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Multiagent Approach to Adsorption-Diffusion-Reaction Processes Modeling by the Method of Likelihood Cellular Automat

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Abstract: The discrete three-dimensional model of the adsorption-diffusion process was developed with three states using the corners of blocks within the framework of the theory of CA (cellular automata). The construction of an asynchronous cellular automaton was used for the modeling. The implementation of the algorithm leads to a huge variety of dynamical regimes some of which are moving from the general chaos into a state of local and then global synchronization (within the framework of the model).

Key words: Adsorption, diffusion, cellular automata, ca-diffusion, multi-agent approach, autowave soliton.

1. Introduction

The micro- and nano-object related scientific researches and technical developments are nowadays actively held. There is also a growing interest in low-dimension structures research. It is known that low-dimension structures show several extraordinary properties. That is connected with specific energy redistribution in such structures. Special chemical processing and anodizing are most frequently used methods to obtain such structures. It is known that surface properties modifications have a significant influence on solid body volumetric properties especially in low size crystal regions when the surface area and the body volume are comparable. Both methods are based on adsorption processes i.e. these processes are basic atom (ion) crystal penetration mechanisms [1]. Current flow in porous silicon is described in Ref. [2]. In particular dynamic characteristics periodical change depending on time was discovered. Molecules (atoms) that can change their charge state adsorption and desorption are able to show process in time dynamic periodicity. For example similar self-oscillating effects were found during potassium field desorption from the surface that has potassium-gold adsorbates mix [3, 4]. A data set acquired from different experiments reveals a need for theoretical basis that can qualitatively and quantitatively describe and explain them. Discrete adsorption model with three states is described in Refs. [5, 6]. The modeling results of solid body surface in adsorption process leading to dynamic characteristics change of time are presented in those papers. Acquired results are similar to instant surface snapshots received during experiments in Refs. [3, 4]. Charged and uncharged external substance molecule on the surface roaming process is described in Ref. [7] using cellular automata with three states. Selected molecule roaming and interrogation description approach is similar to the one in that paper. So the instant

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snapshots are similar to the ones of Ref. [7]. Qualitative similarity to experimental data proves that the chosen direction is correct. That approach does not take into account near surface layers influence though. Besides adsorption processes on the solid body surface, reaction-diffusion processes are active in real experiments. Three-dimensional model is needed to take into account not only adsorption processes, but also near surface layers reaction-diffusion processes. Experiments that could have shown dynamic processes in near surface layers do not exist yet though. The lack of experiments provides difficulties when building a three-dimensional adsorption-diffusion processes model. That's why experimental data received from solid body surface modeling were taken as basis.

2. Classic Problem Description

Dynamic processes in active environments (reactionary-diffusion processes in physics and chemistry) are traditionally presented by differential equations (or simultaneous equations) with particle derivatives of the following kind:

$$\frac{\partial U}{\partial t} = D\frac{\partial^2 U}{\partial x^2} + F(U) \quad (1)$$

where D is diffusion coefficient, U—distribution function, $F(U)$—derivable non-linear function. In three-dimensional case these equations appear to be the following:

$$\frac{\partial U}{\partial t} = (\nabla, D\nabla U) + F(U) \quad (2)$$

if D = const:

$$\frac{\partial U}{\partial t} = D\Delta U + F(U) \quad (3)$$

where

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (4)$$

So, in equations (or SE) that describe reactionary-diffusion processes, the right part consists of two parts: diffusion, that is presented by a Laplacian, and reactionary ($F(U)$) that reflects active part.

It is because of the non-linear part $F(U)$ analytical solutions are very hard to find. The problem becomes more difficult when increasing the number of particles and even unsolvable when going into three-dimensional environment. Numerical methods are either hard to parallel and have non-evident solving schemes or restricted by stability conditions. CA-algorithms, in their turn, does not have such restrictions. This means that such problems can be solved using discrete asynchronous cellular automata model as an alternative to classic dynamic process description.

3. Diffusion Part Algorithm

Turning blocks method was used, that is described in Ref. [8] to design a diffusion part of the algorithm. A set of cellular rectangle areas will be used as coordinates Z^2:

$$Z^2 = \{(i,j)|1 \le i \le N_x, 1 \le j \le N_y\} \quad (5)$$

Alphabet, i.e., the set of states that a cell can obtain:

$$A\{(A_{ij}, [i,j]: [i,j]\ \epsilon\ M, A_{ij}\ \epsilon[-1,0,1]\} \quad (6)$$

Context and basic templates that determine the context of a cell and a basis of a cell, in our case, will be:

$$V = W = \{(1;\ 1);\ (2;\ 1);\ (2;\ 2);\ (1;\ 2);\ \} \quad (7)$$

Θ operator is a transition operator that has a context cells states vector as an argument and basis cells states vector as output, i.e., in general:

$$\Theta(x):\ A^{|V|} \to A^{|W|} \quad (8)$$

Consider the modeling object to be a set of monolayers. Every monolayer represents as an independent cellular set. Joint cellular set of every two neighbor layers is partitioned into 2 × 2 × 2 blocks different ways that it will be call even and odd. Evenly partitioned blocks have an even main diagonal elementary cells coordinate sum. Oddly partitioned blocks have an odd main diagonal elementary cells coordinate sum. Every obtained block can rotate around one of the coordinate axis for π/2.

In the given case the transfer operator changes cell states by rotating blocks clockwise or counter-clockwise around a random axis. Every iteration in every block the following transformation is generally held:

where rand (1) is a random number (0, 1), $[i, j]$—an

$$\Theta_{3D1} * \Theta_{3D2}: \{rand(1) < P_1\} * \begin{Bmatrix} \{(A_0^1,[i,j]),(A_1^1,[i,j+1]),(A_2^1,[i+1,j+1]),(A_3^1,[i+1,j])\} \\ \{(A_0^2,[i,j]),(A_1^2,[i,j+1]),(A_2^2,[i+1,j+1]),(A_3^2,[i+1,j])\} \end{Bmatrix} =>$$
$$=> \begin{Bmatrix} \{(A_0^2,[i,j]),(A_0^1,[i,j+1]),(A_2^1,[i+1,j+1]),(A_2^2,[i+1,j])\} \\ \{(A_1^2,[i,j]),(A_1^1,[i,j+1]),(A_3^1,[i+1,j+1]),(A_3^2,[i+1,j])\} \end{Bmatrix} \quad (9)$$

elementary cell name, *P*—probability, "*" —configuration union.

In Fig. 1 a π/2 rotation around X-axis is illustrated.

That is the way how a random cell roaming is modeled. Similar roaming is described in Ref. [7] by Smolukhovsky equation:

$$\rho(t_0, x_0|t + \Delta t, x')dx = \int \rho(t_0,\ x_0|\ t,x)\rho(t,x|t + \Delta t, x')dx \quad (10)$$

where $\rho\ (t,\ x)$ is probability density of a cell being at that coordinates at that time, $\rho\ (t_1,x_1|t_2,x_2)$ —density of corresponding conditional probability, t_0, x_0 and $t + \Delta t$, x' are starting and ending cell coordinates, x, t—some current values on the observed time segment.

In three-dimensional case every elementary cell can move for Δx along one of the axis. Δx can have one the values from 0, 1 and 2 with the following probabilities:

$$P_1(\Delta x = 0) = {}^7/_{18},\ P_2(\Delta x = 1) = {}^7/_{18},$$
$$P_3(\Delta x = 2) = {}^2/_9.$$

4. Algorithm of a Reactionary Part

Authors will present structure of a firm body in the form of a simple cubic singony. The surface and volume of a firm body are considered ideal, it means that defects and heterogeneity are not considered, there are no dislocations and vacancies. Each particle is an elementary cell of the CA (cellular automaton) and has a certain color. The white cell is a molecule of initial substance, basis, without the adsorbed molecule; the gray cell is a molecule of initial substance, basis, with the neutral adsorbed molecule; the black cell is a molecule of initial substance with the charged adsorbed molecule. The recharging scheme of the elementary cell's condition is presented in Fig. 2.

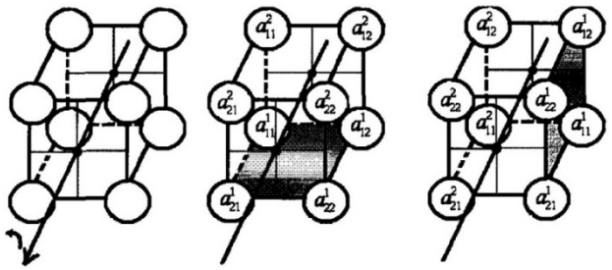

Fig. 1 A π/2 rotation around X-axis.

The final condition of an elementary cell depends on lifetime which defines number of steps (iterations) of the cellular automaton before a recharge and probabilities of transition from one condition to another. Also the final condition of an elementary cell depends on an environment-26 coherent vicinity. Each next cell is in one of three conditions, depending on it there is a transition.

(t) is the condition k system element at the moment of time (t). $(t+1)$ is the condition k system element at the moment of time $(t+1)$. As was told above, each elementary cell accepts, the following values:

$$A_k(t) = \begin{cases} -1 \\ 0 \\ +1 \end{cases} \quad (11)$$

Respectively

$$A_k(t+1) = \begin{cases} -1 \\ 0 \\ +1 \end{cases} \quad (12)$$

The condition to which value -1 is appropriated corresponds to a white elementary cell, 0 corresponds to a gray elementary cell, +1 corresponds to a black elementary cell. Let's enter a number of concepts, which help describe algorithm of realization of a

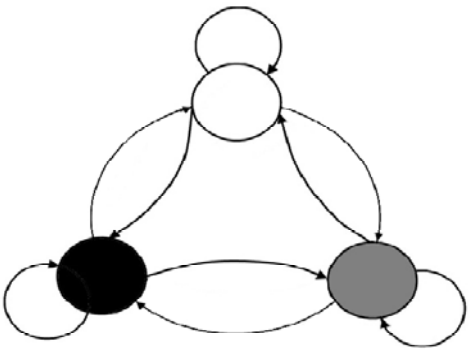

Fig. 2 The recharging scheme of conditions.

reactionary part of KA:

N_{kg}—concentration of "gray" cells in the volume equal to the immediate environment k-oh of an elementary cell;

N_{kb}—concentration of "black" cells in the volume equal to the immediate environment k-oh of an elementary cell;

N_g—the minimum concentration of "gray" cells in the volume equal to the immediate environment of this elementary cell, necessary for transition to a gray condition;

N_b—the minimum concentration of "black" cells in the volume equal to the immediate environment of this elementary cell, necessary for transition to a "black" condition;

$w_g \in [0,1]$—probability of transition to a "gray" condition;

$w_b \in [0,1]$—probability of transition to a "black" condition;

Ttl—life time, time of finding of an elementary cell in current state, depends on current state of a cell. The elementary cell being in a "white" condition can make three various transitions if time of her life expired, i.e. the current counter of steps for an elementary cell became is equal to ttl value. The cell can to pass to a "gray" condition that is caused by certain concentration of "black" and "gray" cells in a vicinity of this elementary cell: $N_{kg} > N_g$, $N_{kb} > N_b$, $w_g > w_b$: $A_k(t) \Rightarrow A_k(t+1) = 0$.

Transition to a black condition is caused by certain concentration of "black" and "gray" cells in a vicinity of this elementary cell of $N_{k\,b} > N_b$, $> N_g$, $w_g <$: $A_k(t) => A_k(t+1) = +1$.

If any of conditions is not carried out, the second cycle of life for a white cell is started, i.e., it passes to herself: $(t) => (t+1) = -1$.

At performance of conditions for transition as in white, and the black condition is checked parameter probability of transition.

If none of the circumstances are fulfilled then a new "white" cycle is launched, i.e., $(t) => (t+1) = -1$. When both "grey" and "white" conditions are fulfilled a "transfer probability" parameter is checked and it determines the final state.

Elementary cell in "grey" state can also transfer three ways when its life time is ran out. The cell can transfer into "black" state depending on defined concentrations of "black" and "grey" neighbor cells:

$N_{kb} > N_b$, $N_{kg} > N_g$, $w_g < w_b$: $A_k(t) => A_k(t+1) = +1$.

Second "grey" cell cycle launch is conditioned by defined "grey" and "black" neighbor sells concentrations also:

$N_g > N_g$, $N_{kb} > N_b$, $w_g > w_b$: $A_k(t) => A_k(t+1) = 0$.

When the conditions for the transition to the "black" state or run a second cycle time life checks the "probability" transition, which determines the final state. If the conditions for the transition of counting neighbors are not satisfied, then the "gray" cell dies and becomes "white": $(t) => (t+1) = -1$. Recharging the "black" unit cells is similar to recharging a "gray" elementary cell. It should be noted that the concentrations of N_g and N_b, required for the transition, different for different unit cells colors.

The implementation of the above algorithm can simulate the reaction of the equations reaction-diffusion type. Algorithm takes into account the behavior of the nearest neighbors and is guided only local regulations.

5. Implementation of Multi-agent System

Described modeling algorithms implies whole volume cell states recalculation every time stroke. But that is obviously ineffective. Memory and performance problems occur when implementing such algorithm in a "raw" way on a significant amount of input data. The algorithm was modified to resolve this issue. The main concepts of modification are:

(1) Minimization of "idle" calculations (i.e., only blocks that can change their cells state are recalculated);

(2) Parallel calculations on independent blocks.

A multi-agent architecture was chosen to implement those concepts. Multi-agent system consists of agents of three types (Fig. 3): agent-actor, paralleling agent and agent-router. Actor performs calculations to determine states of cell in the given segment of a grid. Paralleling agent divides the grid into segments depending on the number of available actors and distributes the whole task between them. Agent-router searches for new actors that are hosted inside other applications and/or other machines. Paralleling agent queries an agent-router to give it a list of available actors. Then it updates its own list of actors with the received information. The grid is divided into segments depending on the amount of actors in the list and the agents are informed about their segments. Every segment is initialized by putting grey cells on the surface. Every time tick an actor recalculates states of cells of its segment if it has grey or black cells inside or at the border. Otherwise the agent stays idle. If there are grey or black cells on the border of a segment after the recalculation that information is sent to an agent responsible of the neighbor segment. That is how the described above concepts work. The implemented concepts allowed to lower memory and processor requirements and also improved timing. Besides that, the chosen multi-agent platform allows to use agents hosted in different applications and on different machines connected via local network, Internet and event located in the cloud. That allows to parallel calculations between different machines that also improves scalability and performance.

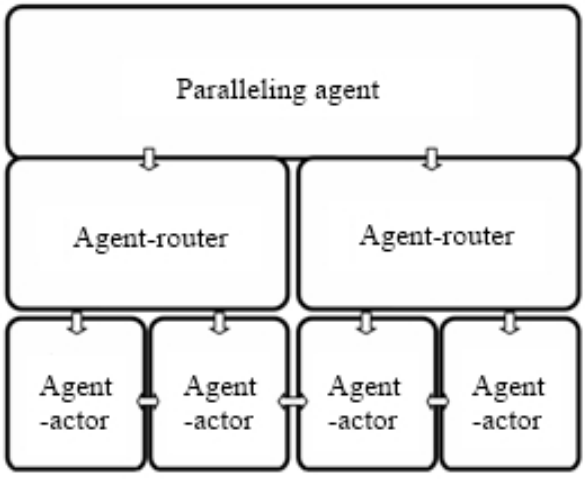

Fig. 3 The block diagram of the multi-agent system.

6. Model Results Analysis

The implemented algorithm was applied to a simple singony structured parallelepiped consisted of 200 × 200 × 50 elementary cells. 2×10^6 cells were processed in this way. Object dimensions were taken randomly. Adsorption on the object surface was made from an endless source perpendicular to the "XY" surface. Diffusion coefficient D is isotropic and equal to 1. Model algorithm made 500 strokes (the number is taken randomly). Given life time values: white—10 strokes, black—5 strokes, grey—5 stokes. All transfers have equal probabilities. Transfer rules for grey and black cells are 4 and 5 cells of corresponding color. In Fig. 4 a set of "XY" section snapshots are presented. They display system evolution in time processed by described algorithm. Similar solid body

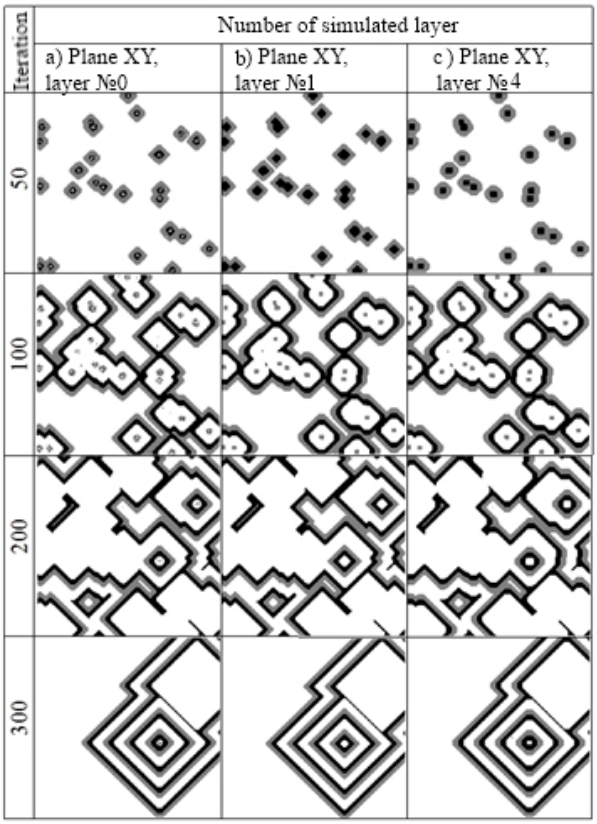

Fig. 4 Evolution of the system, the plane XY.

surface snapshots are presented in Ref. [6]. That automata had different ruling parameters and cell concentration dependencies. It is also 2-dimensional and does not take diffusion processes into view. It should be noted that diagrams and such snapshots are impossible to be built because the number of parameters and modelling concepts differ, nevertheless there is a principal result similarity.

Fig. 4a corresponds to the surface layer, Fig. 4b corresponds to the near surface layer #1, Fig. 4c corresponds to near surface layer #4. At stroke 50 several lead centers start working actively. At stroke 100 those centers start interfering with each other. At stroke 200 most of the leading centers either degrade or are consumed as a result of competition. As a result at stroke 300 only one leading center is left. Leading centers that are formed during the evolution can degrade, be consumed or continue interaction by means of solution waves. Subsequently these centers degrade and the system returns to its initial state. The degradation is a result of several lead centers competition. Similar surface layer snapshots are presented in Refs. [5, 6]. Though, they describe only surface state. The described model on the other side allows to analyze any layer at needed section. CA modelling allows to analyze any layer or section in orthogonal planes. In Figs. 5-6 cell concentration dependencies on time of surface and 4th layer correspondingly. Such measurements can not be obtained during a real experiment. The model on the other side allows to measure at any mono layer in any of orthogonal planes. Dependencies recalculation over the whole volume allows to make comparisons to the real data. For example, in Ref. [9] oscillograms obtained by self-oscillation in electron-hole plasma/exaction in Si with impact ionization in DC research. The measurements were taken from different ends of the sample. Obtained during the modeling dependencies can be interpreted as appearing currents oscillogram. Everything described above leads to the fact that every elementary cell influences neighbor elementary cells. Their transfer between the states is determined by time needed to change state, change state probability and neighbor cells that are in appropriate state to make a transfer. Application of that model allows to observe one of the dynamic processes example-leading centers forming and subsequent consumption both on the surface and in near surface layers.

7. Conclusions

Described above rather simple algorithm implementation illustrates how the system during the transition from chaos to synchronization passes the

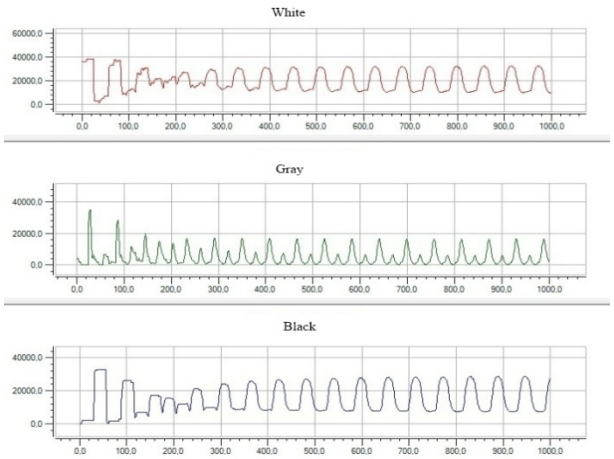

Fig. 5 Depending on the concentration of cells in different states from time to time for the layer№ 0.

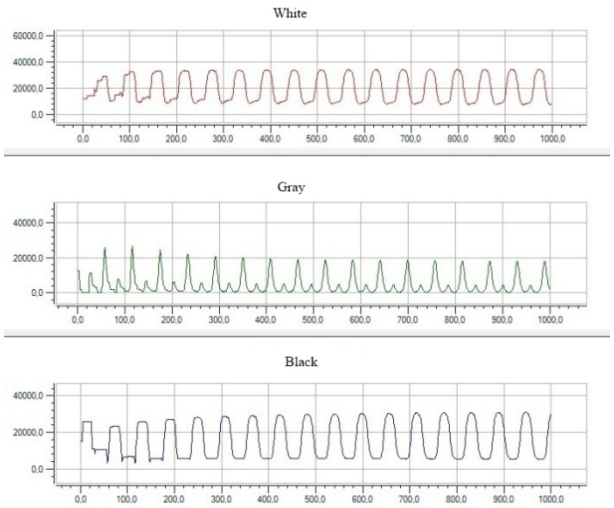

Fig. 6 Depending on the concentration of cells in different states of the time for the layer № 4.

stage of local lead centers synchronization. This means that lead centers with determined oscillation frequencies occur and subsequent evolution is a result of these centers competition and further consumption, degradation or moving into a state of autowave emission. Despite of the algorithm simplicity it is very resource demanding. This fact provides a lot of difficulties and restrictions in its implementation. At the moment a work on dynamic modes diversity increase and structure defects insertion is held. That is done to approximate the modeling object to real crystal systems.

Acknowledgments

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