AN EXPERIMENT-BASED MODEL FOR FOCUSED ION BEAM SIMULATION AND THE PROCESS DESIGN OPTIMIZATION

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ABSTRACT

An experiment-based model, which differs from the current curve fitting and particle motion models, is presented for simulating the Focused Ion Beam (FIB) process and guiding the scan strategy and parameter design. This approach applies Gaussian function fitting on both etching and deposition, and builds an expectation difference function to describe the distance changes between the distribution centers of the etching and the redeposition, which shows good performance in solving the redeposition effect and its attenuation. Through a series of basic experiments, we optimize the model parameters and demonstrate that this method can effectively simulate the dynamic process of FIB sputtering. This model and the optimized parameters are further applied to the scan strategy and process parameter optimization for the complex Micro/Nano-structure realizations using FIB.

INTRODUCTION

Focused Ion Beam (FIB) sputtering is a well-established technique for the micro and nano scale topography creation and modification [1]. This process uses a high-energy focused ion beam to bombard the substrate surface to remove the material and realizes the direct patterning of three-dimensional shapes. The sputtered particles, as a mixture of the incident ion and the substrate atom, are re-deposited on the other fronts of the structure (Figure 1 (b)). The effects from the redeposition are closely related to the beam current, dwell time and the scanning strategies. A rigorous analysis of the parameter influence and the effects is critical for the correct simulation, the process design and their optimization.

For the FIB users, the ion beam current is preset rather than a continuously adjustable variable. It correlates with the beam size and the current density distribution, which determine the extent of irradiation and the distribution of the received ion dose in the area. They further affect the depth and opening width of the formatted structures. However, in practice, it is impossible to calibrate the current and the ion beam of the device every time when it is used, so the condition of the equipment also has a great influence on the ion beam and the processing results. As important parameters in scanning strategies, the dwell time and the scanning times directly affect the morphology of the FIB sputtering results, which are also the key parameters of the redeposition effect. As shown in Figure 1(a), with the same incident ion dose, the larger dwell time results in a deeper and larger opening structure also with more pronounced redeposition effect. Conversely, by reducing the dwell time and correspondingly increasing the number of scans, the redeposition phenomenon is alleviated, but the processing efficiency is also greatly reduced. This is because the subsequent repetitive scans have to remove the re-deposited layer at the previously machined surfaces before processing the substrate. Another reason is that the sputtering process is strongly dependent on the surface topography. The sputtering yield, the ratio between the amounts of the sputtered atom to the incident ion, varies with the incident angle, the ion energy and the target material. Even though all these parameters are fixed, the re-deposited particle flux is still not constant throughout the process. Instead, like in Figure 1(c,d), the deposition amount reduces along with the advancement of scanning and with the increase of the structure opening. An important reason for the attenuation is that the redeposition route for the particles is lengthened from the slowing of the etching deepen and the rise of the deposition receiving surface. All these effects make it difficult to design the scan strategies and obtain the specified parameters for the complicate structure processing in practical applications. This has led to extensive efforts to simulate the FIB milling [2-5].

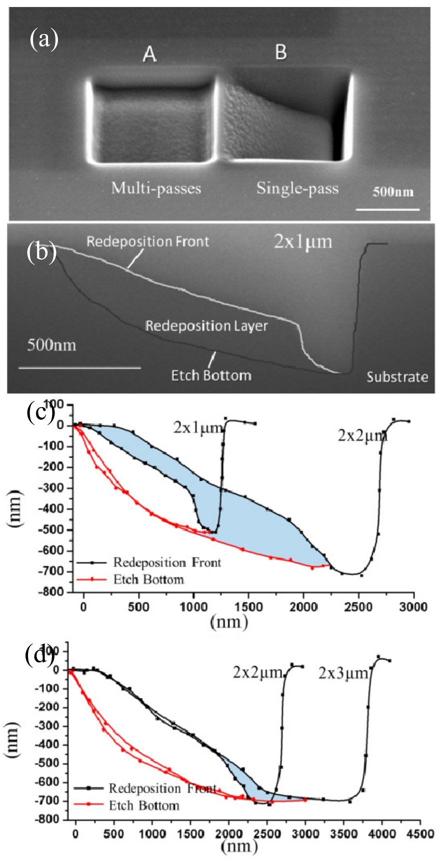

Figure 1, (a) FIB rectangle milling results with multi-pass(A) and single-pass(B) scans.(b-d)Cross-section profile and the redeposition effect at different periods in rectangle scanning (serpentine) with 30kV, 48pA, 1ms dwell time and 1pass on silicon (111). (c,d) The color area is the redeposition amount between the periods.

The current curve fitting algorithms focus only on the profile development with dwell time, while the particle motion models are computationally complex and lack of the attenuation phenomena consideration in the redeposition problem. In this study, we propose a new experiment-based model, which introduces the Gaussian function fitting as an efficient solution for both the etching and redeposition simulations. The particle swarm optimization (PSO) method is introduced to optimize its parameters, and makes the model applicable to different process and device conditions.

FIB MODELING

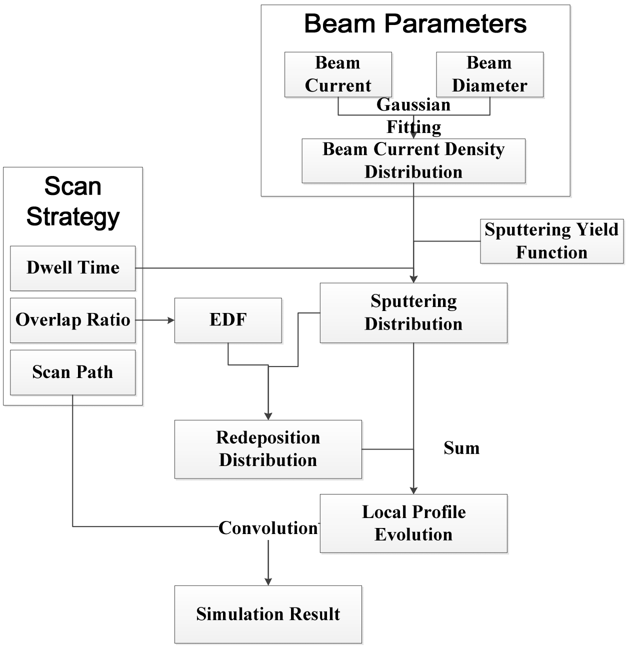

Figure 2. Flow chat of the model.

The actual FIB milling is an accumulation of discontinuous processing at each pixel on the scan path. The same is true with the simulation. As shown in Figure 2, the simulation result is calculated by the convolution of the scan strategy P_s and the line spread function (LSF) J_{tot}, which stands for the local profile evolution.

$$d = P_s * J_{tot} \quad (1)$$

Here, the P_s is a normalized discrete scanning position function, and the J_{tot} is the combination of sputtering and redeposition.

$$J_{tot} = J_{sput} + J_{red} \quad (2)$$

where J_{sput} is the sputtering function, and the J_{red} is the redeposition function. These functions are based on the Gaussian fitting functions, and they are defined as:

$$J_{sput}(x) = Y \cdot I \cdot h_{dt} \cdot P_{sp}(x) \quad (3)$$

$$J_{red}(x) = q(x) \cdot P_{re}(x) \quad (4)$$

where Y is the sputtering yield function, and the mathematical model from Yamamura et al [6] is used in this study (Figure 3), which can provides a good fit to experimental data for all incident angles. x is the distance between the current beam center and the initial scanned position, I is the beam current, h_{dt} is the parameter related to the dwell time dt which stands for the influences on the processing depth, $q(x)$ is the redeposition amount function, $P_{sp}(x)$ and $P_{re}(x)$ are the Gaussian fitting functions, which stand for the sputtering distribution and the redeposition distribution. As the influence of the substrate profile from the ion beam sputtering, the sputtering distribution is strongly dependent on the ion current density distribution, which has been discussed in researches as a single or multiple Gaussian distribution [5, 8]. Here, we assume it as an n-order Gaussian distribution. The emission distribution of the sputtered particles is treated as Gaussian/cosine distribution in current researches [3,4]. We also assume that the growth of the deposition-receiving surface from the emitted particle accumulation is also Gaussian like. We acknowledge that at some stage of FIB processing, the distribution of deposition accumulation is not completely a single Gaussian, but as an approximation, the simulations have substantiated it effective.

$$P_{sp}(x) = \sum_{i}^{n} a_i \cdot \exp(-\frac{x^2}{b_i}) \quad (5)$$

$$P_{re}(x) = \lambda \cdot \exp(-\frac{(x - r(x))^2}{\sigma^2}) \quad (6)$$

where n is the order of the SDF, a_i, b_i, λ, σ are the Gaussian parameters, and $r(x)$ is the expectation difference function (EDF) which describes the distance changes between the centers between the sputtering and redeposition distributions.

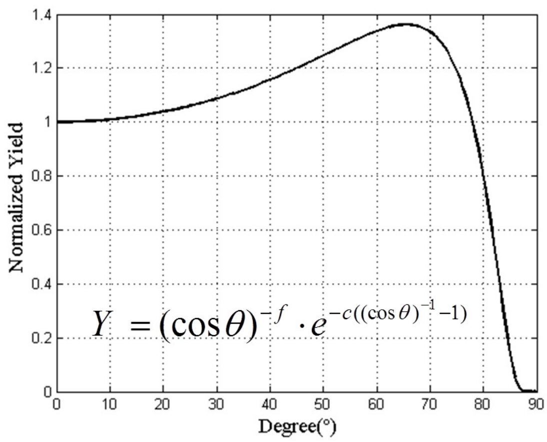

Figure 3. The normalized Yamamura's yield distribution [6].

PARAMETER OPTIMIZATION

PSO is one of the most popular and frequently used nature-inspired optimization algorithms. It searches the best solution by the particle's intelligent motion and its position self-calibration. The particles are considered as a population of candidate solutions, which consist of a set of values for the adjustable parameters. The particles move around in the parameter space according to the velocities that determined by their inertia, local and global best positions. The best positions are also updated after every round of the movement. The relative performances of the particles are decided by a fitness function.

In this model, some basic experiments are designed, not only for a rigorous analysis of the effects and problems, but for the estimation of the parameter ranges and their variation. It is also a preparation of the subsequent optimization for their accurate values.

EDF represents the increasing distance between the redeposition source and the deposition receiving surface. Since the scanning spacing is constant, and the x is linear in the same direction, here we assume that the EDF is also a linear function.

$$r(x) = k \cdot x \quad (7)$$

A series of rectangle milling experiments with one pass scan are designed for the redeposition analysis. The volume changes of the redeposition layers (Figure 1(c, d) color filled area) are used to estimate the variation of $q(x)$, which represents the proportion change of the particles that successfully deposited after the loss from the motion and the re-emission (Figure 5(b)).

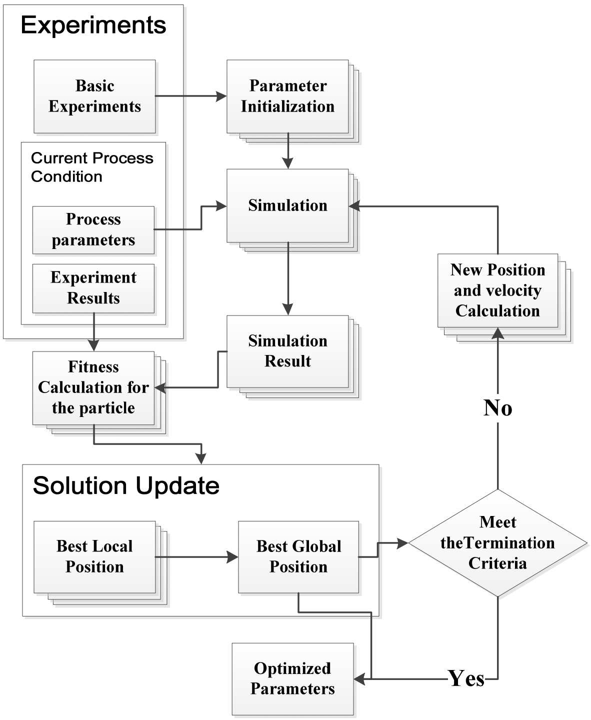

Figure 4. Flow chat of the Particle Swarm Optimization for the parameters.

In our case, the particle is defined as: $X(h_{dt}, f, c, a_i, b_i, k, \lambda, \sigma)$. As shown in Figure 4, the optimal solution is determined through the iterative optimal solution. The particle positions and their velocities are initialized randomly based on the previous estimated ranges. And every simulated profile is compared with the experimental profile in order to determine the fitness of each particle.

$$f = \sum \Delta D_s + \sum \Delta D_{re} \quad (8)$$

where the ΔD_s is the bottom depth difference between simulation profile and the experimental profile at each measured point, and the ΔD_{re} is the thickness difference of the redeposition layer. According to the fitness values, the best individual P_i^t and global positions P_g^t are updated. Based on them, the velocity and position of each particle (i) are updated according to [7]:

$$V_i^{t+1} = \omega V_i^t + c_1 r_1 (P_i^t - X_i^t) + c_2 r_2 (P_g^t - X_i^t) \quad (9)$$

$$X_i^{t+1} = X_i^t + V_i^t \quad (10)$$

where r_1 and r_2 are uniform random numbers in [0, 1], ω, c_1 and c_2 are weight factors for its inertia and motion tendency toward the local and global best positions.

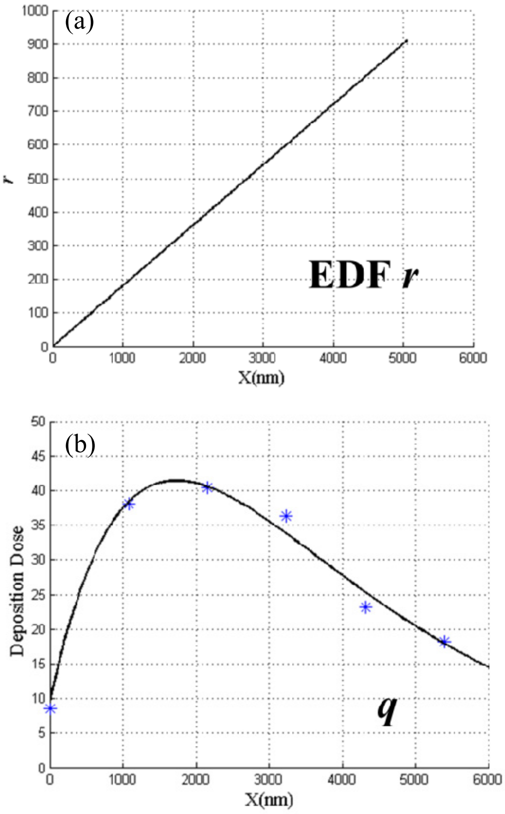

Figure 5. (a) The EDF after the optimization. (b) The valuation and the fitting curve of q.

SIMULATION RESULTS AND APPLICATIONS

For verifying the approach and its parameter optimization, simulations are carried out and compared with the experiments with different conditions on FEI Helios 600. Figure 6 shows two moments of the rectangle FIB millings with 2µm width and 3(5) µm length on silicon (100). The simulations agree well with the experiments on either the etch bottom profile or the redeposition front. The average depth and thickness errors are less than 10%. And the simulation time consuming of every structure are less than 30s.

An immediate application of the model and optimization is the scan strategy and the process parameter design and optimization for the fabrication of some special structures using FIB milling, for example a quadratic curve structure. As shown in Figure 7(a), a general fabrication method of the curve surfaces is a 2-D slice-by-slice scanning method [1]. Although we call FIB milling a direct patterning method, as we have mentioned, the depth and width of the actual machining results are affected by many factors. Once the number of slices is decided, the beam parameters, the scanning path, sequence and the pixel interval are the keys to ensure the accuracy of the final curve surface. To simplify the calculation, we set the depth of every slice the same, and the beam parameters and the scan strategy are inferred through this model. The good agreement among the design, the simulation prediction and the experiment result verifies the correctness of the process design and the model accuracy (Figure 7).

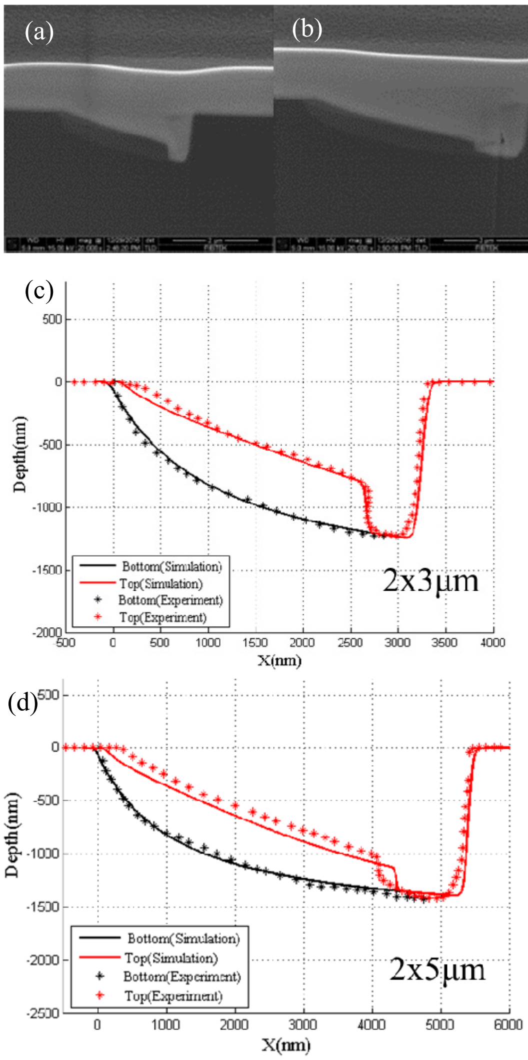

Figure 6. The experiment and simulation results of 2×3μm (a,c) 2×5μm (b,d) rectangle scanning (serpentine) with 30keV, 48pA, 1ms dwell time and 1pass on silicon (100).

CONCLUSION

Targeting the simulation of the FIB, a new experiment-based Gaussian function fitting model is proposed. This model applies Gaussian function to the front evolution from both the sputtering and the redeposition. And the EDF is established to describe the redeposition attenuation effect. Through a series of basic experiments, the variations and the estimation ranges of the related parameters are obtained. And based on these, the PSO is introduced for the parameter optimization. Good agreement with the experiments at different process conditions shows that the method can be used to predict the structure formation and various effects under different conditions. The model is further applied to the design and optimization of complex micro-structures by FIB process. The experimental realizations have demonstrated the accuracy of the optimization and simulation.

ACKNOWLEDGEMENTS

We acknowledge financial support by the National Natural Science Foundation of China No.51375093.

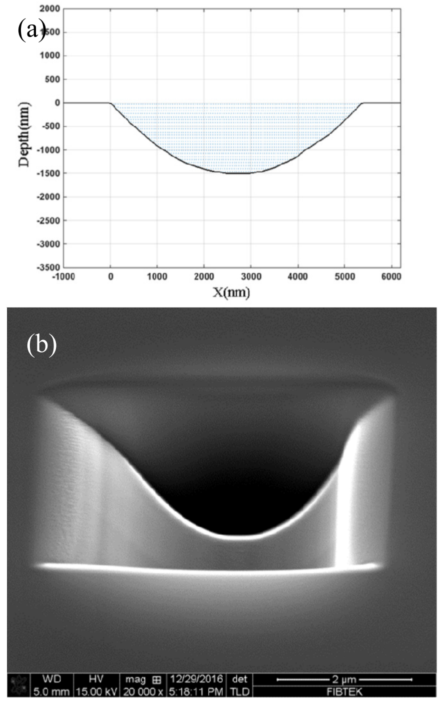

Figure 7. Predictions from the model in the scan strategy and parameters design for a quadratic curve structure and the experimental realization on silicon.

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