RADIATION-INDUCED DEFECT'S CLUSTERING AND SELF-ORGANIZATION DURING SURFACE MODIFICATION

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Defects' clustering model is applied to study of the both: helium blistering in metal lattice and a thin film islands deposition. Plasma surface modification is investigated as a first order phase transition at a fluctuation stage. Wiener stochastic processes which are associated with the clustering evolution as well as with the defects motion are used. Brownian motion due to a long-distance potentials of indirect interaction blisters (or islands): through acoustic phonons and Friedel's oscillations of lattice's electronic density has been modeled. Stochastic simulation has involved the analyse of a follows self-organization structures: vacancy-gaseous bubbles layers (or porosity) and islands chains on the surface with roughnesses.

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1. INTRODUCTION

The evolution of humanity needs new materials with specific properties and as result it, development of nanotechnologies. The paper deals with computer simulation of properties of nano-modified materials and deposited thin films also as defects in materials which are planed as thermonuclear technologies and materials. Self-organization widely known today: among them are the processes of streamlining the particles movement in plasma both recreated in laboratory scale plant and observed in nature. This process depends on transformation of energy received from outside into heat; in that case the groups of waves and particles intensively interact in vast space, and this determines probability for formation in plasma of stable large-scale structures [1,2]. The emergence (without special outside influence) of streamlined structures and forms of movement on the basis of the initially accidental, unregulated ones are described as self-organization. And the fact is that the whole system where this takes place acquires properties that were lacking in its parts [3]. Typical of such phenomena, nonlinear in there nature is of course a great number of closely interacting independent parameters and they always depend on energy received from outside. Also, in this way, it exists the fundamental problem: defects' origin in condensed matter or on the surface solid body models which can be seen as a plasma-like media evolution. It has to be associated with transitions from chaos to self-organization and back: So, here is extremely difficult to working out this problem. The most promising way in this direction is plasma computer simulation [2]. The problem of the phase transition at inequilibrium stage kinetic description is introduced by stochastic simulation method [3,4]. New approach is based on the strict results of the probability analysis of equations of mathematical physics [5]; the kinetic theory of plasma and rarefied gases [6]; the theory and practice of numerical experiment in non-linear plasma simulation [2]. The progress in computer engineering allows us to see the overall picture of initial stage of phase transition in detail the behavior of defects origin, retention of vacancy-gaseous bubbles into lattice. The defects (flaws) have been stratificated in lattice as defects layers near surface. The development of this structure of defects leads to following: porosity, swelling, flacking and others harmful effects. Plasma- surface interaction is depicted as a plasma-like media with the adequate mathematical description of various dynamic processes brought about the construction of models taking into account the random fluctuations of the trajectories of these processes. The large number of stochastic dynamical independent variables {x1(t),...,xN(t)} are obeyed to the set of Ito-Stratonovich stochastic differential equations /SDE/. The SDE system solution is connected with the study of "forward" and "backward" Kolmogorov equations of parabolic type for distribution density of Markov process. The relationship SDE solution to linear parabolic partial differential equation [5,7], absolutely stable algorithms for the given integration step size [7] and modification of Artem'ev method for SDE with non-linear coefficients solution [4,5,8-12] give us a powerful tool for self-organization structures detection. Helium ions and metal lattice would constitute a "open" system as well as the defects interaction each others leeds to specific form of self-organization into phase spaces which associated with blistering problem. We can also to observe the appearance of the fundamental properties of loss of stability in system regarded as a medium with large number degree of freedom. The insight into the kinetic description of phase transition can be extended by determination of distribution function of gaseous phase in a bubbles versus the both: sizes and coordinates. Defects appears into lattice under plasma action on the time scale of interest when the medium state is strongly non-equilibrium. Basic macroscopic characteristics (the so-called moment of the distribution function) are obtained by averaging the non-equilibrium kinetic distribution function. The defects (flaws) have been stratificated in lattice as defects layers near surface. The development of this structure of defects leads to following: porosity, swelling, flacking and others harmful effects. High temperature blistering (or uncharged defects clustering model) of He ions on a surface Ni is developed in two time scales no later than 10^{-4} s. under follows parameters of plasma beam: energy E=10 keV, ions flux density and dose approximately is equal to 10^{16}.

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2. STOCHASTIC SIMULATION MODEL

We start simulation the phase transition by numerical approach, using the model of diffusive Markov's process (MP) in a phase space **{G}** with size g of arising bubbles as well a liquid metal thin film islands: {g(t),t≥ 0}, g>2. Here the $g(t=0)=g_0$, size g means the number of unit volumes of "condensing" substance in the bubble nucleus (however, it is possible also to consider the radius r of spherical bubbles or hemispheres drop of liquids on the surface). The maximum of cluster size (let us name this nucleus- cluster) is determined by conditions of stability of bubble. Collisions and fluctuation processes has produced the nuclei of new phase (gaseous into lattice as well liquid on the lattice surface) out of "super saturation" condition which can be described by Ito stochastic differential equations/SDE/the both are statistically equivalent to equations of Fokker-Planck-Kolmogorov (FPK) and Boltzmann-like (or Leontovich), this allows us to take the numerical solution of SDE systems is to be seen a method for the solution of Mathematical Physics Equations (MPE) for study non-equilibrium first-kind transition processes. The coefficients of both problems (SDE and MPE) are related by definitions and properties of non-look-ahead functionals of Marcov's random processes. The algorithms for solution of a set of linear Ito-Stratonovich SDE [5] by with constant coefficients have been modified for simulation and analysis of the problems with functional-coefficients [3,7,8], in case of heterogeneous to non-equilibrium stage of "condensation" of gaseous particles. We assume that formation of clusters of defects and evolution of their size is to be described by kinetic equation for f(x,y,t) of transitional probability density of a random MP {X(t),t≥0}. Here we talk about Kolmogorov's equation (i.e., about partial differential equations of parabolic type), which is related with Wiener process. The kinetic equations for Brownian particle are partial integral-differential equations [3,7] and its have laborious methods for solving. Rate of bubble/cluster growth (or degradation) and its migration have different characteristic time scales which equal for blistering $\tau_g \approx 10^{-9}$, $\tau_r \approx 10^{-8}$ s and $\tau_g \approx 10^{-8}$, $\tau_{xy} \approx 10^{-7}$ s for film covering correspondingly. Thus, kinetic equations on a discrete time grid are solved by technique of splitting in terms of physical processes, and every stage is represented by its stochastic analogue. Interaction between bubbles/clusters is indirect, through lattice phonons and electron density oscillations [9-16]. The kinetics equations after physical processes split look like following, *W* is Wiener process. The kinetic equations for Brownian particle are partial integral-differential equations [3,7] and its have laborious methods for solving.

$$\frac{\partial f_r(g,t)}{\partial t} = \frac{\partial\left[D_g(g,t)\frac{\partial f_r(g,t)}{\partial g}\right]}{\partial g} + \frac{1}{kT}\frac{\partial\left[D_g(g,t) f_r(g,t)\frac{\partial\{\Delta\Phi(g,\vec{r},t)\}}{\partial g}\right]}{\partial g} + S_\alpha(f_\alpha)$$

$$f_r(g,0)= f_{0g},\quad \left.\frac{df_r(g,t)}{dg}\right|_{g\le 2}=0,\quad f_r(g,t)|_{g<2}=0,$$

$$\frac{\partial f_g(\vec{r},t)}{\partial t} = \frac{\partial\left[D_r(\vec{r},t)\frac{\partial f_g(\vec{r},t)}{\partial \vec{r}}\right]}{\partial \vec{r}} - \frac{\partial\left[\frac{\vec{F}(\vec{r},t)}{M_g\gamma} f_g(\vec{r},t)\right]}{\partial \vec{r}},$$

$$f_g(r,t)|_{t=0}= f_{0r},\quad f_g(r,t)|_{x=x_{\text{left}}} = f_g(r,t)|_{x=x_{\text{right}}},$$

$$f_g(r,t)|_{y=y_{\text{left}}} = f_g(r,t)|_{y=y_{\text{right}}}.$$

Rate of bubble/cluster growth (or degradation) and its migration have different characteristic time scales which equal for blistering $\tau_g \approx 10^{-9}$, $\tau_r \approx 10^{-8}$ s and $\tau_g \approx 10^{-8}$, $\tau_{xy} \approx 10^{-7}$ s for film covering correspondingly. Thus, kinetic equations on a discrete time grid are solved by technique of splitting in terms of physical processes, and every stage is represented by its stochastic analogue. Interaction between bubbles/clusters is indirect, through lattice phonons and electron density oscillations [9-16]. The kinetics equations after physical processes split look like following, here is molar volume of liquid molecules, are temperature and density of vapour molecules. We consider single spherical nucleus with radius of gaseous or liquid cluster *r*, comprising *g* single droplets with molar volume. S_α is source of vapour which generates ion with f_α – maxwell ion function, which is characterized by temperature 2500 K, *g* is the number of atoms which is consisted in island-clusters, D_g is the non-linear diffusion coefficient in the space of cluster sizes; *f(g)* is the bubble size distribution function – the probability to find the cluster with size *g* in interval of values of *g* [*g*,*g*+*Δg*], $\Delta\Phi$ is the Gibbs energy, M_g is the cluster mass, γ is constant of friction, distribution function *f(r)* is the islands space function, $\vec{r}$ is the position of cluster mass centre in orthogonal coordinates system: $x_{\text{left}} = -200$, $x_{\text{right}} = 200$, $y_{\text{left}} = -200$, $y_{\text{right}} = 200$, $U(r)$ is the potential of long-range clusters interaction between them through phonons and oscillation of electron density. The modelling 3-dimensional region is periodic across two coordinates (x and y) across the third coordinate (axis z): on top the region contacts with plasma, on bottom we have reflection from crystal lattice layers undisturbed with vacancy and helium impurity negligible concentration (for simplicity vacancies description here is not demonstrated). There are equations involving partial derivatives of blister coordinate into lattice and its size measured in number of gaseous particle without compression.

$$\frac{dg}{dt} = -\frac{1}{kT} D_g(g,t)\frac{\partial\Delta\Phi(g,\vec{r},t)}{\partial g} - \frac{1}{2}\frac{\partial D_g(g,t)}{\partial g} + \sqrt{2D_g(g,t)}dW$$

$$t_0 \le t \le T_k \quad g(t_0)= g_0 \in [g_{\min};g_{\max}] \quad g(t)>2$$

$$H_x = -\frac{1}{\gamma M_g}\frac{\partial U(x,y,z)}{\partial x} - \frac{1}{2}\frac{\partial D_x}{\partial x};$$

$$\sigma = \sqrt{2D_x},$$

$$x(t) = x(t_0) + \int_{t_0}^{t} H_x(\tau, x(\tau), y(\tau), z(\tau))d\tau +$$

$$+ \int_{t_0}^{t} \sigma(\tau, x(\tau), y(\tau), z(\tau))dW(\tau),$$

$$\Delta\Phi(g,\vec{r},t) = \begin{cases} -(a_\Phi - c)g + bg^{2/3} + \Delta\Phi_r, & if \\ \Delta\Phi(g,\vec{r},t) < \Delta_{break}; \\ -(a_\Phi - c)g + bg^{2/3} + \Delta\Phi_r - \Delta\Phi_{break}, & if \\ \Delta\Phi(g,\vec{r},t) > \Delta_{break} \end{cases}$$

$$\Delta\Phi_{break} = N_{br}\Delta_{break},$$

where $a_\Phi = \eta_a(\chi_\beta - \chi_\alpha)$ is part of Gibbs potential connected with difference of chemical potential of phases (gas in blister and metal lattice/vapour and liquid), c is part of Gibbs potential concerned with elastic force of lattice reaction for blister and with weight of cluster for thin films formation, tensions on boundaries between different phase are taken into account using, $\Delta\Phi_r$ considers bubble/cluster place in lattice/on surface, $\Delta\Phi_{break}$ concerns with relcases of part of connections in lattice for blistering, N_b is number of broken bonds, Δ_{break} is the energy required for breaking of a single bond with lattice. $(\chi_\beta - \chi_\alpha)$ is difference of chemical potential of phases

$$\eta_a = \begin{cases} \dfrac{2\pi}{3V} & for\ blistering \\ \dfrac{\pi(2 - 3\cos\theta + \cos^3\theta)}{3V} & for\ thin\ film \end{cases},$$

– form factor, where V is atom volume of He (for blistering) and evaporated material for thin films formation, (θ-angle of contact, α is first metal vapour, β is cluster of liquid metal on surface, S is phase of second more refractory metal (substrate material).

$$b = \begin{cases} b_0(1 - 1/3\cdot\bar{g}^{-1/3}),\ b_0 = (36\pi)^{1/3}V^{2/3}\sigma_{bl} & for\ \ blistering \\ 2\pi(1 - \cos\theta)\sigma_{\alpha\beta} + \pi\sin^2\theta(\sigma_{\beta S} - \sigma_{\alpha S}) & for\ \ thin\ \ films \end{cases}$$

where $\sigma_{\alpha\beta}, \sigma_{\beta S}, \sigma_{\alpha S}$ are surface tension between vapour of metal and metal liquid in island, liquid island and substrate, vapour and substrate.

$$\Delta\Phi_r = \begin{cases} k_x\cos(2\pi(x - \varphi_x)) + k_y\cos(2\pi(y - \varphi_y)) + \\ + k_z\cos(2\pi(x - \varphi_z)) & blistering \\ \dfrac{\Psi}{\sqrt{g}}(2 - \cos(\dfrac{2\pi x}{a_x}) - \cos(\dfrac{2\pi y}{a_y})) & thin\ \ film \end{cases}$$

The common form of diffusion coefficient in the space of defects sizes is $D_g = D_{g0}g^{2/3}$, D_{g0} is calculated coefficient.

The long- range part of the interaction between uncharged defects in dielectric crystals is elastic interaction through the acoustic phonons. The indirect interaction take place in metal lattice also via influence Friedel oscillation in electron density, for spherical Fermi surface analytically derived the dependence upon the distance between defects. Model assumption in approximation of potential: distance R between defects has been selected as a distance between centre of mass blisters. The correlations which it appear in system in consequence of this indirect interaction of defects each with another. The potential of indirect interaction, which influences on migration defects such as bubble in lattice and clusters on surface, can be presented as $U = U_{dd} + U_{ds}$ where U_{dd} is potential of indirect interaction between defects of one kind (blister-blister or cluster-cluster),

$$U_{dd} = \begin{cases} \sum_{i \neq j}^{N} \left\{ \dfrac{b_{rb}\left[\dfrac{3}{5} - \dfrac{(x_i - x_j)^4 + (y_i - y_j)^4 + (z_i - z_j)^4}{(\vec{r}_i - \vec{r}_j)^4}\right]}{|\vec{r}_i - \vec{r}_j|^3} + \right. \\ \left. + \dfrac{a_{rb}\cos(\vec{c}_{rb}(\vec{r}_i - \vec{r}_j))}{|\vec{r}_i - \vec{r}_j|^3} \right\} \\ |\vec{r}| = \sqrt{x^2 + y^2 + z^2}\ \ blister; \\ \sum_{i \neq j}^{N} \left\{ \dfrac{b_{rc}\left[\dfrac{3}{5} - \dfrac{(x_i - x_j)^4 + (y_i - y_j)^4}{(\vec{r}_i - \vec{r}_j)^4}\right]}{|\vec{r}_i - \vec{r}_j|^3} + \right. \\ \left. + \dfrac{a_{rc}\cos(\vec{c}_{rc}(\vec{r}_i - \vec{r}_j))}{|\vec{r}_i - \vec{r}_j|^3} \right\} \\ |\vec{r}| = \sqrt{x^2 + y^2}\ \ nanofilm \end{cases}$$

U_{ds} is potential of indirect interaction between defects of two different kinds (between bubble and surface for blistering and between liquid cluster of less refractory metal on substrate surface of more refractory metal and linear dislocation on surface or in near surface region).

$$U_{ds} = \begin{cases} \dfrac{A_{surf}}{z^2} & blistering \\ \sum\limits_d \left[\dfrac{b_d \left[\dfrac{3}{5} - \dfrac{(x_i - x_d)^4 + (y_i - y_d)^4 + (z_d)^4}{(\vec{r}_i - \vec{r}_d)^4} \right]}{|\vec{r}_i - \vec{r}_d|^3} + \right. \\ \left. + \dfrac{a_d \cos(\vec{c}_d (\vec{r}_i - \vec{r}_d))}{|\vec{r}_i - \vec{r}_d|^3} \right] & nanofilm \end{cases}$$

b_{rb}, a_{rb}, c_{rb}, b_{rc}, a_{rc}, c_{rc}, b_s, a_s, c_s, b_d, a_d, c_d are model coefficients, z of surface is equal zero for blistering and z of dislocation is equal dislocation depth for thin film formation, if dislocation is located under surface and dislocation z is equal zero if dislocation is located on substrate surface.

In case of blistering (the situation of open system) is created by a flux of inert gas atoms: $D_r(r, t) = D_r(x, y, z, t)$ is the diffusion coefficient for space $\{R == (x, y, z)\}$, γ is the dissipation factor. As for coefficients of stochastic diffusion used for modeling of bubble walk, we introduced a temperature dependence and accounted the nonlinear coefficients by expression:

$$D_z = \frac{D_0 e^{-E_m/kT}}{\gamma M_g} \left(1 + \alpha \Delta z^2\right),$$

$D_0 = 3{,}73 \cdot 10^{-7}$ cm^2/s, $E_m = 0.35$ eV, x_0, y_0, z_0 are the initial values of coordinates x, y, z of a cluster. Diffusion coefficient looks similar form for case of thin film formation.

3. STOCHASTIC SIMULATION NUMERICAL SCHEME

Kinetic equation are changed on its stochastic analogs [3,7,11-16], stochastic differential equations /SDE/ are solved used modified authors Artem'ev method [17]. SDE and modifications of Artem'ev method for these models can be found in more early papers of authors [11-16]. To solve a system of SDE with functional-coefficients, it is required to construct a series expansion for exact solution of Cauchy problem:

$$x(t) = x_0 + \int_0^t H(x(\tau))\, d\tau + \int_0^t \sigma(x(\tau))\, dW(\tau),$$

$0 \le t \le T_{\text{fin}}$.

A modified Artemiev's method was used; it is a second-order accuracy method, with infinite domain of stability (according to methods developed for solving of SDEs) [17]. The modification from the original Artemiev's method is that the coefficients in SDE are essentially nonlinear and depend on flaw distributions on their sizes and coordinates. The use of Stratonovich's form for SDE makes possible to take a standard white noise instead of random function $\xi(t)$, and this simplifies the calculation procedure of stochastic integral for the Wiener process in realization of the numerical method. As a sample, we can take the equation for calculation of the bubble size. For the ith trajectory of diffusive Markov's process its values g_{n+1} and z_{n+1} at the time moment $n+1$ can be calculated through these formulas:

$$g^i_{n+1} = g^i_n + \left[I - \frac{h}{2} \frac{\partial H^i_n}{\partial g} \right]^{-1} \times$$

$$\times \left[hH^i_n + \sqrt{h}\sigma^i_{ng}\xi_{ng} + \frac{h}{2} \frac{\partial \sigma^i_{ng}}{\partial g} \sigma^i_{ng} \xi^2_{ng} \right],$$

$$H^i_{ng} = -\frac{1}{kT} D^i_g\left(g^i_n, t_n\right) \frac{\partial \Delta\Phi^i\left(g^i_n, t_n\right)}{\partial g^i_n} -$$

$$- \frac{1}{2} \frac{\partial D^i\left(g^i_n, t_n\right)}{\partial g^i_n},$$

$$\sigma^i_{ng} = \sqrt{2D^i\left(g^i_n, t_n\right)}.$$

$$\begin{cases} z^i_{n+1} = z^i_n + \left[I - \dfrac{h_z}{2} \cdot \dfrac{\partial H^i_{zn}}{\partial z_i} \right]^{-1} \left[hH^i_{zn} + \sqrt{h}\sigma^i_{zn}\xi_{zn} \right] \\ H^i_{zn} = \dfrac{1}{M(g^i_{n+1})\gamma} \cdot \dfrac{\partial U^i(x^i_n, y^i_n, z^i_n)}{\partial z} - \dfrac{1}{2} \dfrac{\partial D^i_{zn}}{\partial z} \xi^2_{zn} \\ D^i_{zn} = D_{z0}(1 + \alpha (z^i_n - z^i_{n-1})^2) \\ \sigma^i_{zn} = \sqrt{2D^i_{zn}} \end{cases}$$

In this method g_n, z_n are the approximation of SDE system solution at grid points by time $\{t\}$, h, h_z is the time step for size and position changes correspondingly, I is the unit matrix, ξ_n is the sequence of independent random numbers with a zero expected value and unit dispersion. While modeling the SDE solution on a computer, the values of ξ_n can be calculated by formula $\xi_n = \sqrt{-2\log\alpha_1}\cos(2\pi\alpha_2)$, where α_1 and α_2 are random numbers uniformly distributed in the interval (0,1).

We are able to present operator's scheme of computer simulation as superposition of the operators $A_{\Delta g}$, A_{Br}, A_{UD}, A_F, where $A_{\Delta g}$ –operator of size change; A_{Br} –operator of lattice broken (for blistering only); A_{UD}- operator of space diffusion, defects interaction and interaction between defects of two different kinds (between bubble and surface for blistering and between liquid cluster of less refractory metal on substrate surface of more refractory metal and linear dislocation on surface or in near surface region); $A_F = A_{Fus} + A_{Surf}$, A_{Fus}- operator of defects fusions. The fusion of defects takes place if $\left|r_i - r_j\right| \le r_d(g_i^{1/3} + g_j^{1/3})/a + \Delta_f$, where $0 \le \Delta_f \le a$ (r_d is radius of He for blistering or radius of adatom for nanofilm, a is lattice parameter of substrate material).

A_{Surf} has meaning only for blistering and corresponds with blister reflection from surface or destruction on it. $z_{\min} = 0$, $z_{\max} = 400$; it is assumed that the cluster dies on the surface if $z \le (2/3)R_b$ (here $R_b = r_{He}\sqrt[3]{g}$ is the bubble radius, r_{He} is the helium radius).

4. RESULTS AND DISCUSSION

Note that blistering and thin film formation have similar stochastic characters and are described similar equations. Used approach allows us to receive nonequilibrium distribution functions of bubbles/clusters contrasted with defect size and its space position, in terms of its we receive evaluation of order parameter for each problems and mathematical expectations of defects size and others characteristics such as distance from the surface, porosity evaluations of several solids layers and the calculated tensions due to blistering, for example. We should like to summurize results of simulation of fluctuation stage of high-temperature blistering. In our opinion, the most interesting results are: the self-organization of bubbles are observed, blisters form quasi-lattice and blisters chains are formed athwart to incident ions fluxes; the greatest porosity and tensions are observed on depths of ~ 0.85 R_p and ~0.35R_p (Fig.1), R_p is middle depth of projection run, these depths correspond to locations of big and small blisters (Fig.2), which are observed in laboratory experiments; the most rapid blistering development is take place if temperature of substrate material equals 0.47 of melting temperature. The porosity can be considered as the order parameter of first-kind transition for blistering. The porosity is

$$p(z_j,t) = \frac{V_a}{V_l}\frac{\sum_{i=1}^{N} g^3{}_i f(g_i,z_j,t)}{\sum_{i=1}^{N} g^3{}_{0i} f(g_0)}$$

(Fig.1), where V_a is total examined volume, V_l is layer volume, $N=10$ is number of blister, g_0 is initial blister size in number He in blister, $f(g_0)$ is initial distribution function from blister sizes. The fluence is 10^{17} ions/cm^2, energy of *He* ions is 10 keV, temperature is 1000 K for presented calculation. Authors used 10^6 trajectory statistics for kinetic distribution functions calculated. Two maximums of porosity are good noticeable.

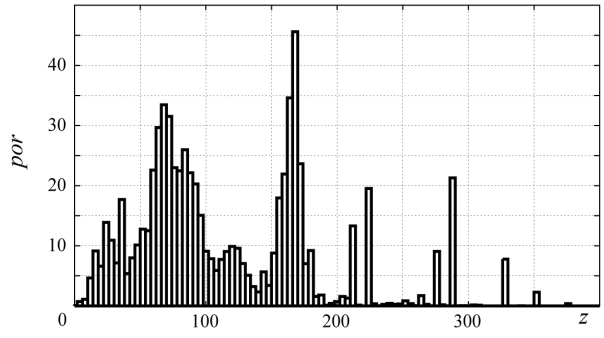

Fig.1. The figure 1 shows the relative porosity of different solid layers as function from layer depth. Z is layer depth from surface under irradiation measured in lattice parameters

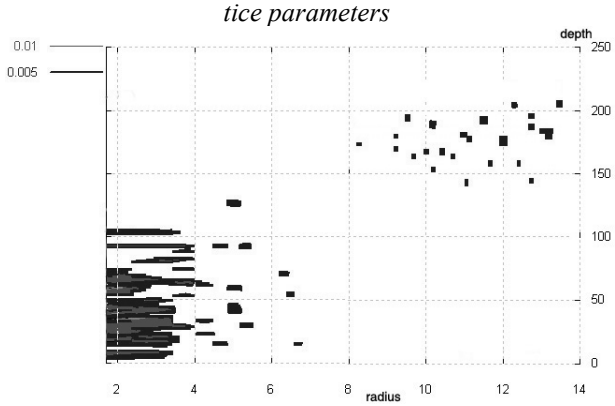

Fig.2. The distribution function from blister size (abscissa axis, size is measured in Å) and depth (ordinate axis, depth is measured in lattice parameter) is presented by colours on this picture

The maximum located on depth approximately 0.85 R_p (R_p is middle depth of projection run, for examined case R_p=70 nm) is corresponded with “big” blisters. “Big” blister can growth to 1 micrometer. The radiuses of "big" blisters at finish of fluctuating stage are 10...14 Å (Fig.2). The maximum located on depth approximately 0.35 R_p is conformed to “small” blisters which end sizes can be 10^{-8}...10^{-7} m. The radiuses of "small" blisters at finish of fluctuating stage are 2...4 Å (Fig.2).

The most interesting results from thin films formation are: I) three stage of cover formation during fluctuation stage are discovered. The first stage lasts from 0 to $8\cdot10^{-7}$ sec, it is stage of slow development. The second stage continues from $8\cdot10^{-7}$ sec to $5\cdot10^{-5}$ sec and it is stage of quick growth of thin film. The third stage lasts from $5\cdot10^{-5}$ sec to 10^{-4} sec and it is notable for deceleration of growth velocity; II) The study of influence of dislocation depth on thin film formation indicates that 1) self-organization of clusters are observed, nanofilm formation begins on surface defects in particular on dislocations; 2) the dislocation influence is important if its depth is less then 5 lattice parameters;

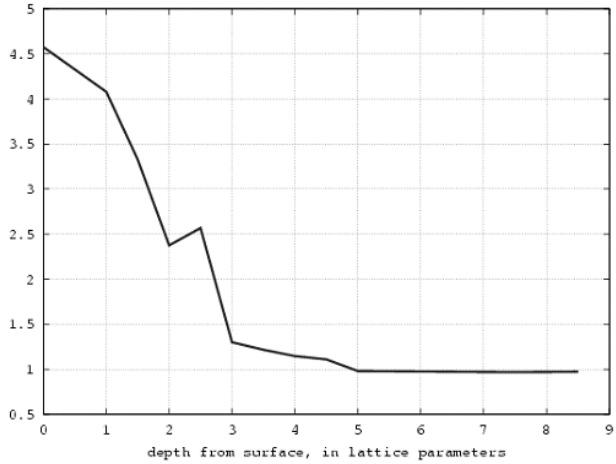

Fig.3. The dependence of the ratio of probability of location clusters on projection of dislocation line on surface from probability of location clusters outside projection of dislocation line on surface from dislocation depth is presented on this pictur

3) if dislocation depth is more then 5 lattice parameters that probabilities of cluster location on dislocation line and outside it are equal; 4) the ratio of probability of location clusters on projection of dislocation line on surface from probability of location clusters outside projection of dislocation line on surface reduces with increase of depth and equals 1 when dislocation depth is more 5 lattice parameters of substrate material. This is non-linear function (Fig.3); 5) the projection of dislocation line on surface can be considered as center of nanofilm formation if dislocation depth is less 5 lattice parameters; 6) if dislocation locates on surface that most heavy growth takes place on dislocation. III) The ratio of covering square at the present situation from covering square at the initial time moment can be considered as order parameter for problem of nanofilm formation. The evaluation of this ratio is presented on Fig.4.

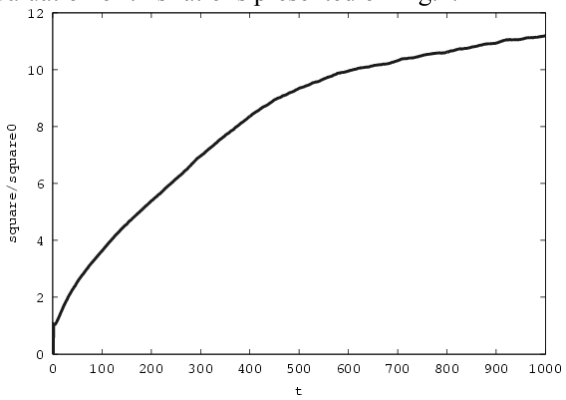

Fig.4. The ratio of total islands square at the present situation from total islands square at initial time moment is shown. The time in τ_{xy}~10^{-7} s is put off on abscissa axis

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КЛАСТЕРИЗАЦИЯ РАДИАЦИОННО-СТИМУЛИРОВАННЫХ ДЕФЕКТОВ И САМООРГАНИЗАЦИЯ ПРИ МОДИФИКАЦИИ ПОВЕРХНОСТИ

А.Л. Бондарева, Г.И. Змиевская

Модель кластеризации приложена к изучению: гелиевого блистеринга в металлах и осаждение островковых тонких пленок. Модификация поверхности плазмы исследована как фазовый переход 1-го рода на флуктуационной стадии. Исследован Винеровский стохастический процесс, который ассоциируется с эволюцией кластеризации и с движением дефектов. Промоделировано броуновское движение благодаря дальнодействующим потенциалам непрямого взаимодействия блистеров (или островов): через акустические фононы и Фриделевские осцилляции электронной плотности. Стохастическое моделирование включает анализ следующих самоорганизующихся структур: слои вакансионно-газовых пузырей (или пористость) и неупорядоченные цепочки островов на поверхности.

КЛАСТЕРІЗАЦІЯ РАДІАЦІЙНО-СТИМУЛЬОВАНИХ ДЕФЕКТІВ І САМООРГАНІЗАЦІЯ ПРИ

МОДИФІКАЦІЇ ПОВЕРХНІ

А.Л. Бондарева, Г.І. Змієвська

Модель кластерізації прикладена до вивчення: гелієвого блистерінгу у металах та осадженню острівкових тонких плівок. Модифікація поверхні плазми досліджена як фазовий перехід 1-го роду на флуктуаційній стадії. Досліджено Вінерівський стохастичний процес, котрий асоціюється з еволюцією кластерізації та рухом дефектів. Промодельовано броунівський рух завдяки далекодіючим потенціалам непрямої дії блістерів (або островів): через акустичні фонони та Фриделевські осциляції електронної густини. Стохастичне моделювання включає аналіз наступних структур самоорганізації: шари вакансійно-газових пузирів (або пористість) і неупорядковані ланцюги островів на поверхні.