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3-D modeling of nanostructures evolution in lateral etching processes

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1. Introduction

Lateral etching is one of the most commonly used technological processes in semiconductor, integrated circuits and micro electromechanical systems (MEMS) manufacturing [1-6]. Micro- and nanostructures whose initial contours are squares, rectangles and their combinations are most frequently used in micro- and nanoelectronics. Some microstructures can form or they cannot form from the initial microstructure when they are initial configurations of nonembossed polygons. The application of such geometry micro- and nanostructures in technologies for manufacturing integrated circuits reduces the number of masks [6].

The progress in computational technologies shifted the efforts towards considering the inside of the material structure on smaller scales [7, 8]. In the case of assumption, that any structure can by represented by the finite set of points with the error, satisfying initial conditions, in the process of evolution only initial set that forms the structure, is changing (change of the parameters' value for all the elements of set) [9].

When modeling evolution process of microstructures with differential methods, usually algorithms are used, based on the analytical differential contour evolution model. These algorithms do not take into account the discrete nature of nanometric dimension structure in space and in evolution process. Also these methods must be modified in order to represent surface roughness of the structure. Some models, that use another assumptions are recently developed to omit described disadvantages [9, 10].

The paper presents further development of two-dimensional lateral etching process model for polycrystalline and amorphous films published in [10]. The aim of this work is to develop and analyze 3D nanostructures geometry evolution model for amorphous and polycrystalline films in the lateral etching process.

2. Modeling algorithm

Etching as a heterogeneous reaction example which takes place on the surface of the object under investigation, thus at any iteration we are interested only in points, that are sufficiently close the active surface. The initial (zero time) medium is generated as the net of uniformly distributed points on the surface under investigation. This is performed for the purpose of convenience only, but has the physical meaning of equally approaching front of reaction at the initial time step.

Any plane nanostructure can be represented by the finite topological set of its points [9]. Nanostructure points of the crystalline films can be arranged in a determined order. Nanostructures of amorphous films can be represented a closed set $A_0\left(O_1, O_2, ..., O_n\right)$ in a space of uniformly distributed randomly arranged points $O_j\left(x_j, y_j, z_j\right)$ whose coordinates depends on the designed device and they are in an area which is limited by the initial nanostructure – space surface $F\left(x, y, z\right)$. The limiting points of the set A_0 make up a new closed set of points $A_K\left(k_1, k_2, ..., k_n\right)$. The set A_K is a set of points $k_i\left(x_i, y_i, z_i\right)$, $i = 1, ..., n$ of environment interaction with the formed nanostructure. These points make up a nanostructure surface.

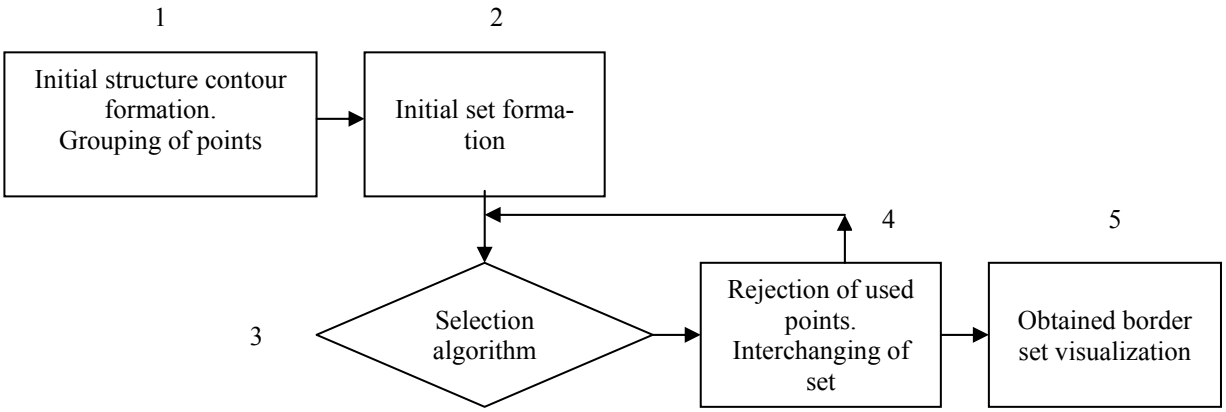


Fig. 1 General scheme of program algorithm

The following model of evolution of the geometry of nanostructure is determined: for the time interval $\Delta t = t_{i+1} - t_i$ the point k_i of the set A_K is represented by the point $O_j\left(x_j, y_j, z_j\right)$ of the set $A_{0_{i+1}} = A_{0_i} / A_{K_i}$, if the distance between these points is less or equal the etching radius

The general algorithm for the calculation and displaying evolution of the geometry of nanostructure during lateral etching is shown in Fig. 1 he program is realized on the basis of personal computer with the Intel Pentium CPU and Matlab software. We shall briefly discuss some points of the algorithm below.

User has to enter the coordinates of the corner points of the structure he is interested in step 1 (Fig. 1) Also the points' density must be entered for model. These parameters define the structure. The density of points can be entered directly or calculated from the etch rate value. In the case that input dimensions are entered in nm, the etch rate would be in nm/s. The resolution of the model and as usual the modeling time depends on the last parameter value. The initial set is formed inside the structure, defined by border points. Each of the points that form the set A_0 is generated in no overlapping cubes with the side equal $2d+a$. This is done to avoid the situation, when points are generated too close to each other. This condition can be expressed as

$$G = \frac{d}{a}$$

here G is the parameter, that specifies the point position inside the unit cube, and a and d are related to the dimensions of the cube. When $G \to \infty$ we get crystalline structure, where the position of each point is strongly determined. In the case we want to model some surface roughness, the value of $G = 0.125$ can be assumed, that gave good results. The probability density function for the point generated inside a unit cube is shown in Fig. 2. Although in the model uniform distribution was used, another distribution functions can be used (normal etc.) in the case it is necessary to model statistical points distribution inside the cube.

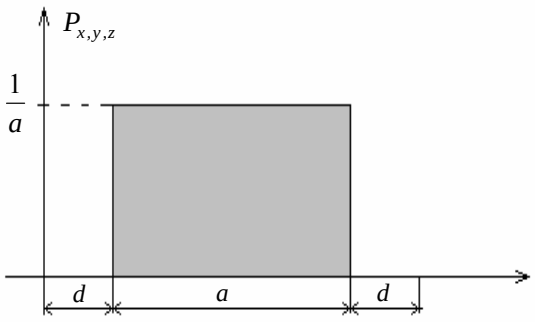


Fig. 2 Probability density function for the point generated in a unit volume element (unit cube)

Together with the initial set etching front is formed at the second step of the general algorithm (Fig. 1). For the convenience purpose it is generated automatically as a set of uniformly distributed points with double density and is shown grey color underlayer in Figs. 4 and 5. It helps us to visualize initial structure topology and simplifies the procedure and the initial (zero-time) step of the program. Selection algorithm (step 3) is quite simple: for any point of the border set a representative point from the A_0 set must be found. If there is no such point at the distance $R = v\Delta t$, etching radius is increased by the value ΔR and the distance condition is checked until at least one representative is found. For any border set point at least one representative point must be found if $A_0 \neq 0$. For the purpose of the algorithm to converge, we have to control the radius increment or at least notice, when the A_0 is empty. The increment can be variable ΔR, but it has to be considered in relation with the etching speed when a question of choosing the value arises. Modeling results showed that $\Delta R = 0.2...0.5R$, where R is initial etching radius gave good results. Here we take, that $R = 0.7...1(2d + a)$, i.e. it is equal or slightly less the unit cube side.

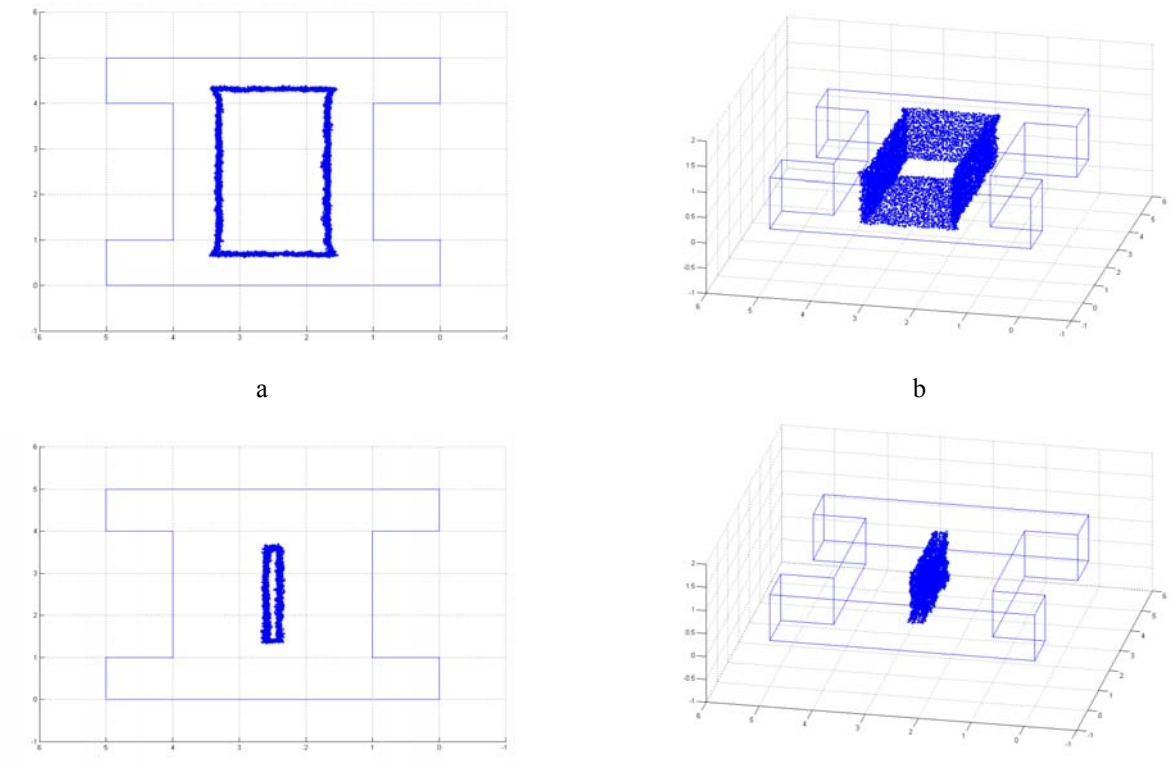
After for each point of the border set, at least one representative is found, all the representative points are taken from initial set to form border set for new iteration procedure. The process is repeated until the required distance is etched or defined number or iterations have passed. Then the border set that represents object surface geometry is obtained.

The exact parameter value depends on nano- or microstructure parameters and surface roughness we want to model. We have to notice, that selection algorithm is independent on the point generation algorithm part. It allows for practical implementation of the models, where $G < 0$. Thus we can form initial sets, where more than point is generated in an appropriate volume unit element. In a case $G \to -\infty$ we can reach filly random point set generation in the whole structure volume that fits the requirements of etching polycrystalline structures.

The total area of investigation is divided up to several hundreds of subarrays and it is drastically decreasing the modeling time. Obviously, their size must be bigger than the square for point generation. Other wise the empty arrays inside the nanostructure can appear. Also dramatic increase of subarrays can decrease the efficiency of managing with such big matrix dimensions.

3. Results of modeling

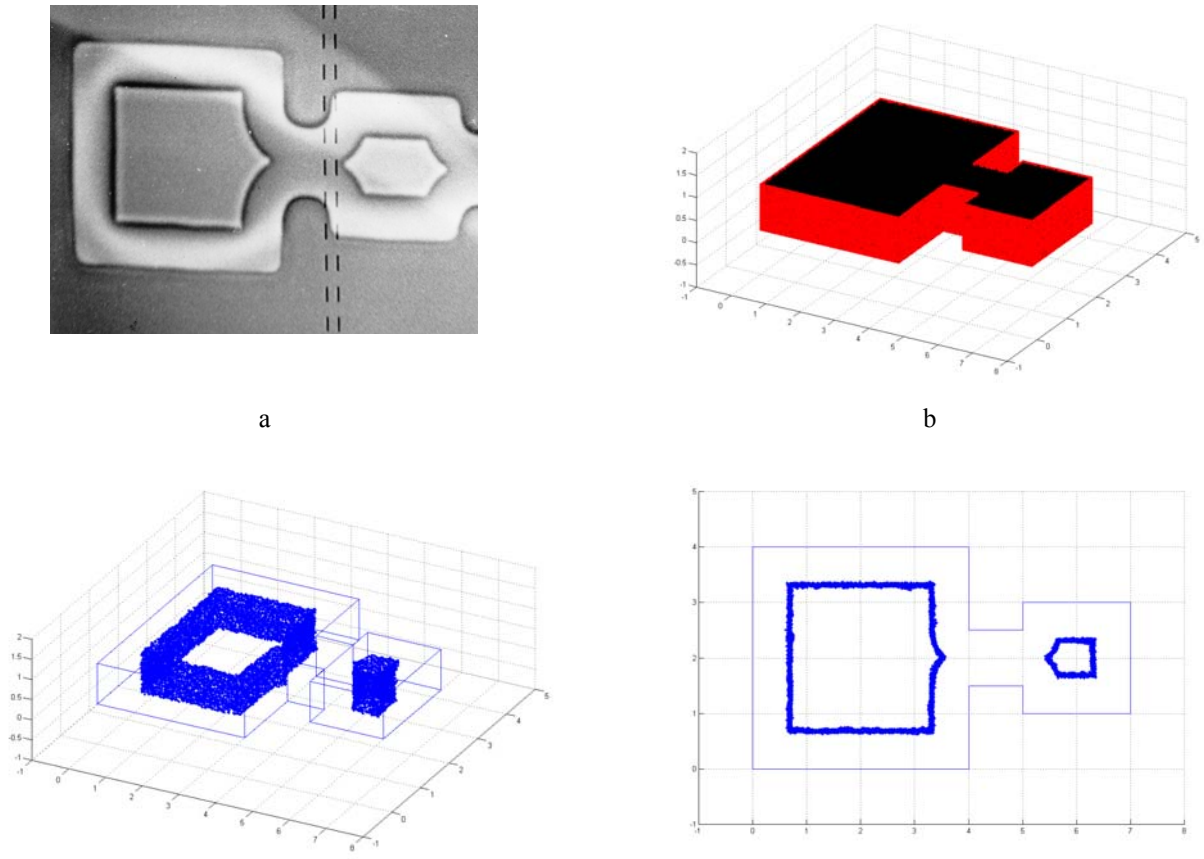
Below the results of modeling and experimental investigation are presented. Any initial structure is formed with from 250 000 up to 390 000 randomly generated points (taking into account boundary conditions described above) depending on the structure size and point density value. Point generation procedure, initial set formation and additional subarrays formation for the purpose of optimization take up to 5-10 minutes of the total program time depending on the number of points used for the model. Set divisions subarrays are done according the assumption, that the reaction can take place only between neighborhood points. Thus for searching procedure only the analysis of neighbor arrays is sufficient, that significantly decreases computational demand of the program. Different evolution steps are presented in Fig. 3. Modeling and practical



a b

c d

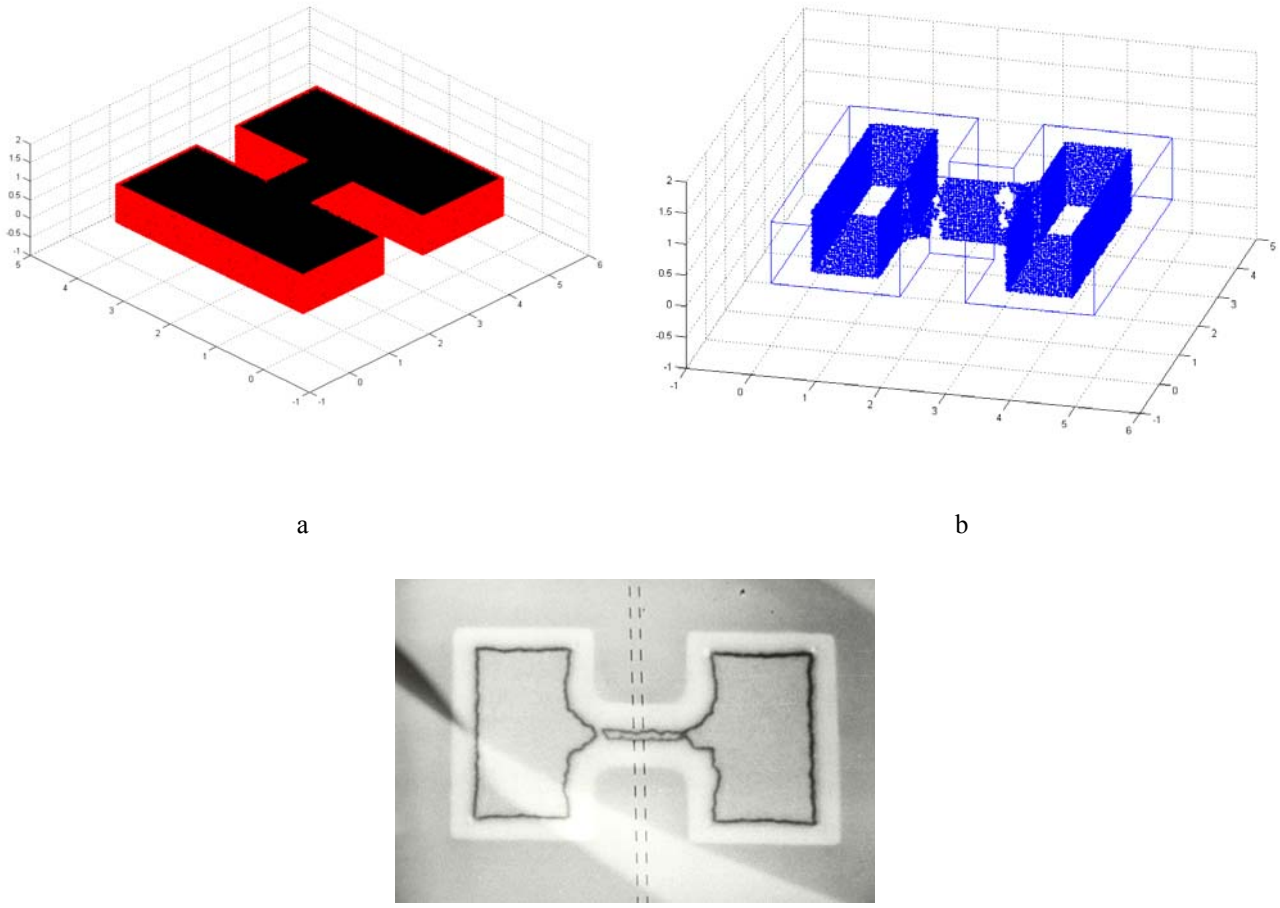
Fig. 3 Different structure evolution steps in lateral etching process. Set of border points. (a,b: $t = 15\Delta t$; c,d: $t = 30\Delta t$)



a b

c d

Fig. 4 Experimental results and modeling of lateral etching: Amorphous microstructure geometry evolution (a): – t = = 1200 s, the distance between markers – 1 μm, external limits – initial microstructure mask of Si_3N_4, (b) – initial structure for modeling, (c, d) – modeling results



a b

c

Fig. 5 Modeling and experimental results of lateral etching: (a) – initial structure for modeling, (b) after modeling; (c) – formed structure after t = 1200 s

investigation results are presented for 2 structures (Figs. 4-5). The number of intermediate border set (surfaces) is between 15 and 30. Time duration of one iteration is approximately 2-3 min.

4. Conclusions

We have developed 3D model of evolution of the nano- and microstructures geometry in lateral etching processes. The modeling results for the different initial geometry structures are presented. The experimental investigations evolution of microstructures in lateral etching processes of amorphous and polycrystalline films were performed and the coincidence of modeling results and the experimental research were received. The results showed, that concrete nanostructures can be defined by the topological set of randomly generated points with border conditions set up to satisfy real physical material properties. The model results are obtained for the infinite selectiveness of etching, although the model allows to model mask etching simultaneous to the film etching. This allows analyzing and designing new self-alignment and self-formation technologies semiconductor devices, integrated circuits and MEMS/NEMS. Also the problem of practical representation for the material of concrete nanostructure with finite set of randomly distributed points was analyzed and some model results were obtained. Results show the possibility of model application in new device manufacturing processes.

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TRIMATIS NANOSTRUKTŪRŲ EVOLIUCIJOS MODELIAVIMAS ŠONINIO ĖSDINIMO PROCESUOSE

R e z i u m ė

Sudarytas trimatis nano ir mikro struktūrų geometrijos evoliucijos modelis paviršinių sluoksnių ėsdinimo procesams. Pateikti modeliavimo rezultatai skirtingos pradinės geometrijos struktūroms. Atlikti eksperimentiniai mikrostruktūros evoliucijos paviršinio sluoksnio ėsdinimo proceso metu tyrimai amorfiniams ir polikristaliniams ploniems sluoksniams. Modeliavimo bei eksperimentinio tyrimo rezultatų palyginimas parodė, kad betono nano struktūras galima identifikuoti naudojant atsitiktinių taškų rinkinio topologiją, parinkus kraštines sąlygas, atitinkančias realios medžiagos fizines charakteristikas. Gauti modeliavimo rezultatai įvairiems ėsdinimo atvejams, nors modelis gali būti naudojamas dangų ėsdinimui bei plono paviršinio sluoksnio ėsdinimui modeliuoti. Tai leidžia tirti ir projektuoti naujus savaiminio sutapdinimo ir savaiminio susiformavimo puslaidininkinius įtaisus, integrines schemas bei MEMS/NEMS. Taip pat ištirtas praktinio pritaikymo problema betono nano struktūros medžiagoms esant baigtiniam atsitiktinio pasiskirstymo taškų rinkiniui, gauti modeliavimo rezultatai. Rezultatai parodė, kad modelis gali būti pritaikytas naujų įrenginių kūrimo procese.

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3-D MODELING OF NANOSTRUCTURES EVOLUTION IN LATERAL ETCHING PROCESSES

S u m m a r y

We have developed 3-D model of evolution of the nano- and microstructures geometry in lateral etching processes. The modeling results for the different initial geometry structures are presented. The experimental investigations of the evolution of microstructures in lateral etching processes of amorphous and polycrystalline films were performed and the coincidence of modeling results and the experimental research were received. The results showed, that concrete nanostructures can be defined by the topological set of randomly generated points with border conditions set up to satisfy real physical material properties. The model results are obtained for the infinite selectiveness of etching, although the model allows to model mask etching simultaneous to the film etching. This allows analyzing and designing new self-alignment and self-formation technologies semiconductor devices, integrated circuits and MEMS/NEMS. Also the problem of practical representation for the material of concrete nanostructure with finite set of randomly distributed points was analyzed and some model results were obtained. Results show the possibility of model application in new device manufacturing processes.

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ТРЕХМЕРНОЕ МОДЕЛИРОВАНИЕ ЭВОЛЮЦИИ НАНОСТРУКТУР ПРИ ПОВЕРХНОСТНОМ ТРАВЛЕНИИ

Р е з ю м е

Составлена трехмерная модель эволюции геометрии нано- и микро- структур при травлении поверхностного слоя. Представлены результаты моделирования для структур с разной начальной геометрией. Проведено экспериментальное исследование эволюции микроструктуры поверхностного слоя при процессе травления аморфных и поликристальных тонких поверхностных слоев. Сравнение результатов моделирования и экспериментального исследования показало, что идентифицирование нано структуры бетона можно осуществить, используя топологию подборки случайных точек и подобрав краевые условия, соответствующие физическим характеристикам реального материала. Получены результаты моделирования для разных случаев травления, хотя модель может быть использована для совместного моделирования травления покрытий и тонких поверхностных слоев. Это дает возможности изучать и проектировать новые само совмещающиеся и само формирующиеся полупроводниковые устройства, интегральные микросхемы, а также МЕМС/НЕМС. Дополнительно исследована проблема практического применения нано структуры материалов бетона при конечной подборке случайно распределенных точек, получены результаты моделирования. Результаты показали, что модель может быть использована в процессе проектирования новых устройств.

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