



FIB sputtering optimization using Ion Reverse Software

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ABSTRACT

This paper experimentally demonstrates that a quantitative description of focused ion beam (FIB) milling (at least for several 3D profiles with inclination not higher than 45°) can be done by means of an isotropic local etching model. Specific characteristic of this model is that it does not account for re-deposition.

The paper also presents IonRevSim – Software developed specifically for data preparation and prediction of the shape of the FIB machined structures. Those functions and their operating modes are discussed here in detail and FIB experimental results are provided to verify the algorithms embedded in the software.

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1. Introduction

To have a better control on the FIB sputtering process when realizing complex 3D shapes, Novel Simulation Software (Ion Reverse/Simulation Software – IonRevSim) is created. In our previous study, the capability for layer-by-layer FIB machining of complex 3D shapes utilizing 3D CAD models was reported [1]. However, in that method two factors were neglected: the angular dependent sputtering rate and the re-deposition. To take into account the first factor and to increase the accuracy of FIB sputtering process for 3D structuring, IonRevSim was validated for FIB machining of nanoimprint lithography (NIL) templates.

The IonRevSim, developed especially for FIB application implements two basic approaches to dose definition in file preparation for FIB milling as well as a data simulation function. Having the desired structure (a complex 3D shape in most cases) the IonRevSim prepares the input *.gds data file for FIB milling using one of the two main approaches for dose preparation: quasi-stationary or stratification technique. Based on the data generated the software simulates the sputtering process during feature machining. The latter function is based on the isotropic local etching model [2,3].

In this paper, optimized data preparation method is discussed and simulation results for 3D patterning generated by IonRevSim are compared to the ones obtained after FIB machining.

2. Preparation of optimal exposure data with IonRevSim

The software can accept as an input 3D structures designed in different formats (e.g. BMP) and it also provides the option to design 3D structures internally using their mathematical description. For example the pyramid of Fig. 1 was created with internal tools of the software. There are two approaches that can be applied for the preparation of the ion etching dose, i.e. quasi-stationary and stratification.

In case of quasi-stationary strategy, the calculated ion dose $D(x,y)$ is applied in N small portions $D(x,y)/N$. This approach mimics stationary ion etching with “shaped” ion beam, which has different ion density in each point (x,y) . The term “stationary” implies that the ion beam current density does not change with time during sputtering and all parts of the sample are milled simultaneously. Such shaped beams are typically employed for projection ion lithography like CHARPAN tool [4]. The splitting of the desired dose into N portions is shown schematically in Fig. 2b.

In applying the stratification mode, the calculated dose is distributed “horizontally” into M strata, each having a uniform dose but different exposure area. Thus, after exposing all the strata, the calculated (total) dose $D(x,y)$ will be applied. The exposure order of each stratum is very important. The software generates the correct exposure sequence of strata automatically (from bottom to top). Once generated, the exposure data is exported in different lithographic formats, like GDSII etc.

3. Simulation using IonRevSim based on isotropic local model

In this simulation approach it is assumed that the ion beam has stationary current density $J(x,y)$ in the XY plane. The initial etched

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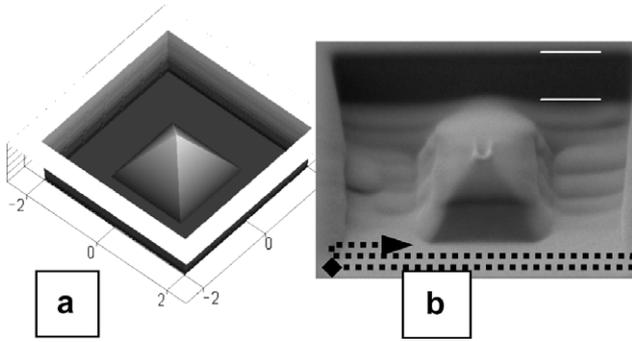


Fig. 1. (a) Test structure of square pyramid with base $2 \times 2 \mu\text{m}$. (b) FIB etching with single loop. The big distortion of the ideal shape is a result from both non-stationary etching and re-deposition.

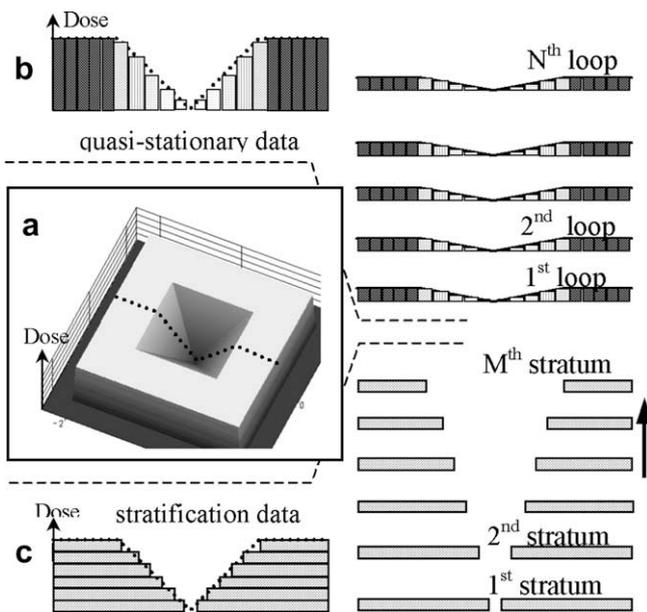


Fig. 2. (a). The total exposure dose $D(x,y)$ used for all experiments and simulations. Schematic illustration of optimal exposure data preparation for the two modes of exposure: quasi-stationary (b) with N exposure loops and stratification (c) with M exposure strata. Rectangles in b and c represent exposure elements corresponding to cross sections along dot-line of a. Vertical arrow shows exposure order.

surface is flat and coincides with XY plane. Incidence ion direction is parallel but opposite to Z-axis. During sputtering the initially flat relief tilts and the surface normal at some points is no longer parallel to Z-axis. Here an assumption is made that the sputtering rate coefficient (quantity of sputtered material per one ion) is proportional to $1/\cos(\theta)$, where θ is the tilt angle (angle between ion direction and the surface normal). The angular dependence is observed for a wide range of angles θ , and for lots of materials, ions and their energies [5]. This dependence is very important as it allows us to consider ion sputtering in the model of isotropic local etching [2,3,6] usually applied for wet etching. (Note that in isotropic local etching model the processes of sputtered material re-deposition and ion re-scattering are not taken into consideration and the etching velocity perpendicular to the surface is independent from θ). Indeed, for inclined surfaces, the number of ions per area decreases as $\cos(\theta)$. This decrease compensates for the increasing of the sputtering rate. Thus the etching velocity $V(x,y) \sim \cos(\theta)J(x,y)/\cos(\theta)$ does not depend on the inclined surface and depends on current density of beam $J(x,y)$ (or exposure dose in quasi-stationary FIB mode) in each point. Of course, proportionality of sputtering yield to $1/\cos$

θ) is not valid for all θ angle values. At angle $\theta_m = 60\text{--}80^\circ$ 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 isotropic local etching model is not applicable for simulation of relief with steep slopes.

Great advantage of that approach is the absence of unknown (fitting) parameters in the model. The only necessary value is that of the exposure dose $D^* [A \cdot s/\text{cm}^2]$, which is needed for sputtering of large areas at $\theta = 0$ at a given depth H^* . A relative value $R_s = D^*/H^* [A \cdot s/\text{cm}^3]$ denotes the sputtering “sensitivity”, which is a physical constant for substrate material, type and energy of ions. The sputtering sensitivity R_s can be obtained from a simple experiment.

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

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

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

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

where $H_0 = 0$ for all the calculations. For $z(x,y,t)$ (a 3D case) the minimum should be located along trajectories in the XY plane [3,4]. The first term in the formula describes the simplest sputtering model, assuming that the etching depth is proportional to the exposure dose. It is equivalent to neglecting the θ dependence of sputtering yield. The total formula is an improvement of the simplest etching model by $1/\cos(\theta)$ dependence of the sputtering yield. Isotropic local model appears to be more difficult for calculation than the simplest sputtering one, but it is significantly easier compared to a sputtering model where re-deposition, reflection of ions and more complicated θ behavior of the sputtering yield (in accordance to experimental data [5] and SRIM simulation [7]) are taken into account [8]. Simulation presented in Fig. 3 (left column, a, c, e) is performed using expression (1) and dose distribution $D(x,y)$ described in previous section (Fig. 2). The corresponding algorithm based on usage of (1) is implemented in the IonRevSim Software.

4. Test structure and results

In order to validate the IonRevSim Software simulation results for FIB sputtering and assess the GDSII files generated through stratification and quasi-stationary modes, a square pyramid model was selected. The pyramid with base $2 \times 2 \mu\text{m}$ was placed in a box of a $4 \times 4 \mu\text{m}$ base, as shown in Fig. 1. The model was generated through an analytical description and exported in GDSII format. The experiments were conducted on a FIB system, XB1540 (combining Orsay Physics gallium ion beam column with an electron beam GEMINI column). For exposing GDSII data, Raith lithography software and hardware, Elphy Quantum, was employed to control the FIB system externally. Amorphous material was used as a substrate - fused silica covered with nanometer-thin Cr layer. The sputtering sensitivity for SiO_2 is: $R_s = 2400 A \cdot s/\text{cm}^3$.

Fig. 1b shows result of naïve strategy when following meander trajectory ion beam exposes flat surface. Dwell time at each beam position was calculated proportional to designed depth (Fig. 1a) considering sputtering sensitivity, R_s . It is clearly seen that the naïve strategy is failed due to effects of re-deposition and non-stationarity.

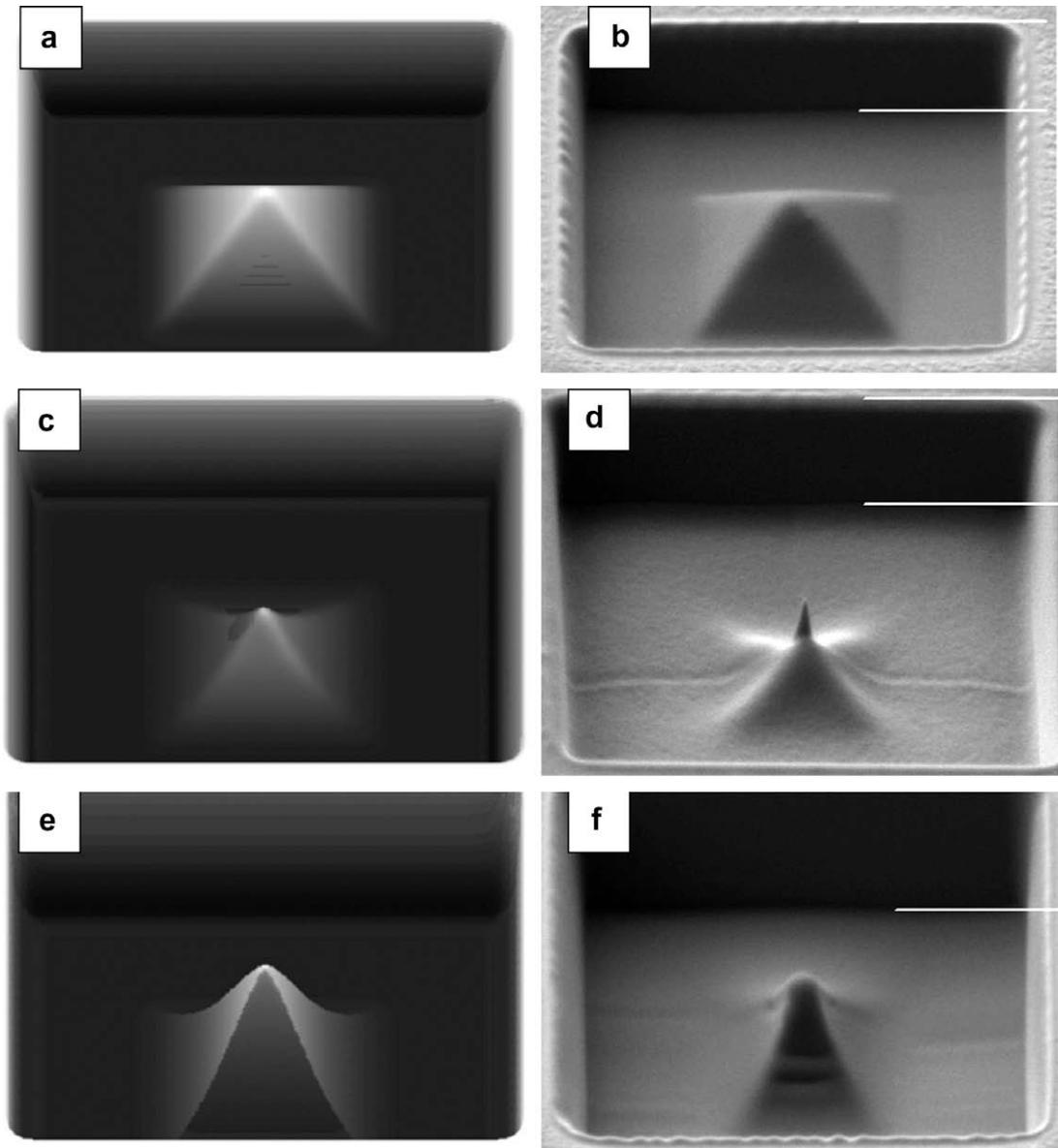


Fig. 3. Ion etching simulation using Eq. (1) (left column, a, c, e) and sputtering results (right column b, d, f) for the different exposure modes shown in Fig. 2. (a,b) Stratification mode $M = 100$, depth H is about $1 \mu\text{m}$; (c,d) stratification mode inverse order $H \sim 1 \mu\text{m}$, $M = 100$; (e,f) quasi-stationary mode (with exposure dose $D(x,y)$ shown in Fig. 2a, $H \sim 1.6 \mu\text{m}$, $N = 30$). Simulation in stratification mode is set of M calculations for all strata doses, Fig. 2c. Observation angle is 36° .

Fig. 3 presents the results from the FIB milling of the GDSII files generated with IonRevSim as well as the expected outcome yielded with the simulation tool of the software. Three types of files were prepared, using the two dose defining approaches: one in quasi-stationary mode and two in stratification mode, both the latter having $M = 100$ strata but different order of exposure execution (right order generated by IonRevSim and inverse). Fig. 3a and b show the results for 100 strata, bottom–top exposure approach and reveal almost perfect coincidence between the expected and the actual outcome. The inverse order of strata (top–bottom execution) is presented in Fig. 3c and d) – simulation and milling result, respectively. The FIB results show that the etching algorithm quite accurately predicted the shape of the produced feature except for the pyramid center where steep slopes appear and the sputtering rate model does not coincide with the experimental one. An explanation related to re-deposition looks unlikely in that case.

To demonstrate that the optimal doses for the two modes (stratification and quasi-stationary) differ, the third simulation using the quasi-stationary mode (Fig. 3e) and the associated FIB

milling (Fig. 3f) were performed. Though the actual pyramid appears to be somewhat steeper compared to the ideal one the overall shape profile of the two features is quite identical. Therefore, it can be concluded that the Simulation Software predicted the shape quite accurately.

5. Conclusion

Several 3D shapes designed and fabricated show that the isotropic local etching model provides a good description of the ion sputtering in quasi-stationary and stratification modes for relieves with small aspect ratios.

The stratification mode provides a viable way for FIB machining of pre-designed complex 3D shapes.

The influence of re-deposition and re-scattering is negligible for relief inclinations of less than 45° .

The ion etching is strongly dependent on the order of ion exposure. It is demonstrated that changing sputtering sequence (for the same total dose) changes the resulting 3D profile.

Acknowledgements

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