3D ion multi-beam processing with CHARPAN PMLP tool and with a single ion beam FIB tool, optimized with the 'IonRevSim' software

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ABSTRACT

The paper demonstrates that the ion beam milling process can be modelled as a local isotropic etching without taking into account the material re-deposition during the sputtering. It also presents a software, IonRevSim, specifically developed to simulate the 3D ion structuring and thus to validate the milling process and if necessary to optimise off-line its processing parameters. In particular, employing the IonRevSim software it is possible to prepare the necessary data for performing 3D ion milling and then to simulate the 3D structuring process with the aim to minimise the deviation of resulting machined surface from the targeted one. These two main functions of the software and their respective operating modes are discussed in the paper. An experimental verification based on an optimised data generated by IonRevSim was performed using both FIB and multi-beam CHARPAN PMLP tools. For both ion-patterning techniques a good agreement between experimental and simulation results was demonstrated when applied for producing relatively low aspect ratio structures.

Keywords: PMLP, FIB, 3D patterning, software, CHARPAN, IonRevSim

1. INTRODUCTION

3D ion-beam milling with the aim to produce predefined shapes at micro and nano scale with a minimum geometrical error is an ambitious task that have attracted the attention of researchers both exploring the capabilities of single Focused Ion Beam (FIB) systems and also those developing novel technologies for Projection Mask-Less Patterning (PMLP). In particular, a method for layer-by-layer FIB machining of complex 3D shapes utilizing 3D CAD models was developed and experimentally tested by some of the authors of this paper in another research [1]. However, in the conducted feasibility studies to validate it, two assumptions were made about the angular dependence of the sputtering rate and the material re-deposition during the sputtering process. Therefore, to increase the accuracy of the 3D FIB milling process it is necessary to investigate and thus minimize the negative effects of these two assumptions. One possible way to achieve this is by developing accurate simulation models for off-line process optimization, e.g. the one discussed in this paper. In addition to single beam processing an ion multi-beam PMLP tool designed and implemented as part of an European project “Charged Particle Nanotech” (CHARPAN) [2] for performing simultaneous sputtering with thousands of focused beams necessitates the development of appropriate methods for off-line process optimization. Especially, again the dependence of the etching rate, V, on the inclination angle θ represents a major uncertainty in calculating accurately the optimal ion dose for the ion multi-beam PMLP processing. In this context, the paper describes a novel software for Ion Reverse Simulation (IonRevSim) that was developed as a tool for calculating and optimizing the processing parameters for performing single beam and multi-beam sputtering of 3D structures.

The IonRevSim software implements two basic approaches for defining the ion doses for the milling process and then to simulate the 3D structuring process. Starting with the geometrical description of the desired 3D structure IonRevSim generates a file in the GDSII data format by employing quasi-stationary or stratification, layer-based, strategies to drive

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both FIB and multi-beam PMLP systems. In addition, by applying these two techniques, the data necessary to simulate the 3D ion milling process are generated, too. Particularly, in this research the sputtering process by the scanning FIB and by multi-beam PMLP system is modeled as an isotropic local etching [3,4].

In this paper, a method for calculating and optimizing the data necessary to carry out 3D ion milling is discussed together with a method to simulate the sputtering process. To validate the data generated by IonRevSim, and also the simulation results obtained with this software, an experimental study was conducted to assess the validity of the proposed method when performing 3D ion beam structuring.

2. EXPOSURE DATA PREPARATION

[c]The IonRevSim software can use as an input data the 3D geometrical description of the pre-defined structures in different formats, e.g. BMP, RSL but also it is possible to generate this data internally by entering the analytical description of the desired 3D shape. For example, the pyramid in Figure1.a was created employing the internal capabilities of the software to create 3D models. In addition, as it was already mentioned two strategies are implemented in IonRevSim to define the ion etching dose for each pixel and thus to be able to perform FIB and multi-beam PMLP, in particular the quasi-stationary and stratification ones.

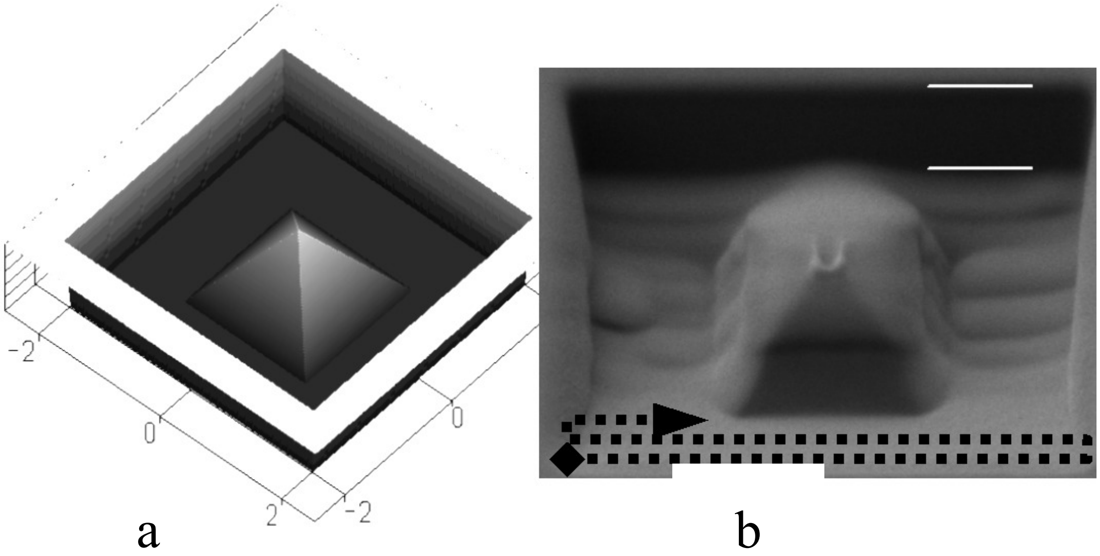

Figure 1. a) Square pyramid with a 2x2 μm base used as a test structure. b) FIB milling results with a single exposure. The big discrepancy with the targeted shape is due to both non-stationary etching and material re-deposition.

When, the quasi-stationary strategy for 3D ion structuring is applied, the total calculated optimal ion dose per pixel, *D(x,y),* is applied in *N* small portions, *D(x,y)/N*. Thus, this ion milling strategy mimics the stationary ion etching with "shaped" ion beam, which has a different ion density for each pixel *(x,y)*. The term "stationary" implies that the ion beam current density does not change with the time during the sputtering process, and all points on the sample are milled simultaneously. Such shaped beams are typically employed in projection ion lithography, e.g. the CHARPAN tool [5]. The splitting of the desired dose into *N* portions is shown schematically in Figure2b.

To calculate the optimal dose in the quasi-stationary mode the angular dependence of the ion sputtering rates is considered. It is assumed that this dependence could be described employing a simple formula, $V(\theta)= V_0 /\cos\theta$. This approximation allows the model of isotropic local etching, firstly developed and implemented for liquid etching, to be used both for optimization and simulation of the ion structuring process. The developed software, IonRevSim, allows the inverse 3D sputtering problem to be solved. In particular, a numerical procedure is proposed to define the optimal dose distribution, D_{il}, in an iterative manner that takes into account the current difference between the reference and calculated profiles. The calculated in this way D_{il} minimizes the profile error up to a preset level. This method for optimizing the sputtering parameters is called quasi-stationary because it is assumed that the ion dose does not change during the process regardless of the beam spatial coordinates. In particular, when the quasi-stationary mode is applied, the number of exposure loops and exposure doses necessary for each pixel are calculated with the objective to achieve non-uniform sputtering similar to that of a stationary beam.

On the contrary, when the stratification mode is applied for 3D structuring the calculated dose is distributed "horizontally" into M strata/layers, each having a uniform dose but different exposure areas. Thus, after exposing all the strata, the calculated so call total dose for each pixel, $D(x,y)$, will be applied. The exposure order of each stratum is also important. The software generates the correct exposure sequence of strata automatically, from the bottom to the top. Once generated, the exposure data can be exported in different lithographic formats, e.g. GDSII, to drive the 3D FIB milling process.

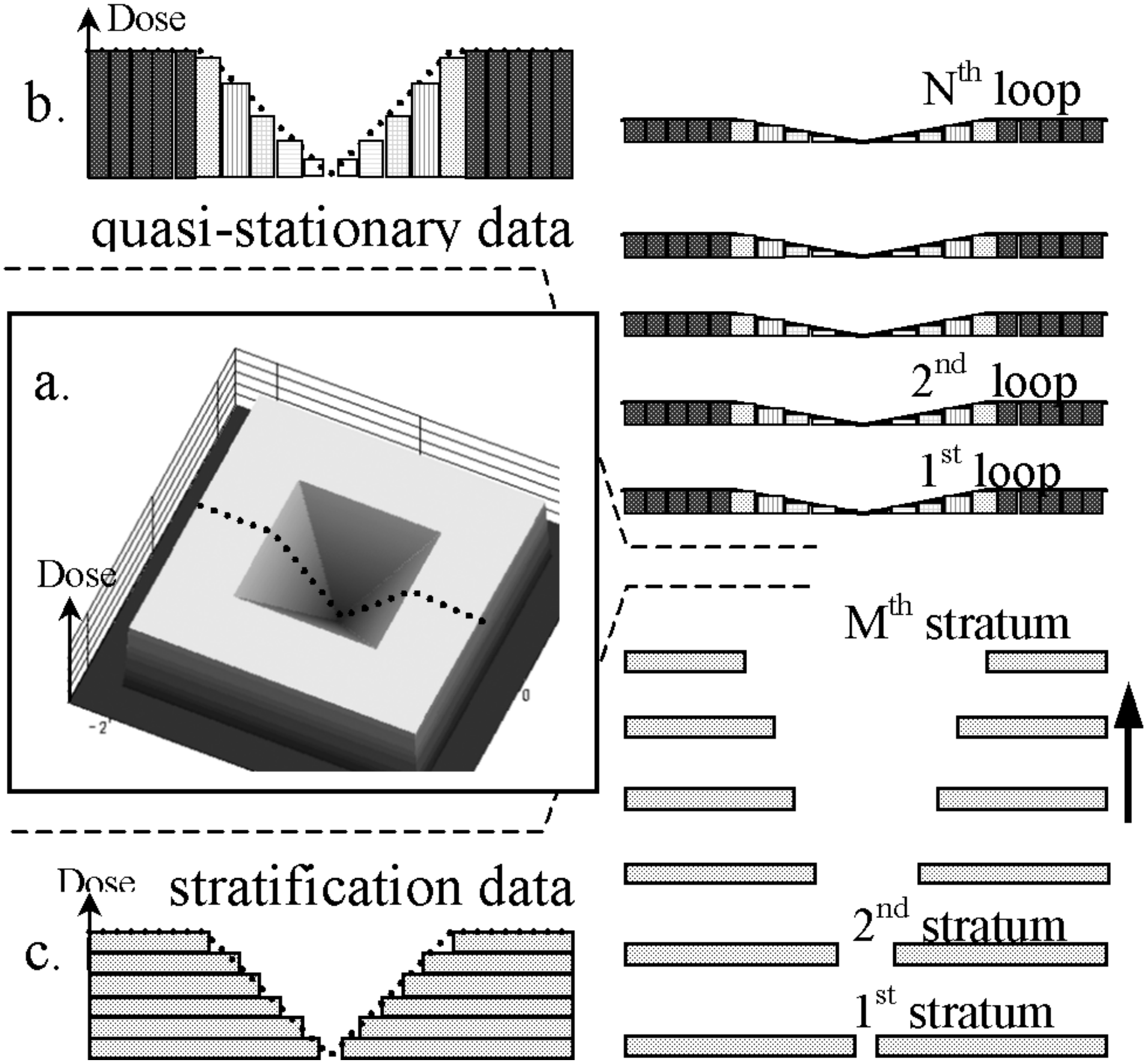

Figure 2. a) The total exposure dose used in all experiments and simulations. b) and c) are schematic illustration of the exposure modes used: quasi-stationary with N exposure loops and stratification with M exposure strata, respectively. Columns in b) and c) represent exposure doses per point/pixel while the vertical arrow shows the exposure order.

3. SIMULATION MODEL

In adopted simulation approach it is assumed that the ion beam has stationary current density $J(x,y)$ in the XY plane and the surface that will be etched is flat and coincides with the XY plane. In addition, it is assumed that the incidence ion direction is parallel but opposite to the Z-axis. During the sputtering process the initially horizontal workpiece tilts and the surface normal is no longer parallel to the Z-axis. Again, an assumption is made that the sputtering rate coefficient, the quantity of sputtered material per one ion, is proportional to $1/\cos(\theta)$, where θ is the tilt angle, the angle between ion direction and the surface normal. The angular dependence of the sputtering rate is observed for a wide range of θ, and depends on the workpiece material, the type of ions used and their energies [6]. These assumptions are very important because they allow the ion sputtering process to be modeled as an isotropic local etching [3, 4, 7] that is usually applied for wet etching. At the same time it is worth stressing that the isotropic local etching model does not take into account the material re-depositioning and ion re-scattering during the sputtering process, and also that the etching velocity perpendicular to the surface is independent from θ. Certainly, for inclined surfaces, the number of ions per area decreases with the increase of $\cos(\theta)$. Thus, this decrease compensates for the sputtering rate increase. Hence, the etching velocity $V(x,y) \sim \cos(\theta)J(x,y)/\cos(\theta)$ doesn't depend on the inclination of the targeted surface and depends only on the current density of the beam, $J(x,y)$, or in quasi stationary ion mode on the exposure dose at each pixel. Certainly, proportionality of the sputtering rate to $1/\cos(\theta)$ is not valid for all θ angle values. At angles, θ_m, in the range from 60º to 80º, the sputtering coefficient reaches its maximum and then decreases due to reflection of ions from the surface. This means that the etching simulation based on the isotropic local etching model is not applicable for simulation of relieves with steep slopes.

A major advantage of this approach is the absence of unknown, fitting, parameters in the model. The only necessary value is that of the exposure dose D^{*} $[A*s/cm^{2}]$, which is needed for sputtering of large areas at θ equal to 0 at a given depth H^{*}. A relative value $R_s=D^{*}/H^{*}$ $[A*s/cm^{3}]$ denotes the sputtering "sensitivity", which is a physical constant for a given substrate material, type and energy of ions. The sputtering sensitivity R_s can be obtained by conducting simple experiments.

Let us consider the results of the isotropic local etching model discussed in [2, 3, 6]. The sputtering velocity (sputtering rate) $V(x,y)$ does not depend on Z. A 2D case, i.e. profile $z(x,t)$ depending on two variables, has a simple solution [4, 7]:

$$z(x,t) = \min_{x_0}\left[H_0 - V(x_0)t + \left| \int_{x_0}^{x} d\sigma \sqrt{\left(\frac{V(x_0)}{V(\sigma)}\right)^2 - 1} \right| \right];$$

where: $z(x,t=0)=H_0$ is the initial profile and t is the sputtering time. This equation can be transformed to take into account the dose distribution, $D(x,y)$:

$$\mathrm{z(x,t)} = \min_{\mathrm{x}_0}\left[-\mathrm{D}(\mathrm{x}_0)/\mathrm{R}_\mathrm{s} + \left| \int_{\mathrm{x}_0}^{\mathrm{x}} \mathrm{d}\sigma \sqrt{\left(\frac{\mathrm{D}(\mathrm{x}_0)}{\mathrm{D}(\sigma)}\right)^2 - 1} \right| \right];$$

where: $H_0=0$ for all the calculations.

In the 3D case, the minimum of $z(x,y,t)$ should be located along trajectories in the XY plane [3, 4]. The first term in the formula represents the simplest sputtering model, assuming that the etching depth is proportional to the exposure dose. Thus, in this case the θ dependence of sputtering yield is neglected. Therefore, the analytical description implemented in IonRevSim is an improvement because of the $1/\cos(\theta)$ dependence of the sputtering yield. Certainly, the computational complexity increases by modeling the 3D ion milling process as an isotropic local etching in comparison to the simplest sputtering one, but it is significantly simpler compared to other sputtering models where re-deposition, reflection ions and arbitrary θ behavior of the sputtering yield (in accordance to experimental data [6] and SRIM simulation [8]) are taken into account [9]. That is especially important when employed to solve the inverse problem and also to model the ion milling of 3D shapes.

It is important to note that in comparison to more sophisticated but much slower IonShaper® [10] IonRevSim showed good agreement with experimental results for structures with low aspect ratio [11].

4. TEST STRUCTURES AND RESULTS

Two different tools were used for experimental verification of optimization procedures and also to validate the simulation model. Due to the multi-beam nature of the CARPAN PMLP tool only data generated by applying the quasi-stationary strategy were used for it while for the FIB system data prepared applying both modes were used for 3D structuring. In particular, a set of experiments was performed on the FIB set-up to demonstrate clearly the advantages and efficiency of using exposure data generated by IonRevSim. Figure1.b shows the result of a "naive" strategy when FIB follows a meander trajectory to expose a flat surface. The dwell time at each beam position was calculated proportional to designed depth (Figure1.a) taking into account sputtering sensitivity, R_s. As it can be clearly seen this naive strategy failed to produce the target structure due to material re-deposition and non-stationary effects.

4.1 CHARPAN PMLP TOOL

To validate the simulation model described in this research, 10x10 arrays of square convex and concave 2.2 µm microlenses with height up to 0.57 µm (Fig. 1a-c) were designed. Then, for these test structures the optimal ion beam dose was generated employing the IonRevSim software and then quasi-stationary milling was performed with the CHARPAN PMLP tool. SEM and AFM images of a 10x10 microlens array fabricated in this way are shown in Figs. 3 a) and b). Figure 3c shows the simulation result obtained with IonRevSim when performing ion multi-beam sputtering with optimal dose.

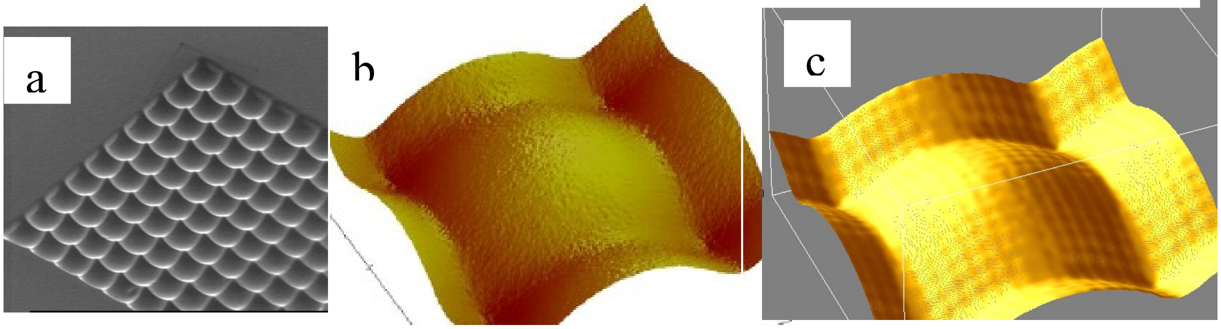

Fig. 3: 10x10 array of square 2.2 x 0.57 µm microlenses fabricated with the CHARPAN PMLP tool with ~ 250,000 argon ion beams (of different sizes)working in parallel, and 10 keV energy. a) SEM image of concave microlenses on a Si surface; b) convex microlenses on GaAs surface (an AFM image); and c) simulation results of IonRevSim for a convex microlens.

4.2 FIB

In order to validate the IonRevSim simulation results for 3D FIB structuring and assess the quality of the GDSII files generated by applying the stratification and quasi-stationary modes, a square pyramid geometrical model was selected. The pyramid with a base 2x2 µm was placed in a box with a 4x4 µm base, as shown in Figure 1. The model was created by employing the IonRevSim build-in capability to generate 3D models by entering their analytical descriptions and then the result was exported in a GDSII format file. The experiments were conducted on a FIB system, XB1540. To carry out the machining with the GDSII data generated by IonRevSim, Raith lithography software and hardware, Elphy Quantum, was employed to control the FIB system externally. A fused silica substrate coated with a 15 nm Cr layer was used. The sputtering sensitivity for SiO_2 is: $R_s = 2400\ A*s/cm^3$.

Figure 4 presents the results from the FIB milling tests together with the simulation results obtained with IonRevSim. Three different files were generated with the software to carry out 3D FIB milling, one employing the quasi stationary strategy and two - the stratification mode with the same number of strata, 100, but with different exposure orders. Fig 4 a) and b) show that the simulation results are almost identical with the experimental one when the 100 strata were exposed from the bottom to the top. The simulation and milling results from the exposure of the same number of strata, 100, in an inverse order, from top to the bottom, are presented in Fig 4 c) and d), respectively. Again, there is a good agreement between the simulation and experimental results except for the pyramid center due to the relatively steep inclinations of the pyramid surfaces. It is unlikely this to be due to re-depositioning effects during FIB milling.

To demonstrate that the optimal doses for the two modes, stratification and quasi-stationary ones, differ, the third set of experiments were conducted applying the quasi-stationary mode, Figure 4 e) and f). Though, the obtained shapes of the pyramid in both simulation and experimental results are different from the 3D model, they are almost identical at the same time. Therefore, it can be concluded that the simulation software can be used to predict quite accurately the results of the 3D FIB milling operations.

5. CONCLUSION

The IonRevSim software generates optimized ion-dose data for performing 3D ion sputtering with both single and multi-beam tools employing quasi-stationary and stratification modes to produce micro and nano scale structures with relatively small aspect ratios. The isotropic local etching model implemented in IonRevSim allows the ion milling of complex 3D structures to be simulated for both FIB and multi-beam (CHARPAN) systems. The effects of material re-depositioning and ion re-scattering can be considered negligible for relief inclinations of less than 45º. It is demonstrated with the simulation results and then confirmed with the FIB experiments that the 3D ion sputtering results are strongly dependent on the order of ion exposure in the stratification mode. Particularly, it is demonstrated that by changing the sputtering sequence without modifying the ion dose, the resulting 3D profiles will be different.

6. ACKNOWLEDGEMENTS

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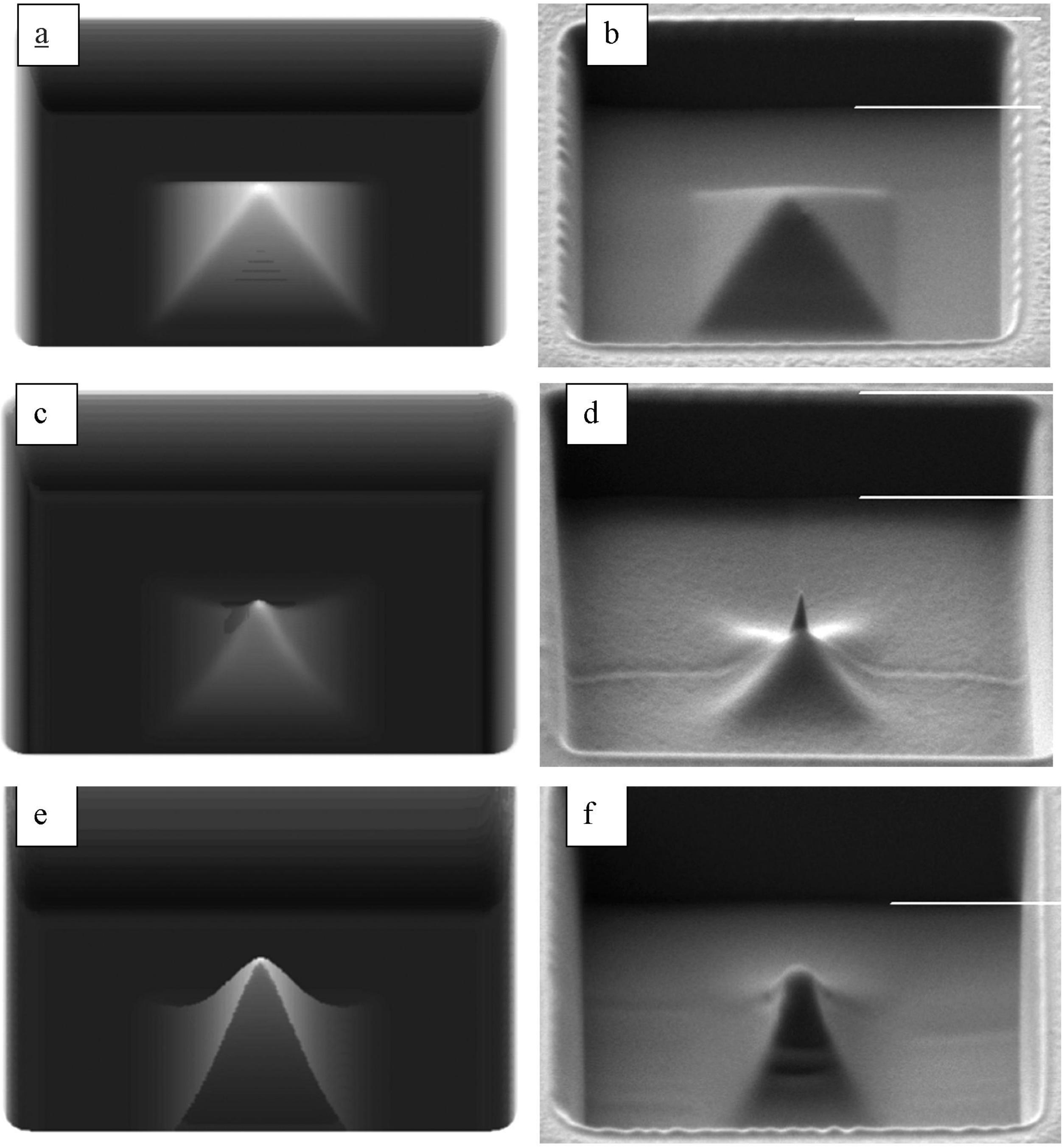

Figure 4. Simulation (a, c, e) and corresponding FIB 3D milling (b, d, f.) results. (a,b)- stratification mode with 100 strata and pyramid height, ~ 1µm; (c,d)- inversed exposure order of 100 strata and pyramid height, ~1µm, (e,f) - quasi stationary mode, number of loops, 30 and pyramid height, ~1.6µm. Observation angle is 36°.

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