [3]. However, despite the aforementioned advantages, the FIB method of submicron profiling is associated with a number of problems, notably the difficulty of achieving limiting values of resolution, accuracy and reproducibility of the parameters of the created structures, as well as the complexity of the method in mass production.

In recent time, the processing technology of solid-state structures with the use of FIBs and the processes occurring during the ion sputtering of solids are studied in comprehensive theoretical and experimental investigations [2–7].

Algorithms and modeling techniques based on FIB etching which were developed and described in the literature allow one to model the two-dimensional surface relief with allowance for the angular dependence of sputtering coefficient, the redeposition effect, the parameters of ion-beam scanning, and the properties of the material under processing [4]. However, the well-known models do not account for the formation of the developed surface of the sample during the process of etching and the influence of parameters of sprayed material, which reduces the accuracy of simulation and increases the time spent on conducting the formation of a solid-state structure using FIBs [6].

The aim of this work is to develop a precise model for calculating the two-dimensional surface topography of solids during FIB etching with allowance for the formation of the developed surface during the etching process and parameters of the sprayed material to improve reliability in predicting the structure of the resultant surface profile.

DESCRIPTION OF THE MODEL

Etching of solids by the FIB is accompanied by a large number of related physical phenomena, such as the penetration of ions into the substrate, the emission of charged and neutral particles, structural disordering and defect formation in the crystal lattice of the sample induced by the diffusion of surface and bulk impurities, the redeposition of the material being sprayed, and others [6]. The impact of FIBs on the substrate is characterized by several parameters of the process, the most significant of which are the following: accelerat-

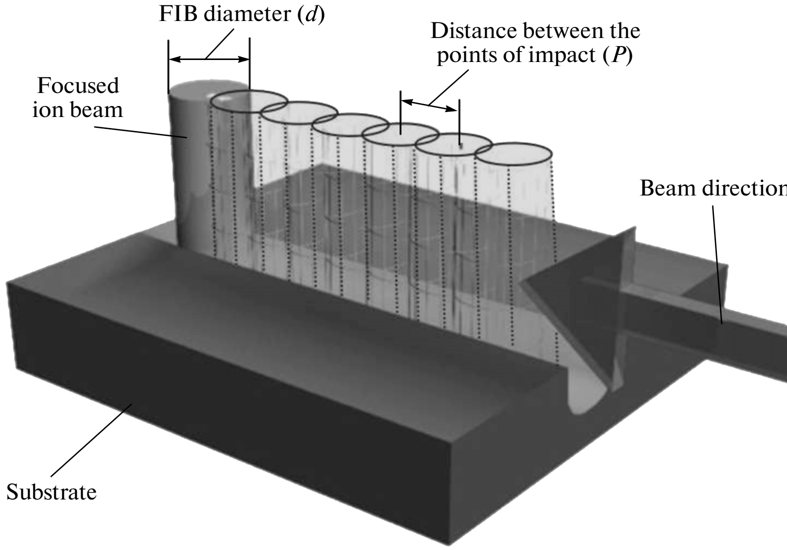

Fig. 1. Scheme of the ion-beam FIB etching.

ing voltage (E), ion beam current (I_p), exposure time at each point of the FIB action (t_d), and the number of beam passages in a predetermined pattern. The uniformity of the etching rate across the area of an irradiated surface is influenced by the energy distribution of ions over the beam diameter (F) and a degree of overlap between the two points of the impact (*overlap*). The intensity distribution of the ion flux in the beam depends on the characteristics and accuracy of the adjustment of specific FIBs equipment; therefore, this parameter is constant at certain values of the ion-beam current and an accelerating voltage. The rate of etching and the profile of relief are significantly affected by the angle of incidence of ions onto the substrate surface due to the ions slowing down in solids. Moreover, the effect of the redeposition of sputtered material onto the surface of the sample significantly influences the formation of the substrate relief upon etching.

The ion-beam etching by FIBs is a discrete process which is determined by the movement of the beam from point to point on the given area (Fig. 1). Partitioning the domain of etching onto the points of discrete impact and setting the number of passages of the ion beam over this region is performed by the specified patterns formed initially by the operator of this setup.

During FIB etching, the resultant geometry of the substrate being treated can be represented as a result of the superposition of discrete impacts of x ion beams. The main contribution to the geometry of the structure is made by the profile of the ion energy distribution over the beam diameter (Fig. 2). For the most accurate determination of the energy distribution of ions over the FIB diameter, it is advisable to use a bi-Gaussian function, which represents the two Gaussian functions describing central and peripheral regions of the beam [6].

In developing a mathematical model of the two-dimensional topography of the solid surfaces during FIB etching with allowance for the parameters of the process, we calculated the beam profile of ions. After that, we calculated the maximum depth of the FIB etching for time t_d according to the expression [8]

$$H = \frac{4YAIt_d}{\pi\rho d^2 e N_A}, \qquad (1)$$

where Y is the sputtering coefficient of the substrate material; A is an atomic mass; I is the FIB current; t_d is the FIB impact time at a given point; ρ is the density of the substrate material; d is the FIB diameter determined at a half-width of the bi-Gaussian curve; and e and N_A are the electron charge and Avogadro number, respectively.

At the next stage, the calculated FIB profile is subdivided onto the infinitely small segments dx, on which the modeling of etching is carried out with allowance for the weight coefficient, which is defined by the intensity of the ion beam for each dx (Fig. 2a).

After that, for the given parameters of the ion-beam scanning (step magnitude and *overlap*) we calculated a sputtering coefficient for a certain type of ions and the substrate material with allowance for the incidence angle of ions on dx [9].

Thus, the expression for the calculation of the surface relief after the ith passage of the ion beam with the

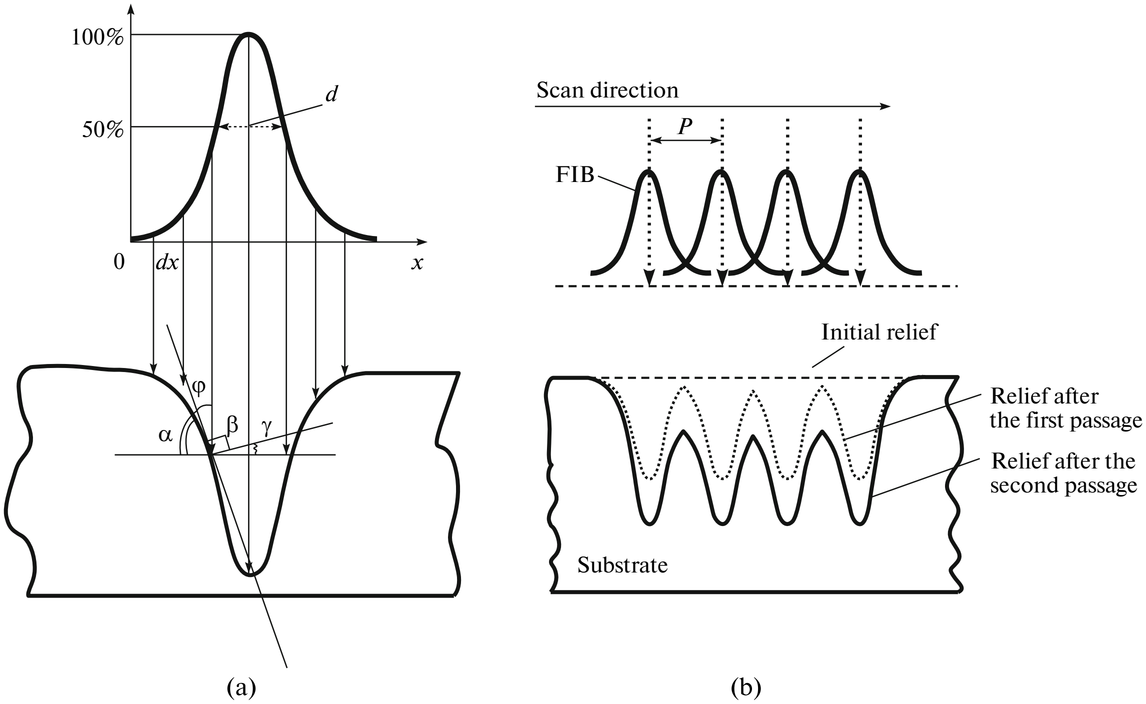

Fig. 2. Scheme of the substrate etching by FIBs: (a) partition profile FIB and (b) formation of the surface relief after the first and subsequent passages.

shape described by a bi-Gaussian distribution is as follows:

$$F_i(x) = \sum_{n=1}^{N} \frac{F_f y(x)}{\eta} \left(w e^{-\left(\frac{x-(n-1)P}{\sigma_1\sqrt{2}}\right)^2} + (1-w) e^{-\left(\frac{x-(n-1)P}{\sigma_2\sqrt{2}}\right)^2} \right), \quad (2)$$

where $F_i(x)$ is the substrate profile after ith FIBs passage; η is an atomic density; σ_1, σ_2 are the components characterizing the standard deviation of the FIB diameter; $y(x)$ is the sputtering coefficient at each point; P is the distance between the points of the FIB impact; and N is the total number of points of the FIB impact on the substrate. Schematically, the process of relief formation at the first FIB passage is shown in Fig. 2b.

When simulating the first FIB passage, it is assumed that the initial surface of the substrate is perfectly planar and the beam falls perpendicularly to the plane at each point. Starting from the second passage of the beam, the surface relief becomes nonuniform and it is necessary to calculate the angle of incidence of the ion beam at each point to obtain the sputtering coefficient.

To calculate the angle of incidence of the ion beam at the given point, we used the diagram shown in Fig. 2. After the first FIB passage, the tangent line is plotted at each point of the substrate relief and the corresponding angle is determined:

$$\varphi = 90° - \alpha = 90° - \arctan\left(\frac{F_i(x+1) - F_i(x)}{dx}\right). \quad (3)$$

The developed substrate topography complicates the analysis of the FIB interaction with the solid, since the material sputtering from the surface occurs at different angles relative to the direction of the ion-beam impact. Figure 3 shows the FIB interaction with the substrate when the ion beam interacts with the surface of the material close to vertical and inclined walls.

An analysis of the two-dimensional model of etching shows that the horizontal surface is sprayed uniformly, but part of the sputtered material falls onto the side wall and is deposited once again (Fig. 3). Since the distribution of the material that is sputtered from the horizontal surface obeys the cosine law, the flux of matter in the direction of a certain point on a vertical wall is given by

$$O(z) = \int_0^l \frac{O_0 \cos\theta \cos\phi}{r} dz, \quad (4)$$

or

$$O(z) = O_0\left[1 - \frac{z}{(l^2 + z^2)^{1/2}}\right], \quad (5)$$

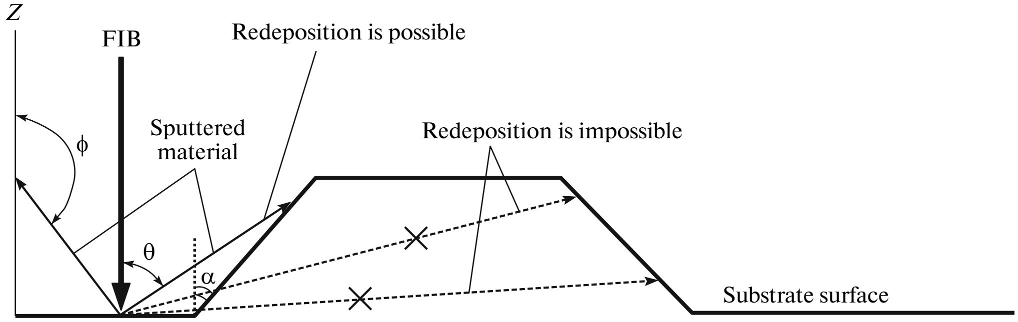

Fig. 3. Scheme of redeposition of the sputtered material during FIB etching.

where O_0 is the flux density of the sputtered material per unit surface area in the direction of solid angle θ, z is the height of the vertical wall, ϕ is the angle between the direction of the flux and surface normal at the point of redeposition, and r is the distance between the points of sputtering and redeposition. The inverse proportional dependence of $O(z)$ on r follows from the analysis of the sputtering model. If the height z of the vertical wall is smaller than distance l between the neighboring vertical walls, flux O does not depend on z. According to the data from literature [10], the real rate of matter during redeposition is lower than the calculated rate, since the coefficient of accommodation is lower than the unit, the walls of the relief on the surface of the structure are not vertical, and the ion beam has a certain divergence.

During FIB etching, a situation is also possible where the inclination angle of the wall of the surface relief relative to the ion-beam direction equals (Fig. 3). If the height x of surface relief elements is much lower than distance l to the point of impact, the flux of matter in the direction of the vertical wall is given by the expression

$$O = O_0(1 - \cos\alpha). \tag{6}$$

In the case under consideration, the rate of sputtering of the side wall is determined by the difference between the rates of sputtering and redeposition.

During FIB etching, the surface relief can be calculated using the experimental values of the sputtering coefficient depending on the angle of incidence of ions, their energy and density current, and the rate of redeposition onto the vertical walls. In modeling the relief, we must also consider the heterogeneity of the substrate surface topography and the situations arising in connection with it when the sputtered material can not be redeposited in some areas of the substrate surface (Fig. 3).

Based on an analysis of the factors influencing relief formation during FIB etching, we developed an algorithm for modeling the surface relief with allowance for the process of redeposition as a function of the angle between the directions of sputtering and FIB (Fig. 4).

We have developed software written in programming language C++, making it possible to calculate the two-dimensional topography of the substrate surface during FIB etching, a quantitative calculation of the parameters of relief, geometric parameters of the ion beam, and the etching rate of the substrate in different directions.

Calculated dependence of the arithmetic mean roughness within the etching area on the magnitude of an overlap

Overlap, %	10	20	30	40	50	60	70	80	90
Arithmetic mean roughness, nm	2.5	2.4	2.0	1	0.7	0.6	0.7	1.5	2.5

RESULTS AND DISCUSSION

Using the software developed in this work, we have simulated surface relief of the substrate obtained during consecutive irradiation by FIBs in several points with the preset overlap (150%) and an impact time of 30 ms. As a result, we have obtained surface profiles of the substrate with allowance for the effect of redeposition of sputtered material and without it (Fig. 5).

To compare these data, we have performed experimental investigations using FIB module based on a NANOFAB NTF-9 (NT-MDT, Russia) multipurpose nanotechnological complex. The morphology and geometrical parameters of the profile were studied in tapping mode of atomic force microscopy using an SPM module of NANOFAB NTC-9 equipment (NT-MDT, Russia) [11]. In experimental studies we used KDB-10 (100) silicon substrate. Etching was performed by the focused beam of gallium ions in regimes which are characterized by the following set of parameters: a beam current of 50 pA and a voltage of 30 keV; the number of passages was assumed to be 100 and the duration of the exposure and overlap were equal to 30 ms and 150%.

In addition, an analysis of an arithmetic mean roughness of the surface relief depending on various

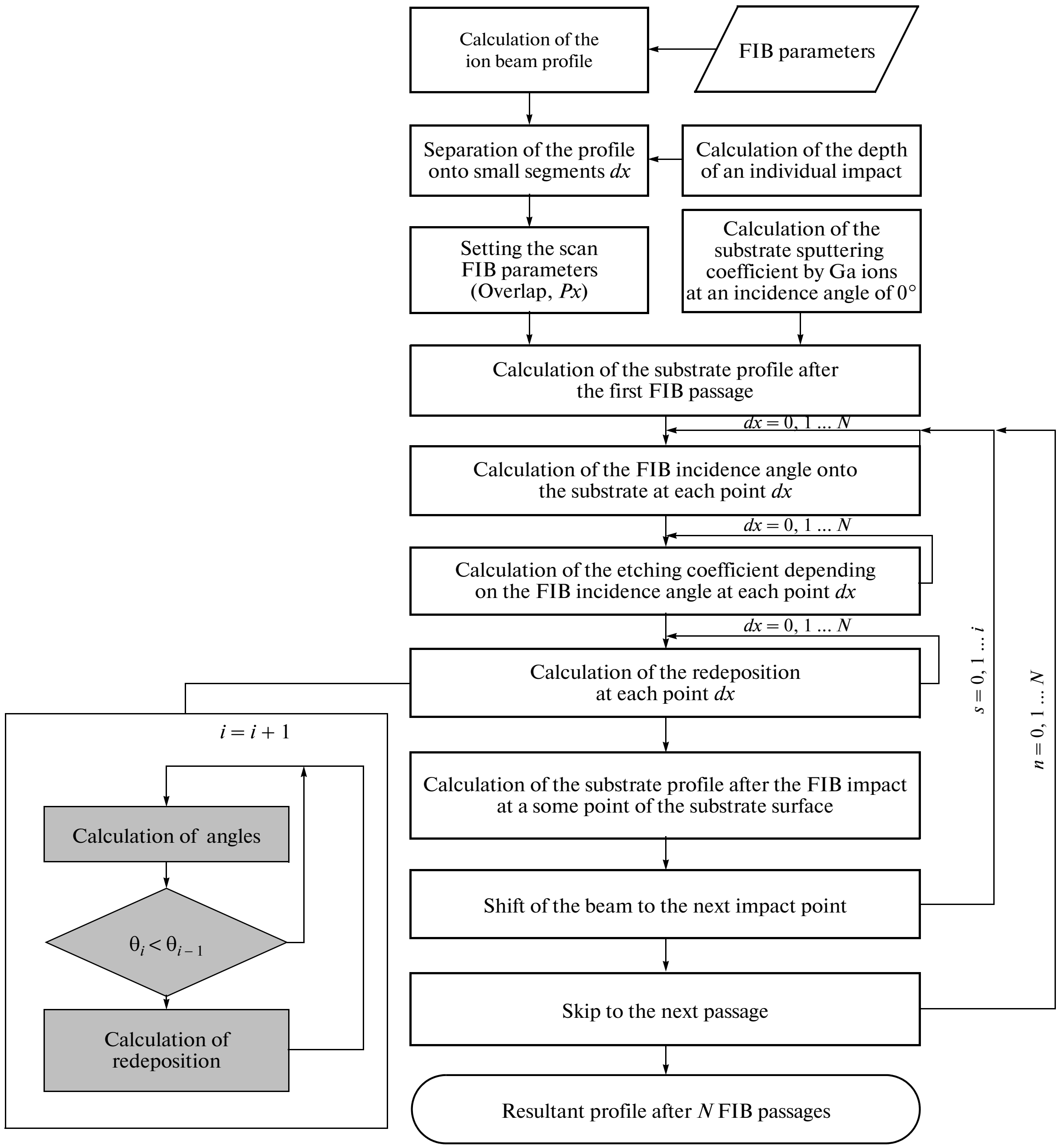

Fig. 4. Algorithm for simulating the dimensional topography of the substrate surface by FIB etching.

parameters of the FIB action on a silicon substrate was performed. This analysis showed that the greatest impact on the formation of the developed etching area has parameter *overlap*. The table shows the calculated arithmetic mean roughness depending on *overlap*. The minimum arithmetic mean roughness is equal to 0.65 at *overlap* = 66%.

Analyzing these results, we can conclude that dependences which are plotted with allowance for the effect of redeposition are in good correspondence with the experimental ones and allow us to calculate the profile of the substrate during FIB etching more precisely (Fig. 5). A certain mismatch of theoretical and experimental curves can be explained by the fact that the simulation does not consider the amorphization effect of the surface layer of the substrate and the difference between the rates of spraying and redeposition of crystalline and amorphous material. Comparing the theoretical and experimental values of the arithmetic mean roughnesses of the bottom of an etched area also showed a good correlation: the roughnesses of theoretical and experimental profiles are 2.5 and 3.9 nm at *overlap* = 90%.

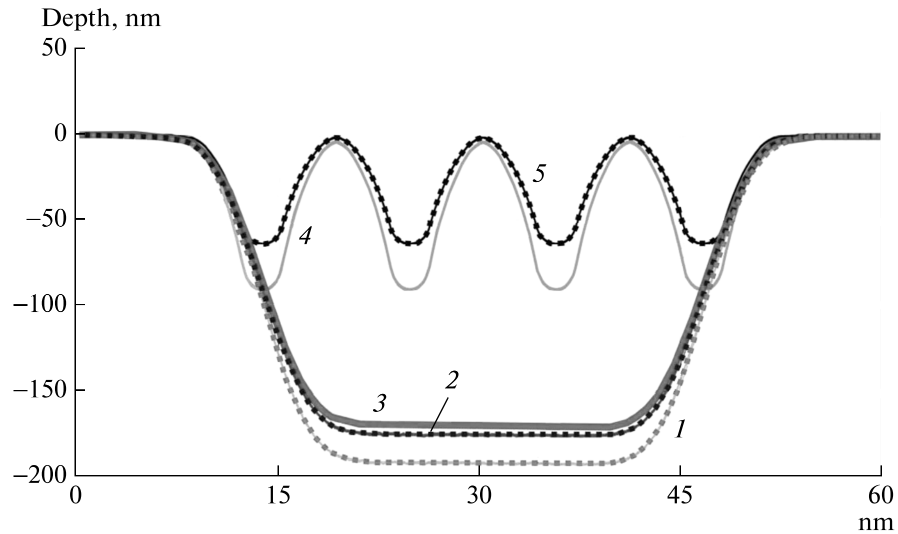

Fig. 5. Profiles of the topography of the substrate surface after exposure to FIB: (*1*) calculation without redeposition (overlap = 50%), (*2*) calculation with redeposition (overlap = 50%), (*3*) experimental profile (overlap = 50%), (*4*) calculation without redeposition (overlap = 200%), and (*5*) calculation with redeposition (overlap = 200%).

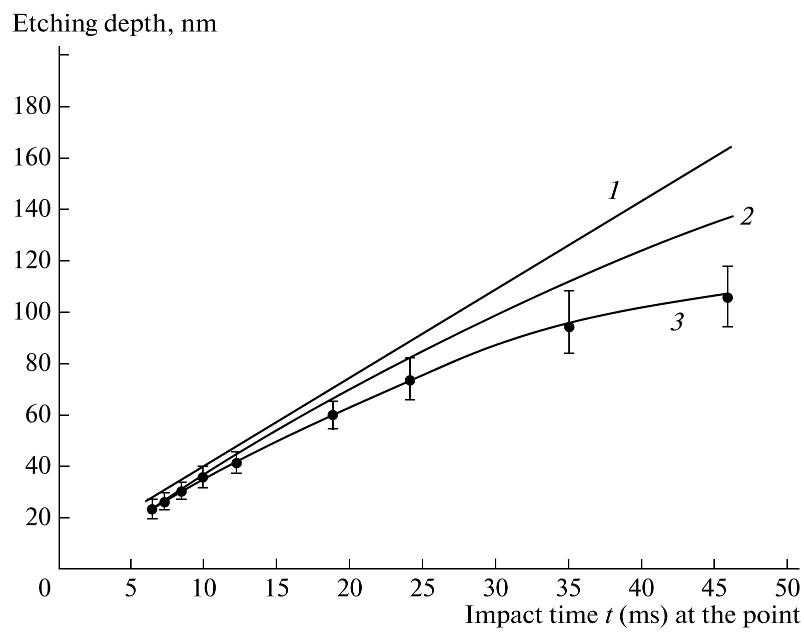

Fig. 6. Dependence of the etching depth on the FIB impact time at the given point: (*1*) without redeposition, (*2*) with redeposition, and (*3*) experimental dependence [9].

Using the results of numerical simulation, we have calculated the depth of the ion-beam etching of the substrate depending on the exposure time at the point of the FIB. Figure 6 shows the obtained theoretical and experimental dependences. Their comparison demonstrates a good correlation for the FIB processing time from 5 to 18 ms and some divergence at larger exposure times. This effect can be related with the fact that, for a small etching depth corresponding to the small impact time at the given point of the impact, the effect of redeposition does not exert a decisive influence on surface relief, while with an increase in the etching depth the effect of material redeposition becomes more important, which explains the difference between dependences 1 and 2 in Fig. 6. The difference between dependences 2 and 3 is caused by the fact that the interaction of the sputtered atoms and the action of reflected ions onto the side walls are not taken into account in modeling, though these effects lead to material redeposition and diminish the total etching depth.

CONCLUSIONS

As a result of the work, we have developed a mathematical model for calculating the two-dimensional topography of the substrate surface using FIBs etching. Based on this model, we simulated the two-dimensional relief of the substrate surface after the FIB action and compared the theoretical and experimental dependences of the etching depth on the FIB exposure time at the given point. Moreover, a correlation of these results was established and the analysis of the substrate profile formation during the FIBs etching was performed. It was established that the main effects during the substrate surface-profile formation are related with the energy distribution of ions over the diameter of the beam, the technological parameters of the beam and scanning system, the sputtering coefficient of the substrate material and its angular dependence, and the effects of redeposition and amorphization of the sputtered material and subsurface layer upon FIB irradiation.

The developed algorithm and mathematical model for calculating the two-dimensional topography of the substrate surface by using FIB etching allows one to forecast the relief parameters of solid surfaces when etching the surfaces by this method. The adequacy of the model is confirmed by a good correlation between the simulation results and experimental data in a wide range of parameters.

To improve the adequacy of the model and reliability of the results, it is necessary to take into account the contribution related to the amorphization of the substrate surface layer. The results can be used in the design and simulation of manufacturing processes of submicron structures and elements of nanoelectronics and the technology of nanosystems.

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