Self-Formation Model Based on Parametric Space Evolution

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ABSTRACT

Topological approximation of self-formation of artificial objects in micro-scale is well established. However expansion of the topological approximation into nano- and molecular scales requires new and more generalized concepts of self-formation. This paper represents a preliminary effort to define self-formation as an evolution of 4-D parametric space in 8-D topological space, as universal concept for micro- and nano-scale

Keywords: evolution, self-formation, self-assembly, parametric space, singleton, object, medium, interaction.

INTRODUCTION

Manufacturing (formation) of any electron device (e.g., solar cell) implies the sequence of technological processes followed by the increase of initial object (e.g., silicon wafer) complexity until the final structure (e.g., solar cell) is obtained. Usually the initial object is homogeneous and contains no elements. The elements are formed during manufacturing when a particular sequence of technological processes (i.e., routing card) is applied.

A technological process can be considered as an interaction between the object and the medium (e.g., gas, liquid, soft matter, light flux, particle flow, etc.). Such processes can lead to the change of element properties, structure and/or its chemical composition. However, interaction with homogeneous (chaotic) medium does not define neither the element geometry nor its planar arrangement. For this purpose structural media (e.g., photomask, electron-, ion-beam, laser, grooving blade) are used which enable the formation of planar structures. Such element formation by using the structural media is known as an external formation.

Under self-formation technology we understand arising of the new structures as a result of the forming object interaction with selected sequence of chaotic media – gas, liquid, light flux, particle flow etc. Any technological process or a sequence of the technological processes can cause self-formation or not. It depends on both the configuration of interacting objects at the interface as well as the media properties [2,3].

Self-formation was proposed in microelectronics in 1974 [1] as an alternative technology for patterning processes. In contrary to photolithography or electron/ion-beam lithography the object is formed under interactions with chaotic media, e.g., chemical etching, electroless plating, spin-on coating etc. SF technology in 1970-1980 was patented in USSR, USA, UK, France, Germany, Czechoslovakia and Hungary. In English the term “self-formation” was first proposed in 2000 [2].

The modelling of self-formation is based on approximation of an object by a representative set of discrete Euclidean space points. Any point of this set is juxtaposed with some parameter (the approximating material). The technological processes are approximated by an interaction matrix which defines parameter change in time [3].

In this paper we present the SF theory which is based on the 8-dimensional (8-D) topological space, comprising Cartesian product of Euclidean space \( \mathbb{R}^3 \times (X \times Y \times Z) \), interaction space \( I = P^4 = P \times P \times P \times P \), and time axis \( T \):

\[
L = \{ R^3 \times I \times T \} = \{ (X \times Y \times Z) \times P^4 \times T \} = \{ P^3 \times P \times P \times P \times T \}
\]

where

\( P^3 = (R^3 \times P) = (X \times Y \times Z \times P) \)

represents the parametric space, as a Cartesian product of Euclidean space \( \mathbb{R}^3 \) and parameter set (axis) \( P \).

An interaction in micro-scale is defined by combination of four parameters, comprising of the initial interacting object-medium pair \( p_i, p_j \) and the resulting pair...


\[ (p_i, p_j, p_k, p_l) \in I \]  \hspace{1cm} (3)

A temporal evolution can be observed as a change of object configuration, when, e.g., the object parameter transforms into the medium parameter \((p_i, p_j, p_k, p_l)\) or the medium parameter transforms into the object parameter \((p_i, p_j, p_k, p_l)\). The change of the object structure is observed when under interaction the object parameter changes to a new one \((p_i, p_j, p_k, p_l)\). However, mechanical motion of the object is not defined. In our model all interactions are considered only between a pair of nearest-neighbour Euclidean points.

Such approximation was sufficient to define the evolution of an object, where interaction takes place on the object interface (the contour between the object and the medium).

As an example let us consider a solid-state object with parameter \(I\) and chaotic medium with parameter \(j\). Also assume that interactions \((1213, 3233)\) are valid. Then the object evolution in time is obtained and a new region with parameter \(j\) is formed (the intermediate evolution states are presented by different grey shades) (see Fig 1). In this case we observe the object evolution when the contour of the object expands.

![Fig.1. Object evolution under interactions (1213, 3233)](image1)

Evolution of the resulting object as in Fig.1 under interaction with different medium \(j\) \((1414, 3444)\) is presented in Fig.2. Here we observe a contraction of the object contour.

![Fig.2. Object evolution under interactions (1414, 3444)](image2)

Such cases of evolutions approximate heterogeneous reactions, e.g., electroless plating, chemical etching, etc. However, the SF based technology development was also extended to other very common processes: oxidation, diffusion, and photoresist or glass sol-gel spin-on coating. The latter are soft matter formation on surface, rather than heterogeneous processes. In this case the SF phenomenological model based on figure boundary motion becomes helpless.

Furthermore, the SF process, also well known as self-assembly (SA), cannot be extended into nanotechnology, since one cannot distinguish between medium and object in the nano-scale and only atoms and molecules can be observed in Brownian motion [5-8].

Therefore there is an obvious need of an universal model, covering the micro- and nano-scales. Presumably it must be phenomenological model for simulation of SF and SA.

### PARAMETRIC SPACE PRESENTED BY SINGLETONS

According to Eq. (2) \(\mathbb{P}^3\) is a parametric space, as a Cartesian product of a Euclidean space \(\mathbb{R}^3\) and parameter set (axis) \(\mathbb{P}\).

The pair \((X, \Omega)\) is called a topological space, where \(\Omega\) is a topological structure or just a topology in \(X\). An element \(x\) is called a point of this topological space, and element \(\Omega\) - an open set of the topological space \((X, \Omega)\). A set \(F \subset X\) is said to be closed in space \((X, \Omega)\) if complementary set \(X \setminus F\) is open \((X \setminus F \in \Omega)\). If \((X, \rho)\) is a metric space, \(M\) is its point, and \(r\) is a positive real number \(r \in \mathbb{R}\), then set

\[ D_r (M) = \{ x \in X | \rho (M, x) \leq r \} \]  \hspace{1cm} (5)

is called a closed ball [4]. Any closed set of Euclidean space \(\mathbb{R}^3\) consists of infinite set of Euclidean points \(M_i\) \((x, y, z)_i\) with their closed neighbourhoods – balls.

\[ S_0 = \{ (S_{01}, S_{02}, ..., S_{0k} ..): i = 1, 2, ... \} \]  \hspace{1cm} (6)

In a Euclidean space the balls can be disjoint, i.e. their intersection is empty: \(S_{0i} \cap S_{0j} = \emptyset\), or otherwise they do intersect: \(S_{0i} \cap S_{0j} = \{ x | x \in S_{0i}, x \in S_{0j} \}\).

In the parametric space \(\mathbb{P}^3\) (see Eq. 2) any Euclidean point \(M_i\) is juxtaposed with parameter \(\{p_i\}\). Let us assume that the interior and boundary points of any parametric ball are juxtaposed with only a single parameter. A set with exactly one element is known in mathematics as singleton. For example, set \{0\} is a singleton. Consequently, when all interior and boundary points of the parametric ball are juxtaposed with a single parameter \(\{p_i\}\), the parametric ball is called a singleton \(\{S_i\}\). There \(S_{0i} \subset \mathbb{P}^3\), \(S = S_{0i} \times p_i \subset \mathbb{P}^3\).

An intersection of Euclidean balls \(S_{0i} = S_{0j} \cap S_{0k}\) in \(\mathbb{R}^2\) is defined by common Euclidean points \(M_0 \in S_{0i}\) and \(M_0 \in S_{0j}\), while \(M_1 \in S_j = M_0 \times p_j\). \(M_j \in S_j = M_i \times p_j\) (Fig. 3). The plane balls \(S_{0i}\), \(S_{0j}\) define parametric balls \(S_i\) and \(S_j\). However in this case any point of intersection \(M_0\) \(\in S_{0j} \cap S_{0k}\) is juxtaposed not only with single parameter \(\{p_i\}\), but also with the second parameter \(\{p_j\}\) simultaneously. Yet \(S_i \cap S_j\) can be treated as a singleton when it includes only a single parameter \(p_i = p_j\).
INTERACTION OF SINGLETONS

Approximation of parametric space by singletons requires a new concept, since it must accommodate interpretation of mechanical motion in Euclidean space, contact essence, rejection and self-assembly.

From the topological point of view the contact of two singletons in the Euclidean space means that they have at least one common Euclidean point, i.e. the singletons intersect. Intersection of singletons can be treated as a new homogeneous parametric ball with parameter \( p_m \), where \( m \in \{ 0, 1, 2, \ldots, i, j, m, \ldots, N \} \). Arising intersection of two singletons can be described by interaction \( p_r, p_j, (p_r, p_m, p_j) \), which in micro-scale under \( p_m = p_r \) or \( p_m = p_j \) transforms to well known \( (p_r, p_j, p_r, p_j) \). Therefore, instead of 8-D topological space used in SF modelling in micro-scale, we have 9-D topological space

\[
\{R^3 \times I \times T\} = \{(X \times Y \times Z) \times P^3 \times T\} = \{P^3 \times T\}
\]

In other words, evolution of the parametric space, approximated by singletons, can be represented by 9-D topological space. The singleton with parameter \( \{p_k\} \) can occupy any place in a Euclidean space, i.e. \( (x, y, z, p_k) \). The minimal topology comprises a single singleton of parameter \( \{p_k\} \) and the complementary space \( (X \setminus \{p_k\} \in \Omega) \), represented by singletons of parameter zero \( \{p_0 = 0\} \).

Obviously, it becomes necessary to provide interpretation for the mechanical motion of singleton in the Euclidean space. This can be described by means of interactions between singletons. Commonly no interaction occurs with parameter zero \( (p_0, p_0, p_r, p_0) \). Parametric system remains in the equilibrium state.

Now let us assume that if a vector field in a neighbourhood of a singleton in a Euclidean space is defined (see Fig. 5 a). Then an interaction with \( \{0\} \), oriented along the vector direction arises

\[
I^\top = (p_k, 0, 0, p_k)^\top.
\]

During the time interval \( \Delta t = t_j - t_i \) singleton \( \{p_k\} \) obtains parameter \( \{0\} \), i.e., it becomes a subset of Euclidean space, while the singleton \( \{p_0\} \) along the vector field direction obtains parameter \( \{p_k\} \). The parameter of any point of singleton

\[
M_i (x, y, z, t_i, p_k) \rightarrow M_j (x, y, z, t_j, p_k)
\]

becomes juxtaposed with the new Euclidean coordinates.

If the couple of singletons \( \{p_i\} \) and \( \{p_j\} \) exist in Euclidean space with oncoming own vector fields (see Fig. 6 a), then they come into contact, i.e. they comprise the intersection \( \{p_m\} = \{p_i\} \cap \{p_j\} \) (Fig. 6 b).

As a consequence of sum of the two opposite direction vector fields, the resulting vector field disappears. An interaction \( I = p_i, p_j, (p_i, p_m, p_j) \) takes place, and we have a new singleton \( \{p_m\} = \{p_i\} \cap \{p_j\} \). If \( p_m = 0 \), then the new singleton is a Euclidean space (see Fig. 6 b and c), and the singletons become autonomous \( \{p_i\} \cup \{p_j\} \) (Fig. 6 d) with their new neighboring vector fields.
In case when $p_m \neq 0$, the new singleton with parameter $p_m$ arises, i.e., we observe self-assembly of a system, consisting of singletons \{\(p_i\}\{p_m\} and \{p_j\}\ (Fig. 7 c).

If the interactions: $I = \{(p_i, p_j, p_m, p_m)(p_i, p_m, p_j, p_j)\}$ exist, we observe self-formation of the self-assembled system, consisting of only the initial singletons \{\(p_i\}\} and \{\(p_j\}\\ (Fig. 7 d).

Therefore, in case of interaction $I = p_i, p_j, (p_i, 0, p_j)$ we have a rejection of singletons. And in case of $I = p_i, p_j, (p_i, p_m, p_j)$ we have self-assembly (or self-formation) of the equilibrium system, i.e., this is an object in molecular or nano-scale.

**PARAMETRIC SPACE EVOLUTION IN MOLECULAR-SCALE**

In nano-scale an object and medium are discreet and consist of autonomous atoms and/or molecules in Brownian motion. There are many models of the molecular self-assembly in the nano-scale [5, 6, 7, 8]. In topological approximation any atom can be presented as a singleton or an object consisting of some singletons.

Let us consider a hydrogen molecule, comprising of three singletons with parameters 1, 2 and an oxygen molecule comprising of two singletons with parameter 3 and 4. The oxygen and hydrogen molecule contact can be of three different configurations. Only one of the contact schemes results in a self-assembly: when the hydrogen singleton with parameter 2 comes into contact with the oxygen with parameter 3 under interaction (3255) (Fig. 8)

The process unfolds as follows. An oxygen atom with the singleton parameter 3 in front moves towards the singleton of the hydrogen molecule parameter 2. Owing to the interaction (2355), the singletons with parameters 2 and 3 change to parameter 5. As long as the two contacting neighbourhoods with identical parameters can be treated as a single neighbourhood, we have the resulting object – a water molecule as it is shown in Fig. 8, right side.

**PARAMETRIC SPACE EVOLUTION IN MICRO-SCALE**

Object evolution in micro-scale, where interactions, as heterogeneous reactions, occur only at the interface of the object-medium system, is investigated extensively [8, 9, 10, 11]. In this case the object and the medium are treated as homogeneous, and the interactions take place when two Euclidean parametric points are located in the same Euclidean point neighbourhood. Let us choose a square singleton shape. Approximation of the object-medium system by mesh of square singletons is shown in Fig. 9.

Any interaction occurs only between the contacting singletons. In such case we can assume the contact as a common boundary, common corners, or both of them. The results will depend on the way how the contact is chosen (Fig. 10).

Moreover, different results of interaction can be obtained when one singleton interacts with one, two, or up to eight neighbouring singletons or one, two, or up to eight singletons interact with just one singleton (Fig. 9). Different modes can be selected, which can be useful for interpretation of both short-distance and long-distance interactions. Some possible modes are presented in Fig. 11.
Simulation of the object evolution can be constructed as follows. Let us select a mode for the first time step from the first line of modes (Fig. 11), for the second time step – from the second line and for the third time step – from the third line, e.g. (1,1,0). Then such kind of combination can be repeated, or alternatively, a new combination can be selected, e.g. (1,0,3). Such couple of two combinations can be repeated during all simulation, or replaced at any time by the other combinations.

An evolution of quadrangle and triangle under interaction (1222) and sequence of modes (1,1,0)(1,0,3), and circle under modes (1,0,0)(0,4-2,0) is adequate to etching process and is presented in Figs. 12-14.

In Fig. 15 evolution of masked silicon dioxide layer after experimental etching is presented. The shapes of figures after inside and outside etching are analogous to the simulated ones (see Figs. 12-14). Any angle under evolution outside transforms to circle shape, while under evolution inside – remains without transformation. Fig. 16 represents the result of evolution, allusive to photoresist spin-on coating (Fig. 17).
It is important to note, that during simulation of object evolution by such process of approximation, the configuration of the object does not correspond to the real object configuration evolution in time. However the final result of simulation does correspond to the result of the technological process. Therefore in this case we have a new type of phenomenological model.

CONCLUSIONS

The parametric space as a subset of 8-D topological space is regarded as infinite set of singletons – the single-parametric balls of Euclidean points. The defined system of singletons can approximate the evolving objects not only in micro-, but in nano- and molecular scales as well. The study of parametric space evolution based on singleton interactions reveals that introduction of the 5-th P axis is necessary. Therefore, parametric space evolution can be approximated only as a 9-D topological space.

In order to examine singleton rejection, or self-assembly in the molecular scale, an intersection of interacting singletons as their contact is proposed.

Some examples illustrating parametric space evolution concept application for self-formation models in micro-, nano- and molecular scales are presented.

Parametric space approximation by singletons can serve as a basis for development of universal model of self-formation simulation in molecular, nano- and micro-scales.

Simulation in micro-scale demonstrates possibility to use parametric space simulation results as a data basis for their identification with results of technological processes. In this regard any new incoming technological process can be identified and incorporated into existing software without need to create its physical model.

REFERENCES