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Recommended form of bibliographic references: Bondareva A.L., Zmievskaya G.I. Computer simulation: radiation damaging of multilayer solids and thin film formation on solid surface. Keldysh Institute preprints, 2012, No. 1, 40 p. URL: http://library.keldysh.ru/preprint.asp?id=2012-1&lg=e

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Computer simulation: radiation damaging of multilayer solids and thin film formation on solid surface

Moscow, 2012

Abstract. Mathematical model of the first-order phase transition due to fluctuation of thermodynamical parameters presented as system of equations of mathematical physics in partial derivatives of the Kolmogorov-Feller and Einstein-Smolukhovskyi and stochastic differential equations of Ito -Stratonovich. Computer simulation study of the nonlinear stage of nucleation can be used in the powders synthesis and thin films of silicon carbide. Model processes of condensation and crystallization, as well as vacancy-gas defects clustering are presented as superposition of Wiener random processes such as stochastic diffusion in phase space cluster sizes of nuclei and spatial their brownian motion, which are stimulated by long-range self-consistent potential indirect elastic interaction of the clusters of nuclei on the surface and in the volume of the substrate. The effective algorithms for stochastic differential equations with nonlinear functional-coefficients worked out. Kinetic functions of distribution clusters of nuclei from size and spatial coordinates for the conditions of model numerical experiments are calculated. The stressed state of crystal lattice which is proceeded to a solid phase epitaxy thin film of silicon carbide in a silicon substrate has been studied. The results can be used to optimize the coating processes, to control of uniformity and application speed deposition of fine films.
Key words: silicon carbide, crystal powder, thin film, clustering, brownian motion, phase transition, nucleation, porosity, self-organization, stress into crystal lattice.

Аннотация. Численно исследовано флуктуационное зародышеобразование как нелинейная стадия фазового перехода в приложении к задачам получения порошков и тонких пленок карбида кремния. Модели конденсации паров и кристаллизации расплава, а также образование пористости субстрата представлены суперпозицией Винеровских случайных процессов: кластеризации зародышей или стохастической диффузией в фазовом пространстве размеров кластеров зародышей и их броуновским движением под действием дальнодействующего самосогласованного потенциала косвенного упругого взаимодействия кластеров зародышей. Математическая модель представлена системой уравнений математической физики в частных производных Колмогорова-Феллера и Эйнштейна-Смолуховского и стохастическими дифференциальными уравнениями Ито-Стратоновича. Разработаны эффективные алгоритмы решения систем стохастических дифференциальных уравнений с нелинейными функционал-коэффициентами. Результаты представлены кинетическими функциями распределения кластеров зародышей по размерам и пространственным координатам для условий модельных численных экспериментов. Исследованы численно условия напряженных состояний в решетке субстрата, предшествующие твердофазной эпитаксии пленок карбида кремния на кремниевом субстрате для оптимизации процесса создания покрытий с заданными свойствами, для контроля однородности и скорости нанесения тонкой пленки.
Ключевые слова: карбид кремния, порошки, тонкие пленки, кластеризация, броуновское движение, фазовые переходы, зародыши, пористость, самоорганизация, напряжения

Contents

1 Introduction

Among the processes, altering the functional properties of surfaces, an important role is played the heterogeneous phase transitions of the first kind, such as condensation of vapours on surfaces, the origin of pores in crystalline lattice of the substrate, as well as many other phenomena, due to the interaction of plasma with a surface of instruments, facilities and etc.

The formation of the crystalline lattice defects accompanies the aging of materials, the impact of radiation, laser processing, seasonal and diurnal changes in weather's conditions as well as and other many kinds of active influence on the surface which has structure of layers nanometer sizes. Painting and fresco are an example of multilayer structures. Majority objects of cultural heritage are under the influence of natural and antropogenic factors. Frequently the qualities of multilayer structures are able to be lost under influence of dampness, of freezing, temperature change, ultraviolet radiation, the deposition of dust, of mechanical damages and others.

The cause of this - nucleation due to the fluctuations of thermodynamic parameters of substrate and creating vacancies clusters and after this filling their by gas at the influence of powerful streams- quick, and under the weather factors - slow, the accumulation of defects into solids leads to amorphous structure.

These factors can leading to gas atoms accumulation and blistering (gas-vacancy bubbles formation) in the future. As well know, porosity is one of defects of sculptures. Development of porosity here is similar to the influence of ions fluxes on materials leading to the phase transition. Voids under surface is described in detail using computer simulation as well as the roles of roughness and multi-layer structure of substrate in damaging processes, that are presented in this paper. Using this data it is possible to evaluate what are the limits of the damaging action for the materials which allow to preserve its functional properties, you can analyze the position of the defects, if adequately take into account the forces that shape defects, and their diffusion into the crystal lattice under the action of gradient stresses in it. This may be the force of elastic interaction of defects each with other, with borders of layers and with dislocations or grains of structure materials.

May occur thermo elastic stresses, as well as the inconsistency of the structure of lattices of neighbouring layers, gradient of pressure arises due to chemical transformations and changes of concentration of impurities and other. Changes taking place in solids, are not limited to the formation of small inclusions or gas impurities, real conditions accumulation of defects has to be find in computer simulation that leads to a phase transition in the "open" physical system such as "gas flow of gas bubbles in a crystal lattice", which turn into the porosity of the sample. So, it reduces the hardness of the material, then happen layers of pores and cracking. If the cracks are oriented parallel to the sample surface, this leads to the phenomenon of exfoliative layer or flaking. The formation of chains of defects along the gas flow, which occurs in the process of blistering of an amorphous layers, which preceded to destruction of the sample.

In future diagnosis of noise in the samples with defects , as well as the existing numerical models of their emergence as well as self-organization in thin layers of models can be combined in the method of non-destructive damage control in technological installations and objects of cultural values. Moreover known methods for use of natural defects for the hardening of the material by a solid phase epitaxy which is successfully applied in practice and is being studied by the authors in the calculations.

Blistering conformity from computer experiments on surface treatment of silicon by stream of inert gas gives us criteria of the porosity formation. Stress which caused by blistering into silicon substrate and its dependence from the conditions of the experiment as well as the both: Distribution of blisters from its sizes and dependence of the layers and the chains of vacancy-gaseous pores in silicon substrate have been calculated on characteristic times the initial stage of the first type phase transition. Technique of numerical simulation of defects in the surface layers of technological mirrors are used for fundamental conclusions concerning different conditions of experiments.

A new technology has been introduced for creation of materials and structures with special properties. The formation of nanoparticles in plasmas, the charging of nanoparticles and the first order phase transition are investigated by simulation stochastic simulation methods /SSM/ [1,2]. It has been applied to study of the silicon carbide model formation. SiC experimental producing has attracted considerable attention [3]. The feasibilities of both: SSM on the base of stochastic differential equations /SDE/ and dusty plasma 3D3V kinetic object-oriented code [4] allows to study non-equilibrium stage of charged particles clusterization in plasma and crystal powder formation as an adjunct to other methods of experiments interpretation [3]. Collisions and fluctuation nature processes are investigated by Mathematical Physics Equations /MPE/ for non-equilibrium first order phase transition processes (clusterization, crystallization) and MPE for electron-ion plasma and dust grains. The coefficients of both problems (SDE and MPE) are connected by strong relationship [1]. The algorithms for solution of a set of Ito-Stratonovich SDE have been modified for simulation and analysis of the problems with functional-coefficients.

Non—steady state stochastic simulation models of the first order phase transition /PT/ at initial stage (when nuclei of new phase are able to appear) open up a new area of kinetic theory application and computer simulations development [1]. Kinetic approach is newcomers to study of nucleation. Examples of SSM (presented below) put attention on complex problems of kinetics among which are melted charged droplets formation. It is known that the problem is important for dusty plasma investigations.

A numerical method of stochastic simulation of nonequilibrium collision processes which lead to the fluctuation of thermodynamic parameters of rarefied gases, plasma and plasma-like media such as dusty plasma, lattice defects in form vacancy-gaseous bubbles and other can be applied in the interpretation of laboratory measurements (in studies of the laser plasma, vacuum technology, space physics), when it is important to analyze different scenarios collision processes, their relative

role, and, in ultimately, to determine the mechanism of the process, as well as in those cases, when the physical experiment only is scheduled. Theory of brownian motion - the chaotic movement of small, but all the same macroscopic particles in the liquid was developed by Albert Einstein, Marian Smolukhovskii and Paul Langevin. Multiple inelastic collision molecules with this particles (named "brownian particle"/BP/) are the reason of its motion as well as of its grows (together with accounting process of molecules evaporation from the BP's surfaces) can be presented as a stochastic process, or its superposition. Thus, a system of BPs is an example of an "open physical" system [5]. The theory of brownian motion gives us possibility to consider the many physical phenomena such as first order phase transition at initial stage when fluctuation of thermodynamic parameters are the reason of new phase nucleation (liquid drop among vapor molecules, gaseous bubble in lattice with solved vacancy and inert gas molecules et al.), The process of nucleation as the clustering of particle has been put forward by Ya. Zel'dovich [6] under assumption of the Gibbs energy of cluster formation weakly variable during time. This has been needed for the derivation of formula for rate nucleation. More later this theory has been developed using the abilities of computer simulation and the statistical theory of open systems. This required new ideas, new images and concepts: self-organization, synergetics, physics of open systems [7-10]. Larger role in the theory of open systems play a work A.M. Lyapunov - one of the founders of the theory of stability of motion, mathematics academician RAS A. N. Kolmogorov and many others [7,8]. Among the founders of the theory of self-organization one of place belongs, no doubt, L.Arnold [11] and its theory of stochastic dynamical systems which has been used in models of stochastic analogues of processes are caused by fluctuations in medium with condensation or coagulation . This method of computer simulation had been carried out during last decade [2,5,12].

Vacuum is maintained in reaction chamber during charged drops formation. The deposition of thin films is carried out with the help of the most modern vacuum technologies. Is spraying in order to give the product an additional strength, wear resistance, electrical conductivity, etc. But already today there are drawings and ideas of the device, which can radically change the process of spraying, making it a more economical and high-quality. Future technologies nano-spraying too, require uniform application of the film (e.g., metal), but the thickness of it will be a lot smaller, can be significantly increase the durability of the product without increasing its weight, using not only the metal particles. This is especially important for the space industry. Using nano-coating, will actually run reusable spacecraft in space, not once. Nano-spraying as long as it does not have the proper development, is a new word in the industry, and therefore is not used. Therefore the model of formation of nanoparticles, suitable for spraying, are in demand.

Nano-spraying as long as it does not have the proper development, is a new word in the industry, and therefore is not used. Therefore the model of formation of nanoparticles, suitable for spraying, are in demand. Computer simulation methodologies for Nanoscience will be available for objects of Cultural Heritage conservation and its restoration if tools borrowing from Nanoscience will be oriented

on deepening study origin of nanoparticles in plasma discharge, for estimation the number of emerging micro-crystals on the substrate or in the unit volume of the solution as well as a behavior of gels in a large number of applications.

2 Parameters of model of blistering simulation

The term ‘stochastic analog computer simulation' refers modeling of material on the base of molecular-kinetic theory of simulation of gas, plasma, liquid and solids using model its properties and behavior across length and time scales related with the atomistic sizes (parameter of crystal lattice) and duration diffusion into lattice comparable with time particles collision. Under consideration here are defects of lattices such as vacancy-gas bubbles, or blisters, its sizes are measured in unit volumes (masses) of gas molecule penetrating into lattice (or vacancy volume). Evolution of blisters sizes is presented as Marcov stochastic process named here «clustering», when individual collisions of gas particles with nucleus of bubble can be presented by model of diffusion in phase space of clusters sizes *{G}* takes into account postulates of kinetic theory of phase transformation " vapor - liquid" or similar them transition from gaseous particles distributed into lattice to state of " bubble(blister) into lattice" using the same collision process but without calculations each impact. The limitation of many models of materials (i.e. Molecular Dynamics /MD/) come from the limitation of computer power. Simulation MD integrate numerically Newton's law of motion for single atoms (or molecules) where M_i is the atom mass, r_i the position of atom i, and F_{ij}, the interatomic force between atoms i and j is interaction potential. Potential used in simulations range from the Lennard-Jones two body potential. In stochastic simulation approach each trajectory of stochastic process of clustering is not describes atom (or blister) site in the computer simulation box, it is not corresponds to the atomic positions which limit the size of this model box (in MD - approximately to 50 nm). Model based on theory of stochastic process allow us to calculate the mathematical expectation of clusters size and its site using the simulation parameters of nano (up to micro) scale systems over a realistic range of time, length, temperature as well as in multiple physical conditions and environments. This method is interested to apply in order to understand the redistribution of cluster in nanometer scale of model sample. The studying of a microstructural evolution at long times, where the size of each defect is bigger than the size of simulation box can be evaluate using constant velocity of clustering at the end of initial nonequilibrium stage of first order phase transition (or blistering) under action of inert gas beam. In recent years the phase transition model was largely used [13-27] and give us possibility to increase in the application of stochastic computational materials research using partially (or semi) implicit solvers of stochastic differential equations /SDE/which have been developed to deal with instabilities of numerical solution Ito-Stratonovich SDE effective solution. In the last decades this concurrent simulation models have been developed to reproduce the microstructural evolution of defects evolution in metals and dielectrics. The kinetic approach to calculation of the evolution nuclei of liquid as well idea to use model nucleation for microstructure in solid was firstly proposed in [24-26]. This approach

gives the probability density function of clusters on sizes on the fixed atomic positions of lattice. This model was successfully applied to describe many different phenomena like phase transitions in plasma of discharge and islands of melted drop of silicon carbide on the substrate of *Si(100)* [15,16,19,27]. For example, it has been used to explain many of the morphological evolutions in coherent solids islands including *Ge*- nuclei, crystallization for silicon carbide and many others. Despite the tremendous success of phase-transition modeling in predicting many of the experimentally observed microstructures in solids, additional progress is required in order to apply it to predict the microstructure evolution in real multi-component solid systems. For example, there exists no systematic approach for obtaining the thermodynamic and kinetic needed data to the phase-transition models although a number of efforts have been reported in connecting models with existing thermodynamic and kinetic databases. Space and time parameters of model are following: duration is approximately 10^{-4} s , linear substrate sizes are 100 nm × 100 nm, total substrate thickness is 64 nm, layers substrate thicknesses are 10 nm for *Mo* and 54 nm for *Si*, substrate temperature is from 600 to 1000 K, irradiation dose is $10^{14} \div 10^{17}$ cm^{-2}, Xe^{++} ions energy 5 ÷ 15 keV, temperature and supersaturation of *Xe* atoms into substrate are supposed constant, blister density is approximately $3.5 \cdot 10^{24}$ m^{-3}, *Si* lattice parameter 5.43Å, *Mo* lattice parameter 3.15Å, *Si* Young's modulus is $1.89 \cdot 10^{10}$ Pa, *Si* modulus of rigidity is $7.99 \cdot 10^{10}$ Pa, *Mo* Young's modulus is $3.29 \cdot 10^{11}$ Pa, *Mo* modulus of rigidity is $1.22 \cdot 10^{11}$Pa, *Si* fusion temperature is 1688K, *Mo* fusion temperature is 2890K. Scheme of numerical experiment looks like following:

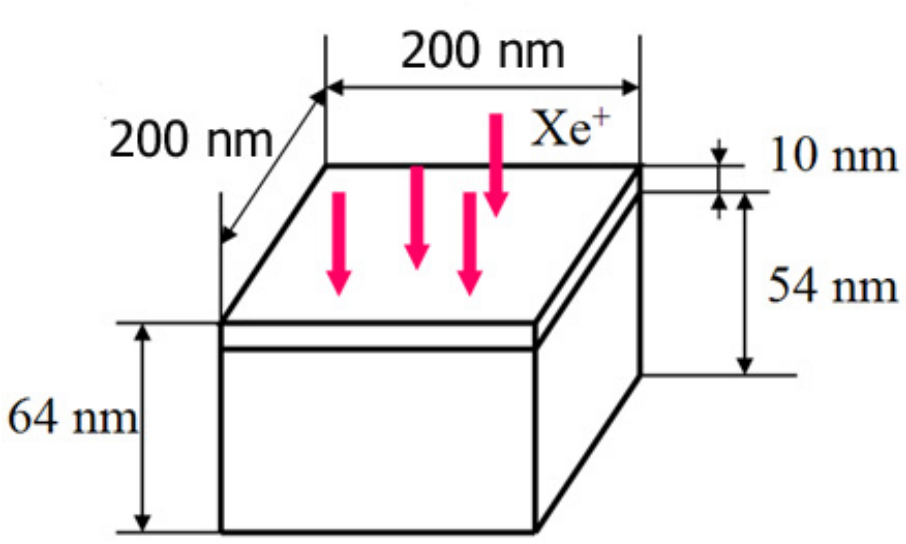

Fig. 1 Scheme of numerical experiment.

Characteristic time for blister size change is $\tau_g = \dfrac{a}{12\pi r_{Xe}^2 \beta(g) c_{Xe} D_0 e^{-Em/kT}} \approx 10^{-9} s$, where D_0 is diffusion coefficient of Xe atom into substrate, $D_0 = 1.8 \cdot 10^{-8}$ cm^2/s,

E_m=0.1 eV is the energy of migration of *Xe* atom into substrate, r_{Xe} ≈2.18 Å is *Xe* atom radius, k is Boltzmann constant, T is temperature of substrate, β is the coefficient of heterogeneous condensation on the surface of blister, c_{Xe} is *Xe* density in substrate.

Characteristic time for blister motion is $\tau_r = \frac{r_{Xe}^3}{D_{r0}a} \approx 1.06 \cdot 10^{-8}$ s, here a is lattice parameter of substrate material.

3 Kinetic and stochastic equations of model

Many problems of probability nature are described by statistical mechanics are also in good agreement with models governed by Fokker-Planck-Kolmogorov equation. This process can be complemented by clusters Brownian motion. First-order phase transition at fluctuation stage into non-linear dissipative "plasma-like" media is considered. The clustering of new phase's germs (or nucleation) is represented by stochastic Wiener processes. Brownian motion of clusters induced by long-range potential of indirect (through acoustic phonons and Friedel's oscillations of electron density) interaction between themselves is taken into account. For solution of quasilinear kinetic equations (Fokker-Planck-Kolmogorov and Einstein-Smolukhovskii [11,28]) are used new, stable and effective, computer simulation method.

Kinetic model of nucleation is based on both: the concept of particle's clustering/ blisters which leads to PT and clusters Brownian motion which is produced by the long-range potentials of clusters indirect elastic interaction due to acoustic phonons of substrate lattice. Mathematical model of diffusion MP into phase space of cluster sizes sufficiently well described by Kolmogorov-Feller equation and its computer simulation. Stochastic process (which is the solution of the Ito SDE with unique existence) satisfies the backward Kolmogorov equation [1] which is uniquely related with SDE Ito in Stratonovich form. We are able to interpret solution SDE in term of probability density of stochastic processes or another way of a distribution function /DF/ of partial differential kinetic equation. The same problem can be applied to Brownian motion /BM/ and Wiener stochastic processes SSM. The clustering of nuclei and its Brownian motion (in terms of clusters DF) are depending on set of stochastic dynamical variables, such as cluster's size and its coordinates in configuration phase spaces.

The model of microporous substrate formation includes the defects formation which are distributed by its size, their migration in the layers of the substrate nanometer thickness, the accumulation of defects and tension in a lattice model, which should be measured by the nonequilibrium distribution functions of clusters defects in size and coordinates. The solubility of inert gases in the materials are extremely small. So, xenon, injected into materials under ion implantation, has the tendency to the formation of gas pores in metals and dielectrics, in crystalline and amorphous materials. Vacancy-gas pore (blister) formation, its grow or degradation and its migration into layers of substrate are considered as fluctuation stage of first

phase transition. Blister is considered as a Brownian particles /BPs/ with spherical shapes and variable masses. Blisters into metal and silicon layers interact by the perturbation of acoustic phonons and Friedel oscillations of the electrons in the metal lattice. The coordinate of the BP center of masses changes under the effect of the total potential of the elastic interaction between BPs, external and internal surfaces of the substrate, and crystal lattice defects of the dislocation type and grain boundaries. Kolmogorov kinetic equation is written for BP. Different characteristic time periods of blister nucleus clusterization (10^{-9} s) and Brownian motion (10^{-8} s) allowed us to divide the problem into physical processes and present each kinetic equation by its stochastic analog.

The total form of kinetic Fokker-Plank-Kolmogorov equation is

$$\begin{cases} \dfrac{\partial f(X,t)}{\partial t} = -\sum\limits_{i=1}^{N} \dfrac{\partial}{\partial X_i} a_i^{\alpha}(X,t) f(X,t) + \dfrac{1}{2} \sum\limits_{i=1}^{N} \sum\limits_{j=1}^{N} \dfrac{\partial^2}{\partial X_i \partial X_j} b_{ij}^{\alpha}(X,t) f(X,t) + S_{\alpha} - Q \\ f(X,t)\big|_{t=0} = f_0(X) \\ \oint \left[a_i^{\alpha}(X,t) f(X,t) + \dfrac{1}{2} \sum\limits_{j=1}^{N} \dfrac{\partial}{\partial X_j} b_{ij}^{\alpha} f(X,t) \right] d\Gamma = 0, \qquad i = 1,...m \end{cases} \tag{1}$$

where Γ is the boundary of all possible values of the Markovian random process, $a_i^{\alpha}(X,t)$ is the drift vector and $b_{ij}^{\alpha}(X,t)$ is the diffusion matrix, which are functionals of MP distributions, should be limited and sufficiently smooth. The functionals $a_i^{\alpha}(X,t)$ and $b_{ij}^{\alpha}(X,t)$ entering the equation have the meaning of meansquare limits in time $\Delta t \to 0$ of the conditional expectation of increment of MP coordinates $\{X(t),\ t \geq 0\}$: $\Delta X(t) = X(t + \Delta t) - X(t)$ (this is $a_i^{\alpha}(X,t)$) and conditional dispersion - $b_{ij}^{\alpha}(X,t)$. S_{α} is source of particles forming a nucleus and Q is monomers and blister drains.

The stochastic analog of Fokker-Plank-Kolmogorov equation is

$$X(t) = X(t_0) + \int_{t_0}^{t} \underbrace{H(\tau, X(\tau))d\tau}_{drift} + \int_{t_0}^{t} \underbrace{\sigma(\tau, X(\tau))}_{stochastic\ diffusion} dW(\tau), \tag{2}$$

$$X\big|_{t=0} = X_0 \quad t \in [t_0, T_{end}]$$

where X is the stochastic dynamical variable, accounting in (1) diffusion and jump-like part . *dW(t)* is increment of Wiener stochastic process, which is used in model of nuclei clustering as well in BM description. X_{coll} is jump-like stochastic process contribution into superposition of processes in (1). The consideration of chemical reactions can be calculated using point-vise. The functionals $H(\tau, X(\tau))$ and $\sigma(\tau, X(\tau))$ should be limited and smooth. $H(\tau,X(\tau))$ and $\sigma(\tau,X(\tau))$ are nonanticipating functionals of the Markov Process.

The relation between coefficients of Fokker–Planck–Kolmogorov equation and coefficients of the SDE is follows:

$$a_i = \underset{\Delta t \to 0}{l.i.m.} \frac{1}{\Delta t} \mathrm{E}\left[X(t+\Delta t) - X(t) \middle| X(t) = x\right]$$
$$b_{ij} = \underset{\Delta t \to 0}{l.i.m.} \frac{1}{\Delta t} \mathrm{E}\left[\left[X(t+\Delta t) - X(t)\right]^2 \middle| X(t) = x\right] \quad (3)$$

and in the one-dimensional case, the H and σ coefficients take the form

$$H(E(X),t) = a_i(E(X),t) - \frac{1}{4}\frac{\partial b_{ij}(E(X),t)}{\partial X}, \quad (4)$$
$$\sigma(E(X),t) = \frac{1}{q}\sqrt{b_{ij}(E(X),t)},$$

here q is white noise intensity. The solution can be simplified by replacing the Wiener process with white noise only if the Ito SDE takes the Stratonovich's form.

The Kolmogorov–Feller equation for blister size/ particle's clustering evolution at the point with the coordinate **r** has the form

$$\partial f_r(g,t)/\partial t = \partial\left(D_g(g,t)\cdot\left(\partial f_r(g,t)/\partial g\right)\right)/\partial g + \frac{1}{kT}\partial\left(D_g(g,t) f_r(g,t)\cdot\left(\partial\Delta\Phi(g,\vec{r},t)/\partial g\right)\right)/\partial g + S_\alpha, \quad (5)$$
$$f_r(g,0)=f_{0g}, \quad df_r(g,t)/dg|_{g=2}=0, \quad f_r(g,t)|_{g<2}=0, \quad g>2$$

here $f_r(g, t)$ is the size distribution functions /DFs/ of nuclei at the point **r** of the lattice volume; D_g is the diffusion coefficient in the phase space of nucleus sizes; $\Delta\Phi(g, \mathbf{r}, t)$ is the thermodynamic potential of the nucleus formation, $\Delta\Phi$ is measured in kT.

$D_g = D_{g0} g^{2/3}$, $D_{g0} = a^2/\tau_g$

The Einstein–Smoluchowski equation for BPs with the mass M_g has form:

$$\frac{\partial f_g(\vec{r},t)}{\partial t} = \frac{\partial\left[D_r(\vec{r},t)\dfrac{\partial f_g(\vec{r},t)}{\partial r}\right]}{\partial\vec{r}} - \frac{\partial\left[\dfrac{\vec{F}(\vec{r},t)}{M_g\gamma} f_g(\vec{r},t)\right]}{\partial\vec{r}} - Q,$$
$$f_g(\vec{r},t)|_{t=0} = f_{0r},$$
$$f_g(\vec{r},t)|_{x=x_{\text{left}}} = f_g(\vec{r},t)|_{x=x_{\text{right}}}, \quad f_g(\vec{r},t)|_{y=y_{\text{left}}} = f_g(\vec{r},t)|_{y=y_{\text{right}}}, \quad (6)$$

here $f_g(\mathbf{r}, t)$ is the distribution function of a BP with mass M_g over the substrate lattice coordinates, M_g is calculated for each time t from Eq. (5) and it is measured in vacancy mass for blistering and in in silicon mass for *SiC* clusters formation. Such, for blistering $M_g = g_{atom}\cdot m_{at} + 0.8\cdot m_{sub}\cdot g_{vac}$, where m_{at} is mass of injected gas atom, m_{sub} is mass of substrate lattice atom. In common case total blisters mass can be written as $M_{bl} = \frac{4\pi}{3}\rho\int\frac{\partial f}{\partial g} g^3 dg$, where ρ is density of gas/vacancies in blister. Q is cluster drain. Monomers and blisters/clusters drains locate on grains boundaries, dislocation and others lattice defects, γ is friction coefficient.

$F_x = -\frac{\partial U(x,\ y,\ z)}{\partial x}$, where $U(x, y, z)$ is the superposition of potentials of the indirect elastic interaction of BPs through the crystal lattice factors.

3.1 The thermodynamic potential of the nucleus formation in problem of computer simulation of structure of porosity in solids

The change of thermodynamic potential of the nucleus formation (change of Gibbs energy) $\Delta\Phi$ can be presented as:

$$\Delta\Phi(g,\mathbf{r},t) = -(a_\Phi - c)\cdot(g_{atom} + g_{vac}) + b\cdot(g_{atom} + g_{vac})^{2/3} + \Delta\Phi_r - \Delta\Phi_{break} + \Delta\Phi_d, \quad (7)$$

In common case blister contains gas atoms and untied vacancies if vacancies into blister are more than gas atoms into it. So, g_{vac} is number of untied vacancies in blister and g_{atom} is number of atoms in blister. a_Φ is the difference of chemical potentials of the phases (gas in the form of injected atoms and a blister); the coefficient $b = \eta\cdot\sigma_{bl}$; σ_{bl} is the surface tension at the bubble–lattice interface; η is form factor, and c is the elastic reaction of the lattice to the nucleus formation. $c = 2\mu^\alpha \cdot \frac{3K}{3K+4\mu^\alpha}\cdot\frac{(V_{sub}-V_{gas})^2}{3V_{gas}}$ where μ^α - modulus of rigidity of substrate material, K – modulus of condensability of substrate material, V_{sub} – volume on atom of substrate material, V_{gas} – atom volume of irradiating material. c is small for brittle material (*Si*), c for *Si* is less than c for elastic material (*Mo*).

When blister grows it can break several lattice bonds at same time, it is taken into account in $\Delta\Phi_{break}$ If $\frac{\Delta\Phi}{N_b\Delta_{break}} = n_{br}$, where Δ_{break} is the energy of one bond rupture (1.76 eV for *Si*, and ~2 eV for *Mo*), and N_b is the number of bonds at one lattice site (14 for *Si* and *Mo*), n_{br} is integer number, $n_{br}\geq 1$ that $V_{blister} = V_{blister} + 14\cdot V_{vac}$, where $V_{blister}$ is blister volume, V_{vac} is vacancy volume. V_{vac} is approximately 0.8 volume substrate atom for diamond-like face-centered cubic lattice and body-centered lattice. i.e. the volume of blisters increases in the volume of vacancies which generate when lattice bonds were broken. The pressure inside the blisters abruptly decreases when lattice bonds were broken.

$\Delta\Phi_d$ is part of change of Gibbs energy corresponding tensions field (for example, tension corresponding discrepancy between lattices *Mo* and *Si*). In common case it can be written:

$$\Delta\Phi_d = \mu(U_{ik} - \frac{1}{3}\delta_{ik}U_{ll})^2 + \frac{K}{2}U_{ll}^2,$$
$$K = \frac{E}{3(1-2\delta)},\quad \mu = \frac{E}{2(1+\delta)},\quad -1 < \delta < 0.5, \quad (8)$$

where δ is Poisson's ratio, K is compression modulus, μ is modulus of rigidity (modulus of compression and shift), E is Young's Modulus, U_{ik} is deformation tensor, U_{ll} is the amplitude of deformation, δ_{ik} is Kronecker symbol, $\delta_{ij}=\begin{cases}1, & i=j,\\ 0, & i\neq j\end{cases}$

The difference between lattice points and interstices are taken into account in $\Delta\Phi_r$:

$$\Delta\Phi_r=\frac{\Psi_r}{\sqrt{g}}\left[k_x\cos(2\pi(x-\varphi_x))+k_y\cos(2\pi(y-\varphi_y))+k_z\cos(2\pi(z-\varphi_z))\right] \quad (9),$$

here k_x, k_y, k_z, φ_x, φ_y,φ_z, Ψ_r are lattice parameters.

3.2 Thermodynamic potential of the nucleus formation in problem of computer simulation of islands liquids droplets and clusters of crystallization accumulated on substrate

Two series of calculation were used:

1. charged melted drops with gradual change of drops compositions from *Si* to *SiC*, finish C composition in *SiC* were different. Motion of charged melted drops in plasma discharge are not examined;
2. *SiC* drops precipitation on *Si(100)*. Drops segmentation and sputtering of its part are not taken into account during precipitation. Drops velocity are supposed zero when its precipitates on *Si(100)*. Substrate temperature is less vapor temperature on 300K. Neutralization and clusterization with polytypic discrimination are taken into account after precipitation on *Si(100)*. Model of instantaneous cooling of *SiC* nuclei on *Si(100)* is assumed. Results of calculations of charged melted drops (DF of drops from its sizes) are initial data for calculation of *SiC* nuclei development on substrate surface. We taken into account that different polytypes have different unit volumes and accordingly different values of coefficients in equation of change of Gibbs energy. Correlation factors will be taken into account in future.

For each mentioned model of PT the change of Gibbs energy has form:

$$\Delta\Phi=\begin{cases}\Delta\Phi_{\text{vol}}+\Delta\Phi_{\text{surf}}+\Delta\Phi_z+\Delta\Phi_{\text{ch}}=\Delta\Phi_{drop} & \text{melted spherical drops in plasma discharge}\\ \Delta\Phi_{\text{vol}}+\Delta\Phi_{\text{surf}}+\Delta\Phi_r=\Delta\Phi_{am} & \text{amorphous clusters on solid surface}\\ \Delta\Phi_{\text{vol}}+\Delta\Phi_{\text{surf}}+\Delta\Phi_r+\Delta\Phi_{\text{edge}}+\Delta\Phi_{\text{edge el.}}=\Delta\Phi_{cr} & \text{crystal nucleus}\end{cases} \quad (10)$$

where $\Delta\Phi_{\text{vol}}=-a_\Phi g$ is connected to the difference between chemical potential of vapor and melt phase, vapor and crystalline and other, $\Delta\Phi_{\text{surf}}=bg^{2/3}$ is connected to the change in the surface free energy of the system, $\Delta\Phi_z=cg^{-1/3}$ corresponding with charge on SiC melted drops in plasma (or ionized gas). The drop charge can be written as $Q=-\frac{kT_e r_d}{e^2}\ln(1+\frac{K_e}{K_i})$ [23], here α is electron or ion, f_α is DF of electrons

or ions, v is velocity of electron or ion, S is surface square of particle, m_α is mass of electron or ion, Q_d is drop charge, T_d is drop temperature, e_α is charge of electron or ion, k is Boltsman constant, T_e is electrons temperature, r_d is drop radius, K_e is mobility of electrons, K_i is mobility of ions. The charge density on *SiC* melted drops is assumed constant.

The change of chemical composition of nuclei in presented model is considered as additive part in change of Gibbs energy accounted as $\Delta\Phi_{ch} = -a_{chem} g^{2/3}$ and change of a_Φ and b, chemical reactions are taken into account as equilibrium process that is $a_{chem} = kT \cdot \ln \frac{K_{ch}}{K_{ch}^{eq}}$, here T is temperature of surface of nuclei, K_{ch} is constant of chemical reactions, K_{ch}^{eq} is equilibrium value of constant of chemical reactions.

Dependence of the thermodynamic potential of the nucleus formation for melted spherical drops in plasma discharge from drop size g for several charges of drops is presented on Fig. 2.

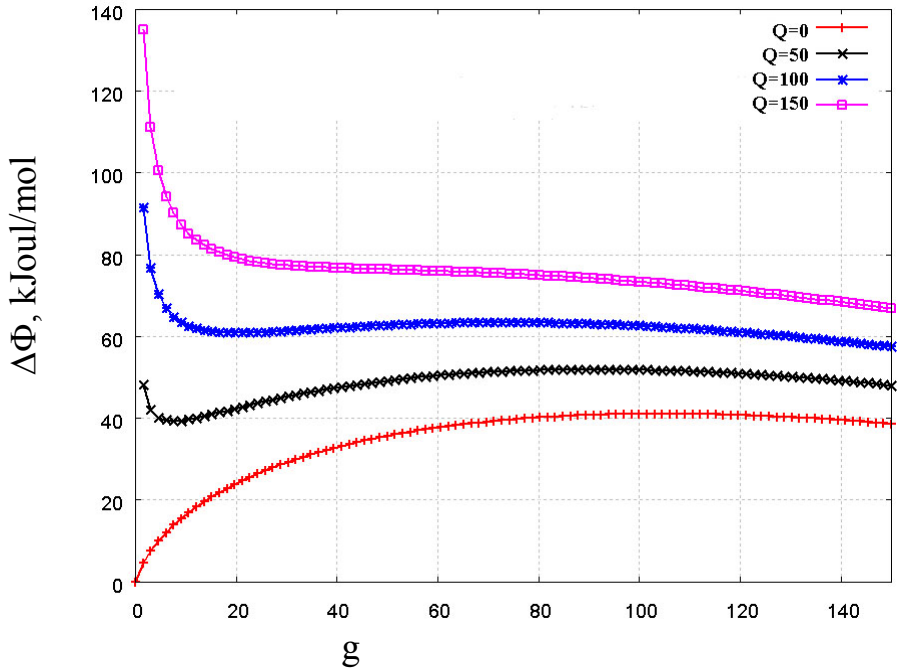

Fig.2 Dependence of the thermodynamic potential of the nucleus formation for melted spherical drops in plasma discharge from drop size g for several charges of drops is presented. g is size of cluster, g is measured in number of *Si* and *C* atoms in cluster. Q is drop charge. Q is measured in in $1.6 \cdot 10^{-16}$ coulomb.

Stability of melted drops to large deformations is determined by the Rayleigh condition:

$e^2 Q^2 < 17.65 \cdot r_d^3 \sigma$, here Q is drop charge, r_d is drop radius, σ is the surface tension of material drops. Taking into account that the surface tension of silicon $\sigma_{si}=763 \cdot 10^{-3}$ H/m, the surface tension of silicon carbide $\sigma_{si}=740 \cdot 10^{-3}$ H/m we can write stability condition as $Q < 3.46 \cdot 10^4 \cdot g$.

The differences between the energies of nucleus formation over the site or interstice of the substrate lattice are accounted by

$$\Delta\Phi_r = \frac{\Psi}{\sqrt{g}}\left(2-\cos\left(\frac{2\pi x}{a_x}\right)-\cos\left(\frac{2\pi y}{a_y}\right)\right) \qquad (11)$$

The short-range contribution of edges to the Gibbs energy $\Delta\Phi_{edge}=d_1\, g^{1/3}$ also has an effect on the crystal cluster formation. The contribution of cluster edges to the elastic relaxation energy is given by $\Delta\Phi_{edge}=-d_2\, g^{1/3} ln(g)$.

Change of Gibbs energy of melted drops and unit volume corresponding different *SiC* polytypes are governing factor in presented model of development of *SiC* nuclei on substrate surface.

If at precipitation time $\Delta\Phi_{drop}\geq\Delta\Phi_{hexag}$ and $\Delta\Phi_{3C\text{-}SiC}\geq\Delta\Phi_{hexag}$ that hexagonal nuclei form on solid surface, $\Delta\Phi_{drop}\geq\Delta\Phi_{3C\text{-}SiC}$ and $\Delta\Phi_{hexag}\geq\Delta\Phi_{3C\text{-}SiC}$ that *3C-SiC* nuclei format on solid surface, if $\Delta\Phi_{drop}<\Delta\Phi_{3C\text{-}SiC,hexag}$ that amorphous clusters format. Here $\Delta\Phi_{drop}$ is change of Gibbs energy for melted spherical drops in plasma discharge, $\Delta\Phi_{am}$ is change of Gibbs energy of amorphous nucleus on solid surface, $\Delta\Phi_{3C\text{-}SiC}$ is change of Gibbs energy for *3C-SiC* on solid surface, $\Delta\Phi_{hexag}$ is change of Gibbs energy for hexagonal nuclei form of *SiC* on solid surface. Amorphous germs have globe calotte forms with wetting angle according to Yung law.

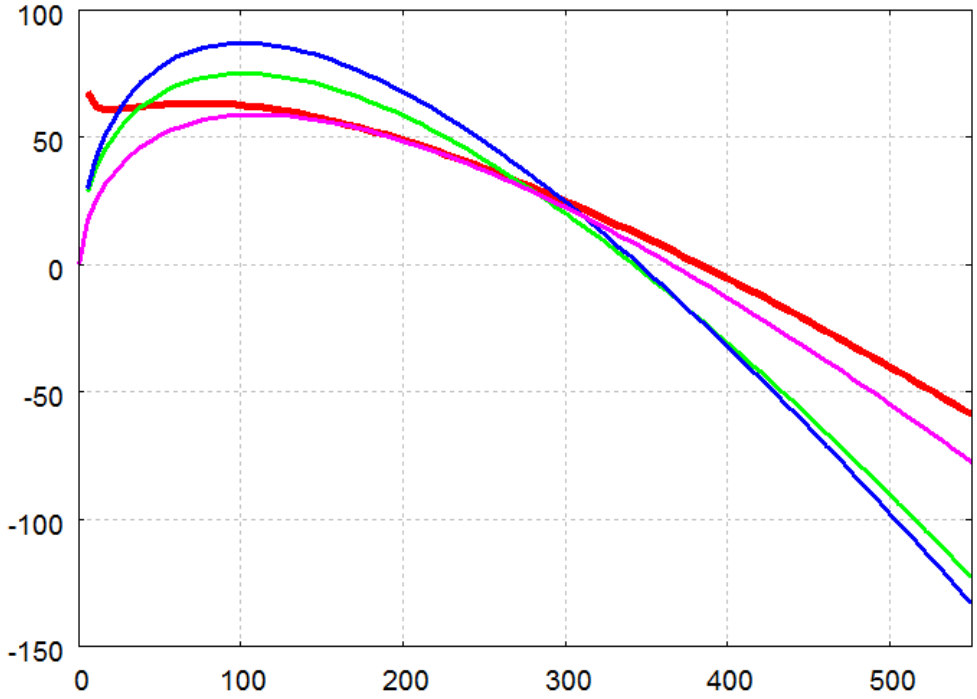

Fig. 3 Change of Gibbs energies for different cases are presented using color visualization: red line corresponds $\Delta\Phi_{drop}$ (change of Gibbs energy for melted spherical drops in plasma discharge), violet line corresponds $\Delta\Phi_{am}$ (change of Gibbs energy of amorphous nucleus on solid surface), green line $-\Delta\Phi_{3C\text{-}SiC}$ (change of Gibbs energy for *3C-SiC* on solid surface), blue line - $\Delta\Phi_{hexag}$ (change of Gibbs energy for hexagonal nuclei form of *SiC* on solid surface).

If silicon carbide nuclei format on sloping surface, then Gibbs energy can be written as $\Delta\Phi_\alpha = \Delta\Phi/(1+\sin\alpha)$, here $\Delta\Phi_\alpha$ is Gibbs energy for *SiC* formation on sloping surface, $\Delta\Phi$ is Gibbs energy for *SiC* formation on surface without slope, α is inclination of plane. Comparison of Gibbs energy for *SiC* formation on sloping surface ($\Delta\Phi_\alpha$) and Gibbs energy for *SiC* formation on surface without slope ($\Delta\Phi$) is presented on fig.2. for inclination of plane from 0 to $\pi/2$. As can see from fig. 4 influence of slope angle decreases with nuclei sizes increase.

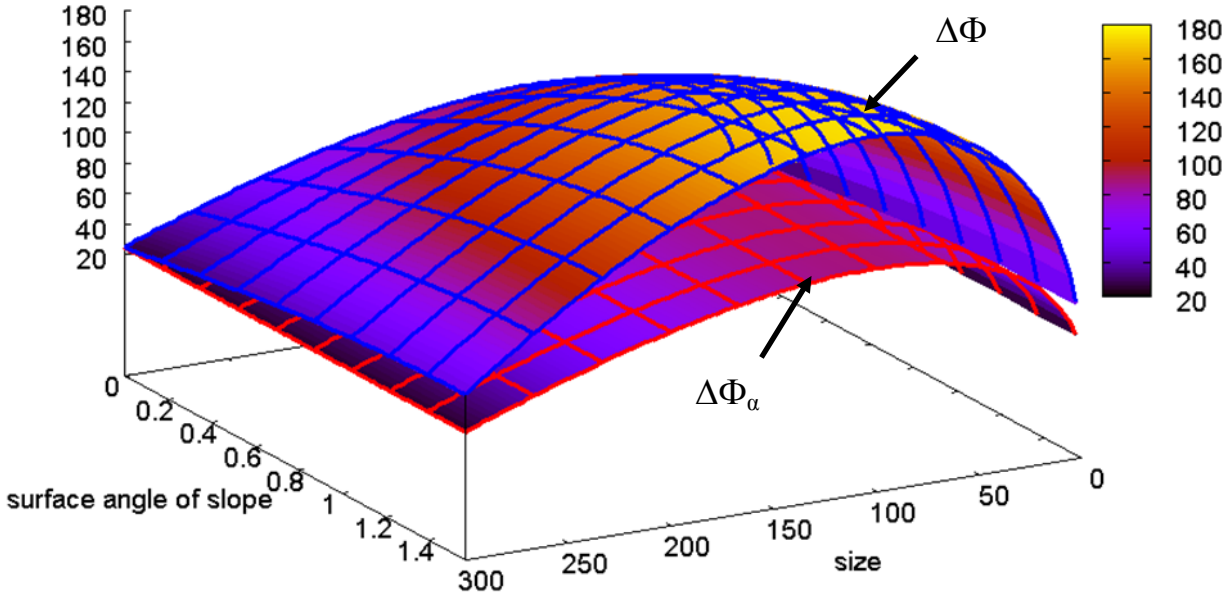

Fig. 4 Comparison of Gibbs energy for *SiC* formation on sloping surface ($\Delta\Phi_\alpha$) and Gibbs energy for *SiC* formation on surface without slope ($\Delta\Phi$) is presented for inclination of plane from 0 to $\pi/2$.

3.3 The potential of long-range interaction on the example of blisters interaction

The potential $U(x, y, z)$ is long-range and sign-variable; interaction occurs through the perturbation of the lattice acoustic phonons and Friedel oscillations of the lattice electron density. In common case, indirect elastic potential can be written as:

$$U(\mathbf{r}) = U_{ij}(\mathbf{r}) + U_{\text{surf}}(\mathbf{r}) + U_{\text{ph}}(\mathbf{r}) + U_{\text{pore}}(\mathbf{r}); \quad (12)$$

Here $U_{ij}(\mathbf{r})$ corresponds to an indirect interaction of blisters with each other;
$U_{\text{surf}}(\mathbf{r})$ corresponds to the blister interaction with all surfaces of the layered structure (the interaction mechanism is the same), including the irradiated surface;
$U_{\text{ph}}(\mathbf{r})$ corresponds to the interaction with lattice defects of the dislocation type and grain boundaries;
$U_{\text{pore}}(\mathbf{r})$ is the potential of the blister–pore interaction for porous materials.
The interaction with pores must be taken into account only inside one porous *Si* layer. The condition $U|_{Mo} - U|_{Si} = \Delta U < U|_{Mo}, U|_{Si}$ is satisfied between *Mo* and *Si* layers. For example, the blister–blister interaction potential similarly to the potentials deduced in [29-32], is presented:

$$U_{ij}(x,y,z)=\sum_{i\neq j}^{N} M_{gi}\left[\underbrace{\frac{b_r\left[\frac{3}{5}-\frac{(x_i-x_j)^4+(y_i-y_j)^4+(z_i-z_j)^4}{(\vec{r}_i-\vec{r}_j)^4}\right]}{|\vec{r}_i-\vec{r}_j|^3}}_{\substack{\text{Interaction through the perturbation of}\\ \text{lattice acoustic phonons}}}+\underbrace{\frac{a_r\cos(c_r|\vec{r}_i-\vec{r}_j|)}{|\vec{r}_i-\vec{r}_j|^3}}_{\substack{\text{Interaction through}\\ \text{Friedel oscillations}\\ \text{of the lattice electron density}}}\right] \quad (13)$$

where i,j are numbers of interacting blisters if we have numerate them from 1 to N, M_{gi} is the BP mass and b_r, a_r,and c_r are lattice model parameters of the respective layer. The blister–blister interaction is much weaker than the blister–boundary interaction.

2D projection of equal potential (blister-blister) values as surface U(x,y=const,z) in *Si* and *Mo* layers for $y=0$ is presented on fig. 5. Temperature is 900 K, irradiation dose is $3\cdot10^{16}$ cm^{-2}, the ions Xe^{++} flow is directed on the normal to the surface.

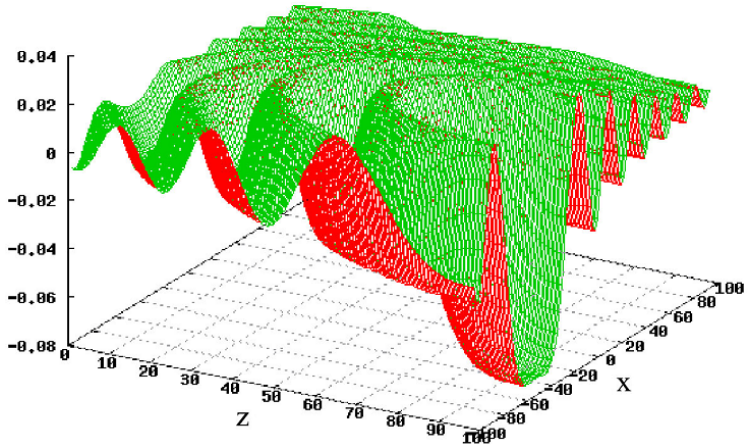

Fig. 5. 2D projection of equal potential (blister-blister) values as surface U(x,y=const,z) is presented for y=0. The value of potential is presented in dimensionless units. X and z is measured in lattice parameters of Si.

Diffusion coefficient in space of substrate lattice for one of coordinate can be written as

$$D_x=\begin{cases}\dfrac{D_0e^{-E_m/kT}}{\gamma M_g}(1+\alpha_x(x-x_{ins})^2) & if \quad |x-x_b|>|x_b-R_b|+\Delta_b\\ A_r\dfrac{D_0e^{-E_m/kT}}{\gamma M_g}(1+\alpha_x(x-x_{ins})^2) & if \quad |x-x_b|\le|x_b-R_b|+\Delta_b\end{cases}, \quad (14)$$

where x is coordinate of mass center of blister; x_{ins} is coordinate of nearest interstice, γ is friction coefficient, x_b is coordinate of the internal boundary layers or coordinate of grain boundaries, $\Delta_b \approx 3$ is model parameter measured in lattice parameters of substrate a=5.43 Å for *Si*. $R_b=r_{Xe}\sqrt[3]{g}$ is blister radius.

4 Numerical scheme for solution of system of Ito-Stratonovich SDEs

Numerical method of non-linear SDE solution is based on Taylor series expansion of exact solution of Ito SDE X(t+ Δt) [33-36].

For the *i*-th trajectory of the diffusion Markovian random process, the values of g_{n+1} and, for example, z_{n+1} the instant $n+1$ are calculated using these formulas

$$g_{n+1}^i = g_n^i + \left[I - \frac{h}{2}\frac{\partial H_n^i}{\partial g} \right]^{-1} \left[hH_n^i + \sqrt{h}\sigma_{ng}^i \xi_{ng} + \frac{h}{2}\frac{\partial \sigma_{ng}^i}{\partial g}\sigma_{ng}^i \xi_{ng}^2 \right],$$

$$H_{ng}^i = -\frac{1}{kT} D_g^i\left(g_n^i, t_n\right)\frac{\partial \Delta\Phi^i\left(g_n^i, x_n^i, y_n^i, z_n^i, t_n\right)}{\partial g_n^i} - \frac{1}{2}\frac{\partial D^i\left(g_n^i, t_n\right)}{\partial g_n^i}, \qquad (15)$$

$$\sigma_{ng}^i = \sqrt{2D_n^i\left(g_n^i, t_n\right)}.$$

$$\begin{cases} z_{n+1}^i = z_n^i + \left[I - \dfrac{h_z}{2}\cdot\dfrac{\partial H_{zn}^i}{\partial z_i} \right]^{-1} \left[hH_{zn}^i + \sqrt{h_z}\sigma_{zn}^i \xi_{zn} \right], \\ H_{zn}^i = \dfrac{1}{M(g_{n+1}^i)\gamma}\cdot\dfrac{\partial U^i(x_n^i, y_n^i, z_n^i)}{\partial z} - \dfrac{1}{2}\dfrac{\partial D_{zn}^i}{\partial z}\xi_{zn}^2, \\ D_{zn}^i = D_{z0}(1+\alpha(z_n^i - z_{its}^i)^2), \\ \sigma_{zn}^i = \sqrt{2D_{zn}^i}, \end{cases} \qquad (16)$$

where I is the unit matrix, g_n^i is the solution to SDE at the grid point, which corresponds to the time t_n and trajectories i, z_{its} is the coordinate of the nearest lattice interstice, h is the constant steps in the algorithm time for calculating the nucleus size evolution equals characteristic time for blister size change and h_z is the constant steps in the algorithm time for calculating the nucleus motion in the substrate space equals characteristic time for blister migration. Set ξ_n is normally distributed independent random number of the succession, with zero mathematical expectation and unit dispersion. $\xi_n = \sqrt{-2\ln\alpha_1}\cos(2\pi\alpha_2)$, where α_1 and α_2 are random numbers uniformly distributed in the interval (0,1). The resulting system of four interconnected SDEs in Ito-Stratonovich form is solved using a modified method having a second-order (or higher) accuracy [37]. Every step of time functional-coefficients of problem are iterated taking account data about DF on previous step of time.

The mathematical expectation of average size at time moment t is $\langle g \rangle(t) = \frac{1}{N}\int_G f(g,t)g dg$.

Total number of blisters is $N = \int_G f(g,t)dg$, $\{G\}$ is region of phase space of blister sizes.

5 Results of numerical simulation of fluctuation stage of high-temperature blistering

Porosity as roughness of same sections of substrate will be examined below. Blisters and its long-size structures, which are perpendicular Xe^{++} ions flow and located on *Mo/Si* surface, will determining for surface rougness after *Mo* layer peeling.

Results of stochastic simulation *Mo/Si* bilayer with *Si* width 100 lattice parameters and *Mo* width 30 lattice parameters are presented on fig. 5-7. Energy of Xe^{++} is 7 keV, temperature is 900 K, irradiation dose is 10^{16} cm^{-2}, the ions Xe^{++} flow is directed on the normal to the surface.

Color visualization of blisters DF in g0z plane is presented on fig. 6. Blister size is measured in Å, z is depth from surface under irradiation and it is measured in Å. Initial blister size g=40 unit *Xe* atom volumes. DF is normalized by 1. 10^5 trajectories are used. Values of DF corresponds color palette. The profile of concentration of interstitial *Xe* atoms is presented on fig.5 by white line and it has maximums on depth of projected run of *Xe* in *Si* and near *Si/Mo* surface. Model terms of the ratio of bandwidth-reflection-absorption on surface are used on boundary between *Mo* and *Si*.

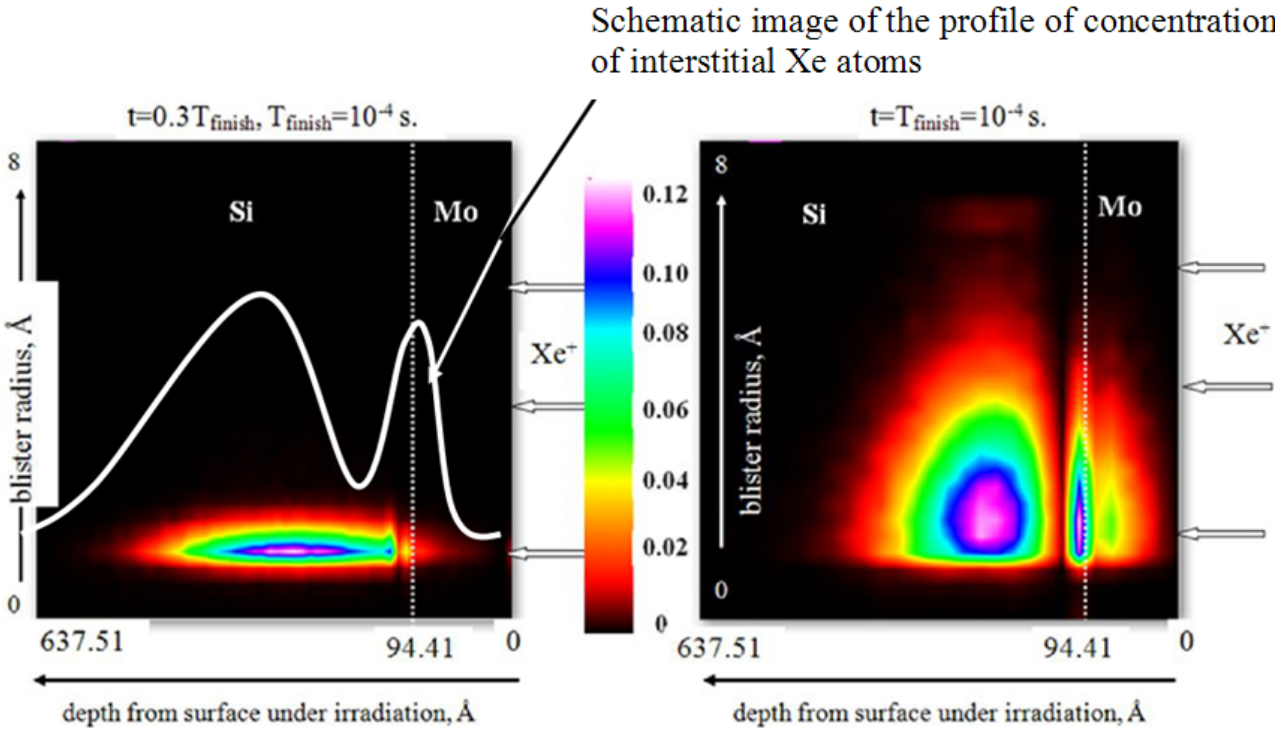

Fig. 6. Color visualization of blisters DF averaged for the x and y coordinates from blister size and it depth from surface under irradiation is presented at two time moments: 0.3 duration of fluctuation stage and at finish of calculation.

Macroscopic characteristics were calculated using DFs: porosity of layers of substrate and stress in substrate layers.

The layer porosity with z-coordinate z_j can be calculated as:

$$p(z_j,t)=\frac{V_a}{V_l}\frac{\sum_{i=1}^{N} g_i^3 f(g_i,z_j,t)}{\sum_{i=1}^{N} g_{0i}^3 f(g_0)} \qquad (17)$$

V_a is total examined volume, V_l is layer volume, N is number of blister, g_0 is initial blister size in number Xe in blister, $f(g_0)$ is initial distribution function from blister sizes, g_i is size of blister at examined time moment, $f(g,z,t)$ is distribution function at examined time, z is distance between surface under irradiation (*Mo* surface) and centre of blister, z is measured in lattice parameter, z=0 is surface under irradiation.
Stress corresponding with bubbles in some sections of substrate is presented on fig.6.
For example, and stress in j-layer of *Si* is calculated by

$$\sigma_j=3.8\times10^8\times\int\left(\sum_i\left(\frac{0.33\ln(<g_i>)-0.1}{\left((x-x_i)^2+(y-y_i)^2+(z-z_i)^2\right)^{3/2}}\langle g\rangle_i^{2/3}\right)+\sum_i\left(\langle g\rangle_i^{2/3}(0.33\ln(<g_i>)-0.1)\right)\right)dxdydz,\quad Pa. \qquad (18)$$

i=1…N,
and stress in j-layer of *Mo* is calculated by:

$$\sigma_j=2.435\times10^9\times\int\left(\sum_i\left(\frac{0.33\ln(<g_i>)+0.57}{\left((x-x_i)^2+(y-y_i)^2+(z-z_i)^2\right)^{3/2}}\langle g\rangle_i^{2/3}\right)+\sum_i\left(\langle g\rangle_i^{2/3}(0.33\ln(g_i)+0.57)\right)\right)dxdydz,\quad Pa. \qquad (19)$$

where N is number of trajectories of stochastic process X(t), $<g_i>$ is expectation of blister size decided on previous size time step using DF of blisters solution of a problem (5) - (6).
Porosity and stress in layers of substrate averaged for x and y coordinates are presented on fig. 7 and fig. 8 at finish of calculated (10^{-4} s). Number of trajectories is 10^6. Depth from surface under irradiation of porosity maximum is 295 Å. Values and location of maximums of porosity and stress can be changed by change of thickness of Xe^{++} flow regulator (*Mo* in presented case).

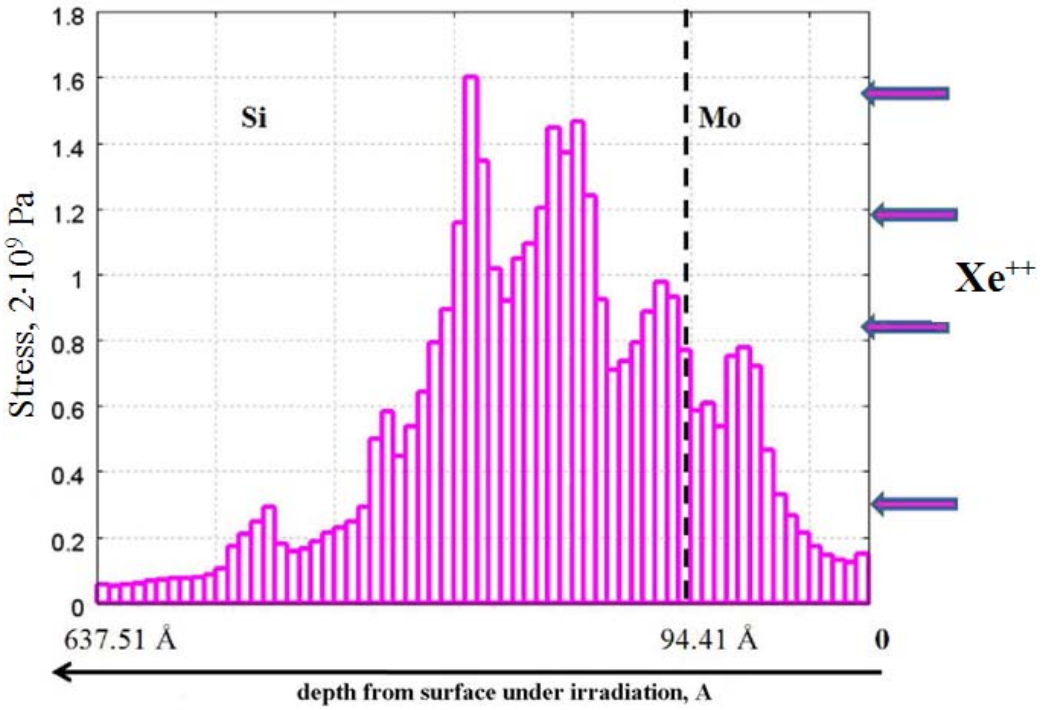

Fig. 7. Stress in layers of substrate averaged for x and y coordinates is presented.

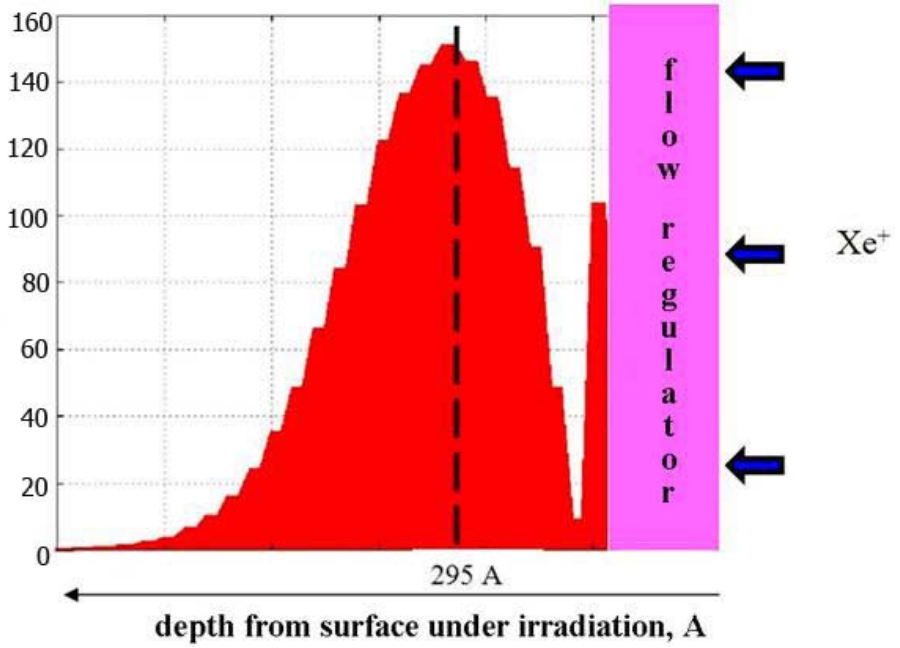

Fig. 8 Ratio of layer porosity from total porosity of all substrate at initial time moment is presented.

Illustration of porosity into layers and long-size structure defects formation is presented on fig.9. Temperature is 900K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}. Black color corresponds porosity and green color lack of porosity in this point. Formation of porosity layer perpendicular to irradiating stream and formation of cracks along irradiating stream are observed.

For fig. 9-18 substrate consists of *Mo* layer (width is 30 lattice parameters a_{Mo}=3.147 A) and *Si* crystal (width is 100 lattice parameters a_{si}=5.431 A). Number of trajectories is 10^6. Square of substrate is 100nm x100 nm, substrate depth is 64 nm approximately. Initial blister radius are distributed uniformly in [6.4Å; 9.4 Å]. At initial time moment blisters locate in *Si* on depth from boundary *Mo/Si* [16 nm; 35 nm] uniformly. Duration of calculation is 10^{-4}s.

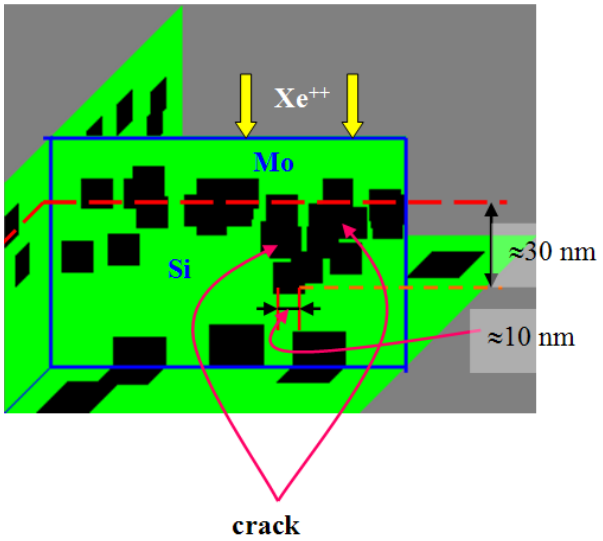

Fig 9 a

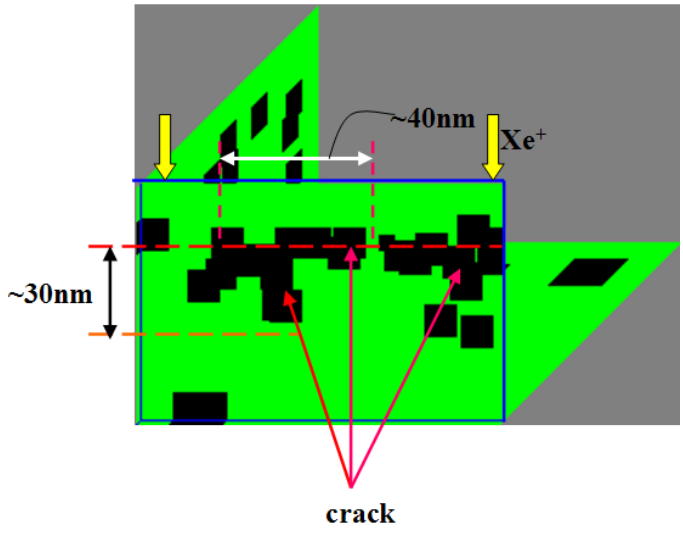

Fig 9 b

Fig. 9 Illustration of blistering develops with the two-layer substrate consisting of layer *Mo* (width is 94 A) and layer of crystal *Si* (width is 543 A) is presented. Black color corresponds porosity, and green color lack of porosity in this point. Temperature is 900K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}.

Divergence between location of maximum of layer porosity which perpendicular to Xe^{++} flow and *Mo/Si* surface is presented on fig. 10 for following physical parameters: temperature is 700K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}. As can see from this figure maximum of porosity locates below *Mo/Si* surface for lower temperature.

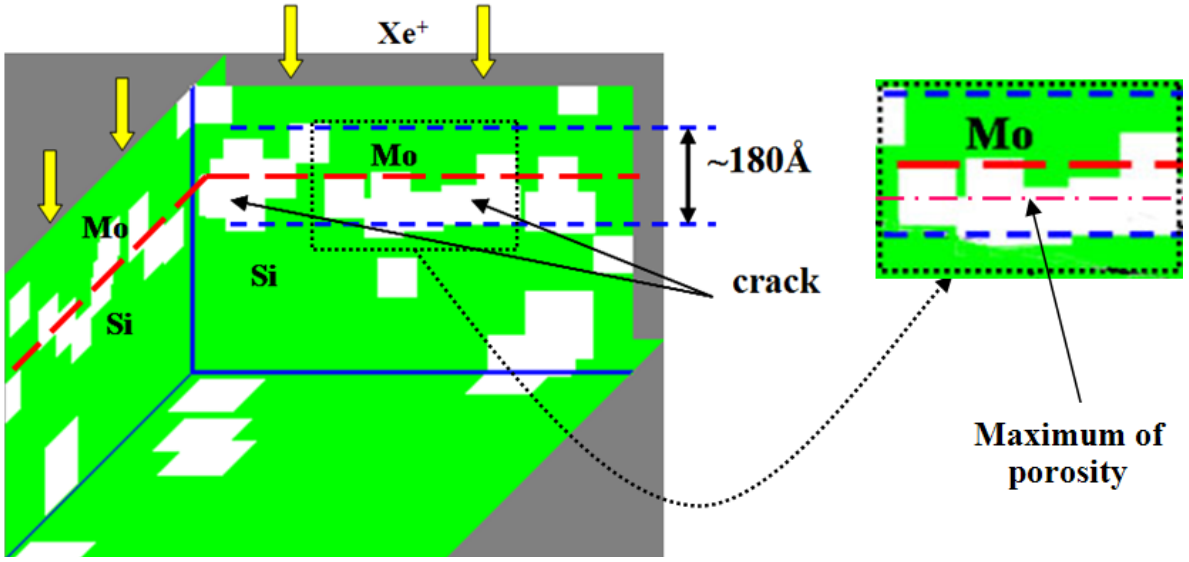

Fig. 10 Illustration of long-size defects structure formation, which perpendicular Xe^{++} flow, in the two-layer substrate consisting of layer *Mo* (width is 94 A) and layer of crystal *Si* (width is 543 A) is presented. White color corresponds porosity, and green color lack of porosity in this point. Temperature is 700K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}.

Maximum of porosity migrates to *Mo/Si* surface with increase temperature. In this case, maximum of porosity is equals to location of long-size defects structure which perpendicular to Xe^{++} flow.

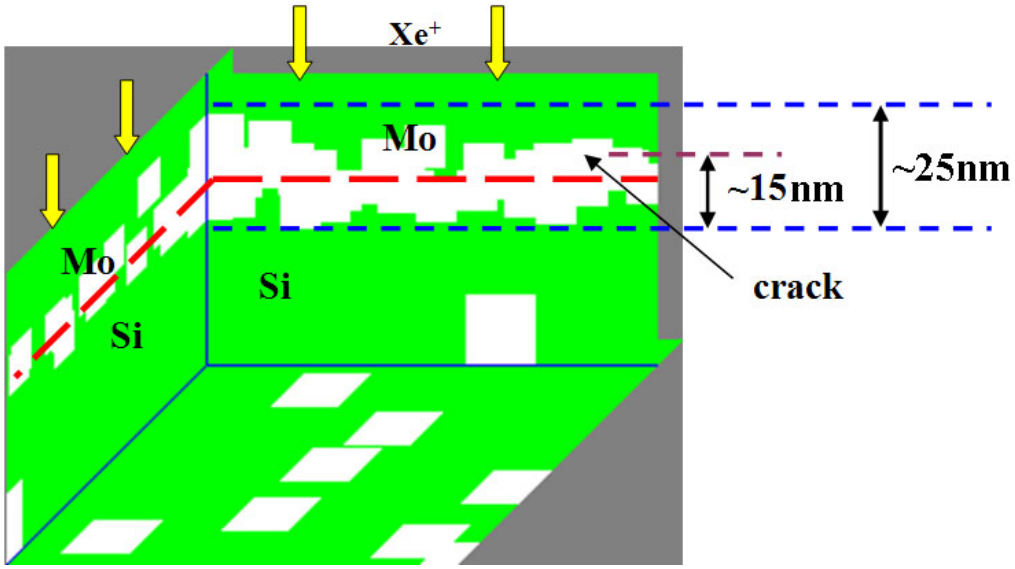

Fig. 11 Illustration of formation of long-size structures of defects in the bilayer substrate consisting of layer *Mo* and layer of crystal *Si* is presented. *Mo* width is 94 A, *Si* width is 543 A. White color corresponds porosity, and green color lack of porosity in this point. Temperature is 1000K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}.

Long-size defects structures don't format when the irradiation dose is 10^{15} cm^{-2}. It is illustrated on fig. 12. But long-size defects structures are observed if irradiation dose is 10^{16} cm^{-2}. Lengths of long-size structure defects, which locate perpendicular to

Xe^{++} flow, and which located along Xe^{++} flow, increase with increase of irradiation dose. It is illustrated on fig. 13. The porosity of substrate and length and branching of long-size defects structures are increase with increase of irradiation dose. Depth of amorphous substrate reaches 30÷35 nm when temperature is 1000K and dose is 10^{16} cm^{-2}, but average amorphization depth is 25 nm. Depth of amorphous substrate reaches 50 nm when temperature is 1000K and dose is 10^{17} cm^{-2}.

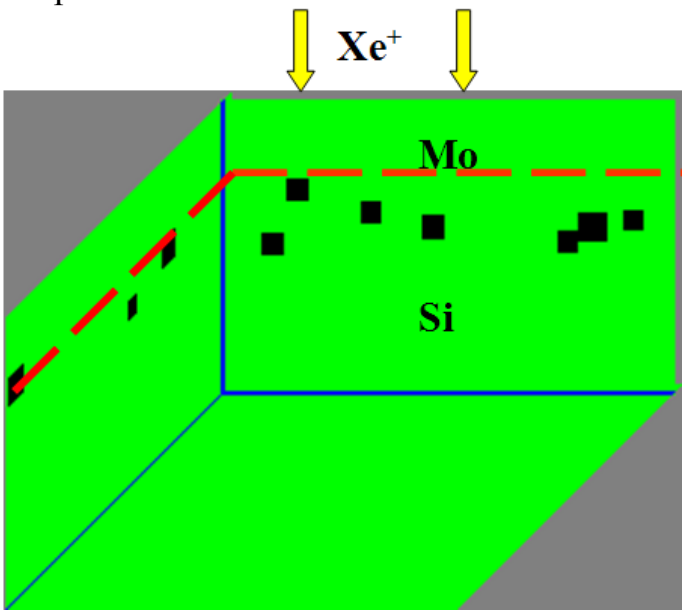

Fig. 12. Illustration of blisters formation in the bilayer substrate consisting of layer *Mo* and layer of crystal *Si* is presented. *Mo* width is 94 A, *Si* width is 543 A. Black color corresponds porosity, and green color lack of porosity in this point. Temperature is 1000K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{15} cm^{-2}. Long-size defects structures don't format.

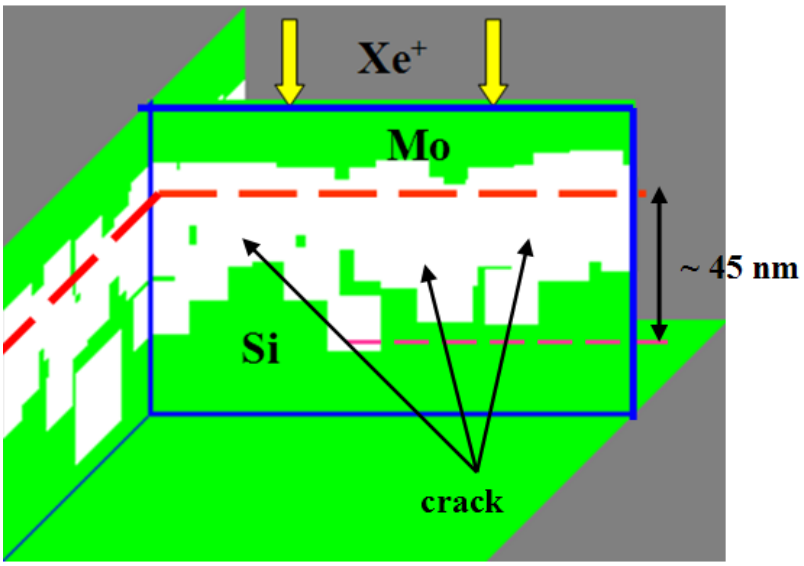

Fig. 13 Illustration of formation of long-size structures of defects in the bilayer substrate consisting of layer *Mo* and layer of crystal *Si* is presented. *Mo* width is 94 A, *Si* width is 543 A. White color corresponds porosity, and green color lack of porosity in this point. Temperature is 1000K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{17} cm^{-2}.

Stress corresponding with blistering in some section of substrate is presented on fig. 14 at finish of fluctuation stage (10^{-4}s). Temperature is 700K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}. Palette of correspondence of stress value and color is presented in right part of picture. As can see from this figure maximum of stress corresponding blistering and long-size defects structures formation locates below *Mo/Si* surface for this temperature.

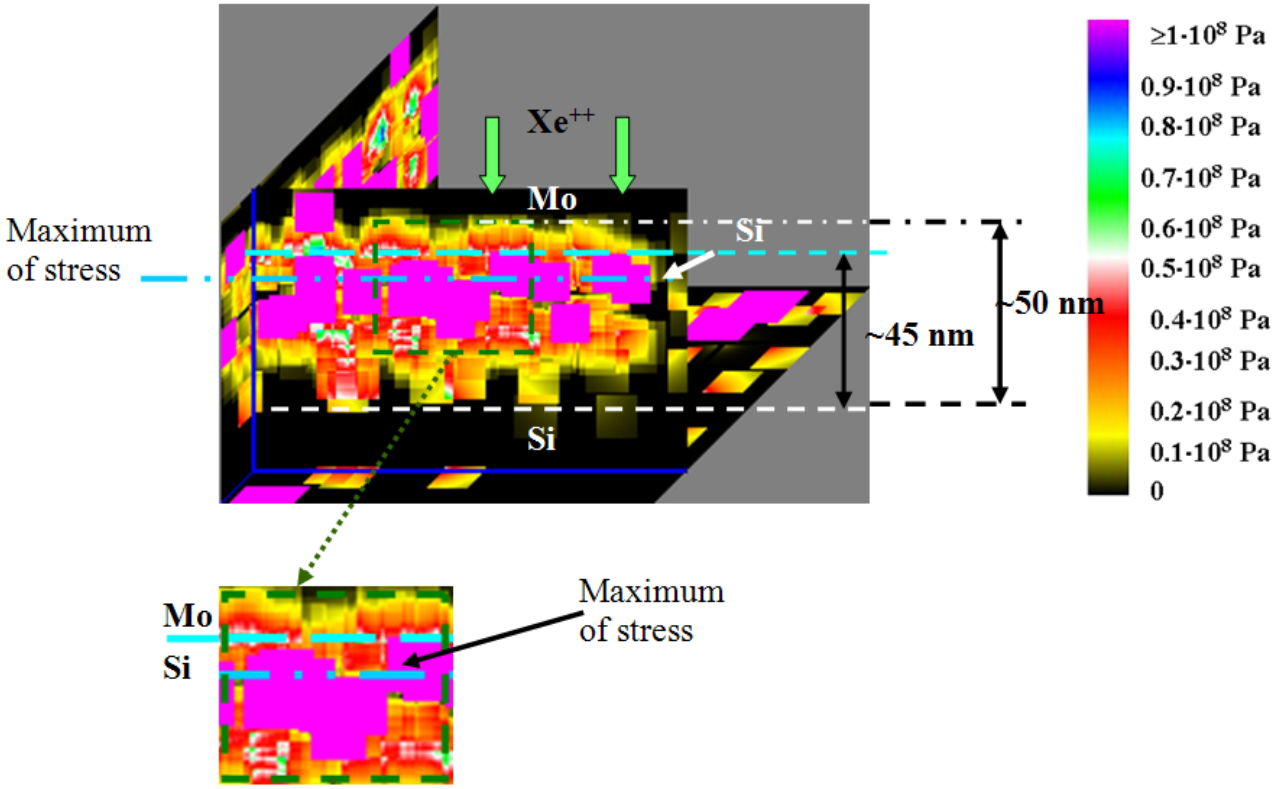

Fig. 14 Stress corresponding with blistering in some section of substrate is presented at finish of fluctuation stage (10^{-4}s). Temperature is 700K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}. Palette of correspondence of stress value and color is presented in right part of picture.

Stress corresponding with blistering in some section of substrate is presented on fig. 15 at finish of fluctuation stage (10^{-4}s) for temperature 900K, Xe^{++} ions energy 5keV, irradiation dose 10^{16} cm^{-2}. Palette of correspondence of stress value and color is presented in right part of picture.

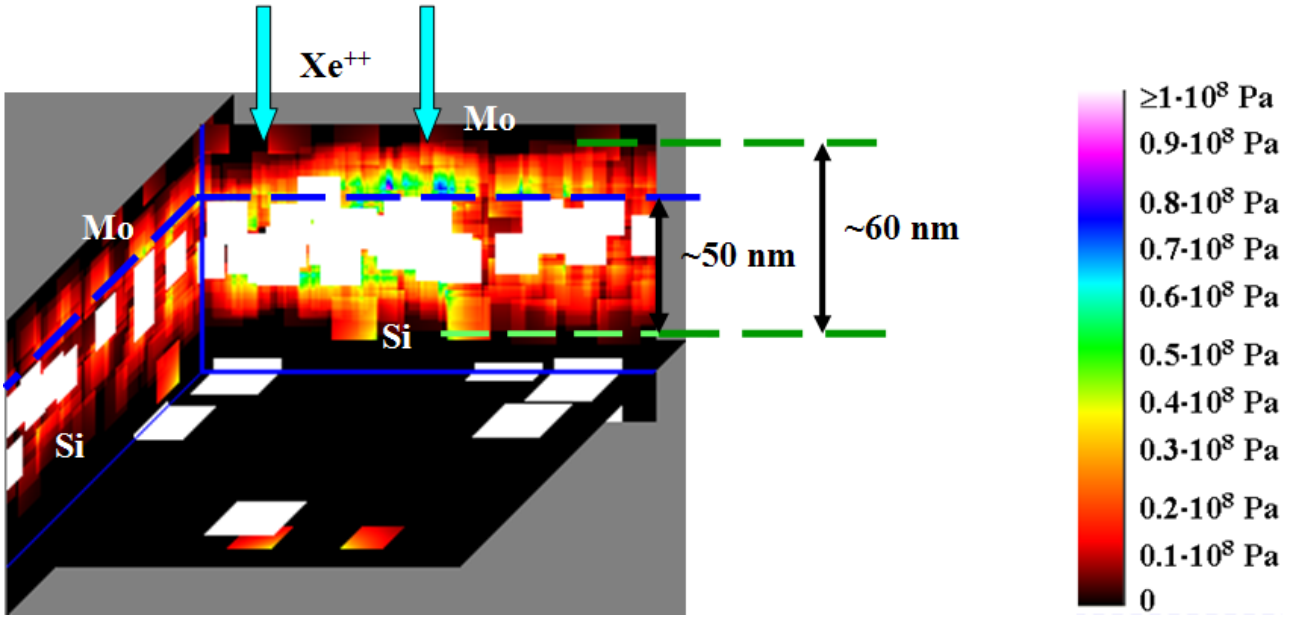

Fig. 15 Stress corresponding with blistering in some section of substrate is presented at finish of fluctuation stage (10^{-4}s). Temperature is 900K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}. Palette of correspondence of stress value and color is presented in right part of picture.

Stress corresponding with blistering in some section of substrate is presented on fig. 16 at finish of fluctuation stage (10^{-4}s) for temperature 1000K, Xe^{++} ions energy 5keV, irradiation dose 10^{16} cm^{-2}. Palette of correspondence of stress value and color is presented in right part of picture.

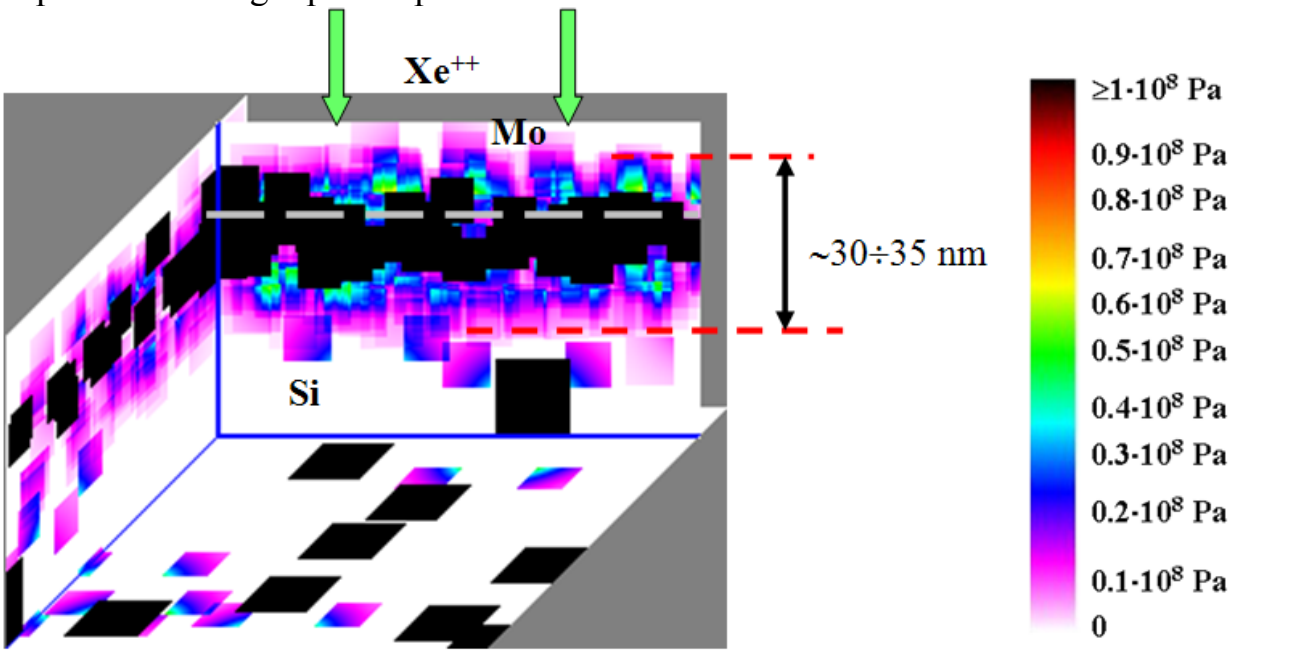

Fig. 16 Stress corresponding with blistering in some section of substrate is presented at finish of fluctuation stage (10^{-4}s). Temperature is 1000K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}. Palette of correspondence of stress value and color is presented in right part of picture.

Tension gradient corresponding long-size defects structure formation for some part of substrate section is presented on fig. 17. Temperature is 900K, Xe^{++} ions energy is 5keV, irradiation dose is 10^{16} cm^{-2}. Palette of correspondence of tension gradient value and color is presented in right part of picture. Tension gradient is calculated with taken into account tension corresponding discrepancy between lattices *Mo* and *Si*. In this case change of Gibbs energy corresponding tension discrepancy between lattices *Mo* and *Si* is not taken into account, discrepancy between lattices *Mo* and *Si* is taken into consideration only when tension and gradient of tension are calculated.

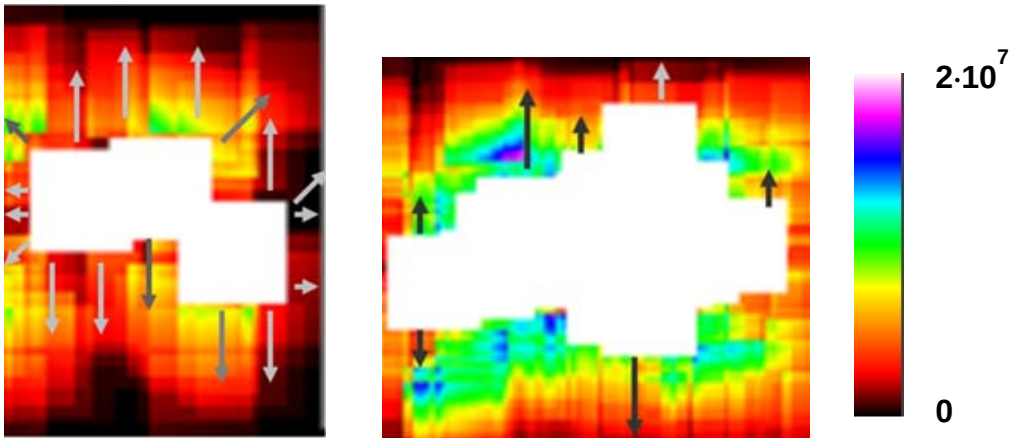

Fig. 17 Tension gradient corresponding long-size defects structure formation for same parts of substrate sections is presented. Palette of correspondence of tension gradient value and color is presented in right part of picture. Grey arrows correspond directions of tension gradient.

Formation of nucleus of long-size structure of defects which are perpendicular to Xe^{++} flow can leads to peeling of *Mo* layer. Possibility of *Mo* layer peeling is illustrated by fig. 18. Black color corresponds long-size structures of defects, and green color lack of porosity in this point.

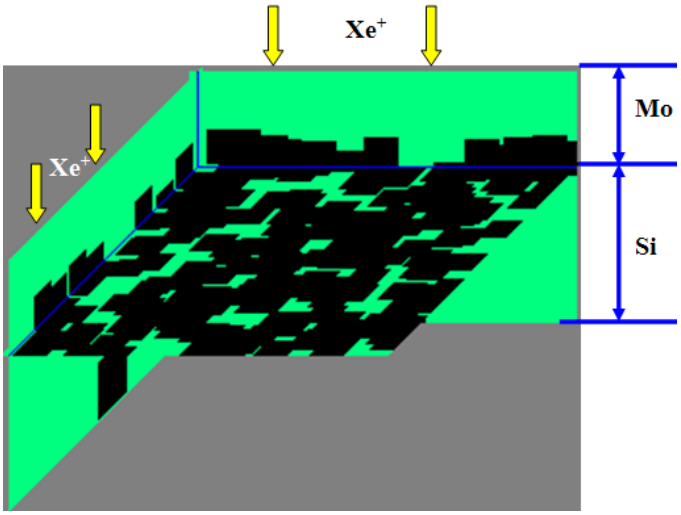

Fig. 18 Illustration of long-size structures of defects on *Mo/Si* surface are presented.

After peeling long-size structure defects, which located along Xe^{++} flow, become permeable. *Mo* islands remain after *Mo* layer peeling. These islands can be catalyst for nanowhiskars formation. If after peeling *Mo* layer are under irradiation of gas mix contained carbon then *SiC* islands several politypes format on *Si* surface and on long-size structures walls and *SiC* nanowhiskar is wire with the diameter of the base of the order of a few nanometers. Schemes of nanowhiskars formation are presented on fig. 19- fig. 20

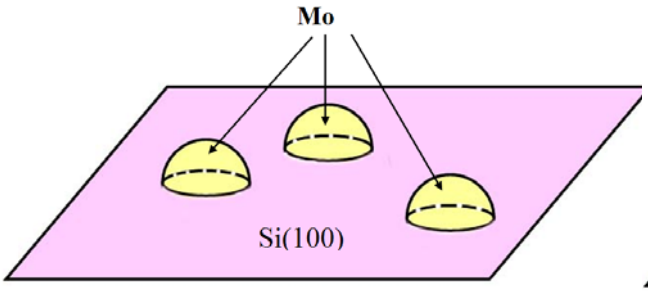

Fig. 19 Scheme of *Si(100)* surface after *Mo* layer peeling is presented.

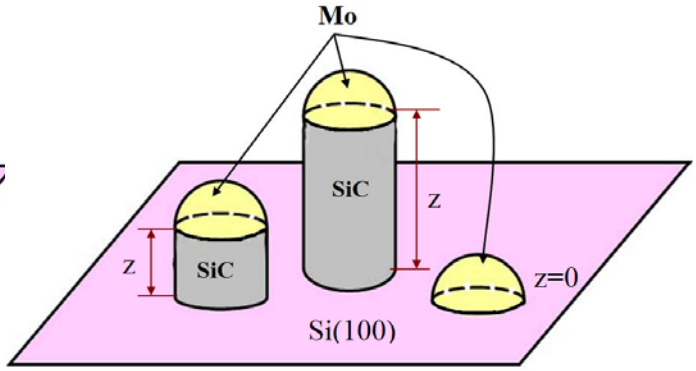

Fig. 20 Scheme of *SiC* nanowhiskars formation under irradiation of gas mix contained carbon is presented.

If suppose that *Mo* is catalyst of *SiC* whiskers growth on *Si(100)* that distribution function of whiskers looks like following (fig. 21):

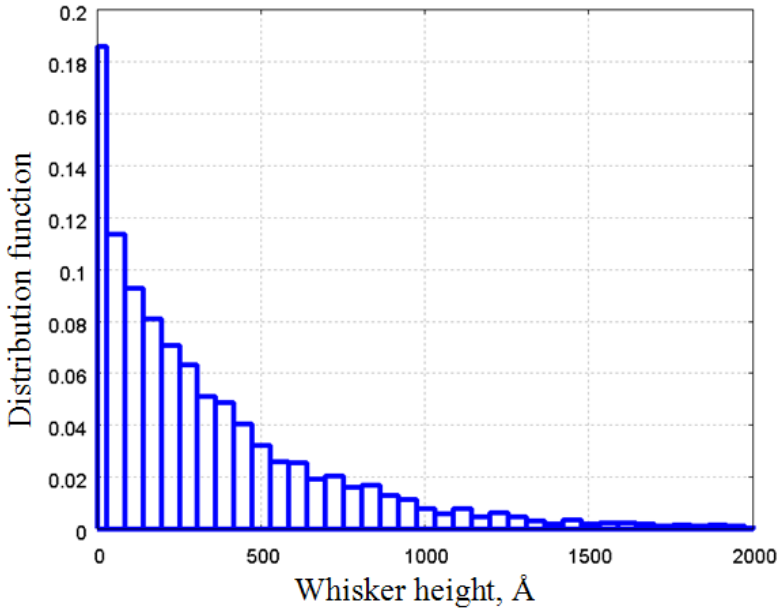

Fig. 21 Distribution function of *SiC* whiskers on *Si(100)* with *Mo* catalysts is presented at finish time of calculation. Radius catalyst is ≈9,8Å (≈3 *Mo* lattice parameters), catalyst density is $3{,}39 \cdot 10^{12}$ см$^{-2}$, substrate temperature is 900 K. 10^6 trajectories are used.

6 Roughness

Usually [38], roughness is measured as standard deviation of height:

$$R_{gh} = \left(\frac{1}{N_x N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \left[z(x_i, y_j) - z_{av} \right]^2 \right)^{1/2},$$

here $z_{av} = \frac{1}{N_x N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} z(x_i, y_j)$ is average height.

In addition, roughness can be measured as average of the module deviation from the average height:

$$z_{av} = \frac{1}{N_x N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \left| z(x_i, y_j) - z_{av} \right|.$$

But in [39] new method measurement of roughness was suggested. Distribution function of height can be written as $f(h) = \frac{2\sqrt{2/\pi}}{C_{2r} r_r} \exp\left[-\frac{2(h - h_c)^2}{r_r^2} \right]$, here h is height, C_{2r}, r_r, h_c are model parameters which depend on angle β. Distribution function from angle β is $f(\beta) = \frac{\sqrt{2/\pi}}{C_{1r} \sigma_\beta} \exp\left(-\frac{(|\beta| - \beta_c)^2}{2\sigma_\beta^2} \right)$, here β_c=0.31118°, σ_β=0.25716°, C_{1r} is model parameter.

Roughness can be result of blistering. Fig. 22 illustrates formation of roughness as result of blistering and fleking. The values of roughness, R(T) (dimensionless ordinate), versus design temperatures (abscissa) *R* is square of defects on surface relationship to total surface square. Lines 1,2,3 correspond to roughness from craters, shapes of bubbles and total, respectively.

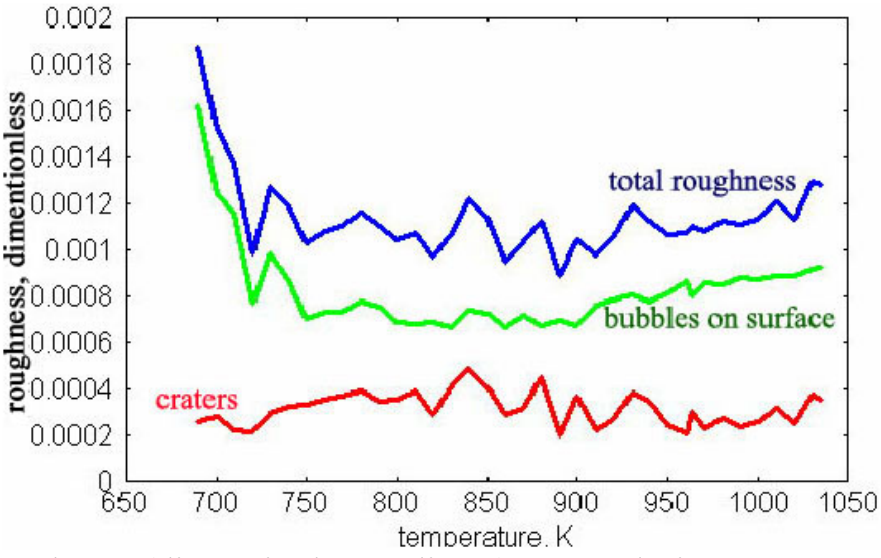

Fig. 22 The roughness (dimensionless ordinate) versus design temperatures (abscissa) is presented.

7 Results of stochastic simulation of islands liquids droplets and clusters of crystallization accumulated on substrate

The results of stochastic simulation of fluctuation stage of *SiC* melted droplets formation at vapor temperature T=1500K and pressure 0.86 Pa, cluster density $3\cdot10^5 cm^{-3}$ for different *C* composition in SiC are presented at Fig. 22-25. Upstream plasma density is equal to 10^{14} cm^{-3}. During fluctuation stage and therefore during calculation vapor temperature and pressure are assumed constants. Change of DFs of charged melted drops from chemical compositions of drops is examined (Fig. 23-25). So, dependence of DF of charged melted drops at finish of fluctuation stage (10^{-4} s) in model with change of chemical composition from drop diameter (Å) is presented on Fig.23-25. *Si* charged melted drops format at initial time moment. Gradual change of charged melted drops compositions from *Si* to *SiC* (maximum composition of *C* corresponding of chemical composition -98.8%) takes place due to joining carbon during fluctuation stage. Time is measured in characteristic time for drops size change $\tau_g \approx 10^{-9}$ s. Fig. 23 corresponds to maximum composition of *C* in *SiC*, DF of *Si* charged melted drops at finish of fluctuation stage (10^{-4} s) is presented on Fig.24 by black lines. Result of gradual change of drops compositions from *Si* to *SiC* with 30% carbon composition due to joining carbon is presented on Fig. 25. Black color lines (black or dark-grey) on Fig. 23-25 correspond to DF of charged melted drops at finish of fluctuation stage, light grey rectangles on Fig. 23-25 correspond to DF of charged melted *Si* drops at initial time.

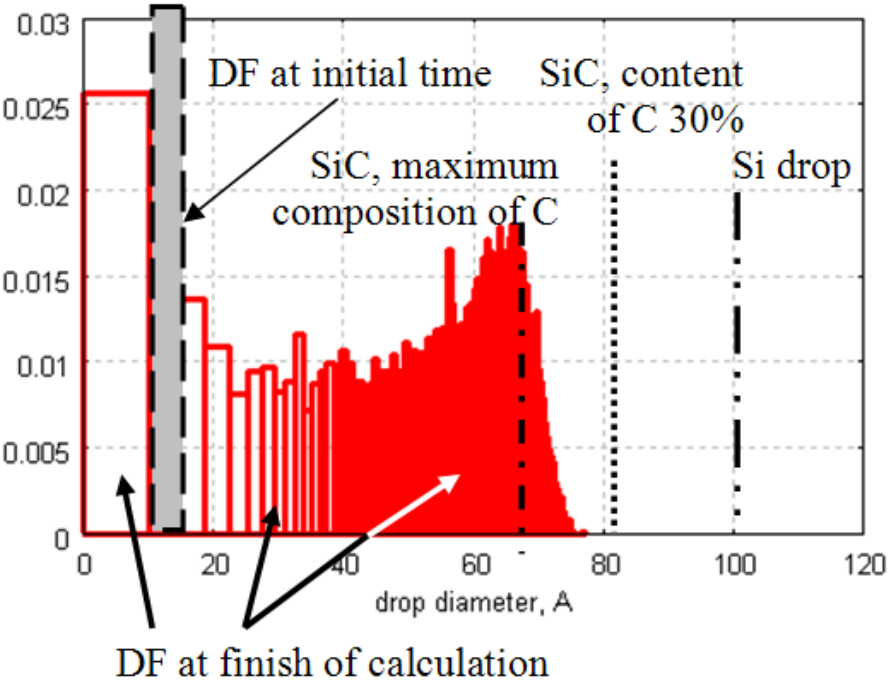

Fig. 23 DF of charged melted drops at finish of fluctuation stage (10^{-4} s) in model with change of chemical composition is presented (black lines). Gradual change of drops compositions from *Si* to *SiC* (full composition of *C* corresponding of chemical composition) takes place due to joining carbon. Light grey color of histogram corresponds to initial value of *Si* drops.

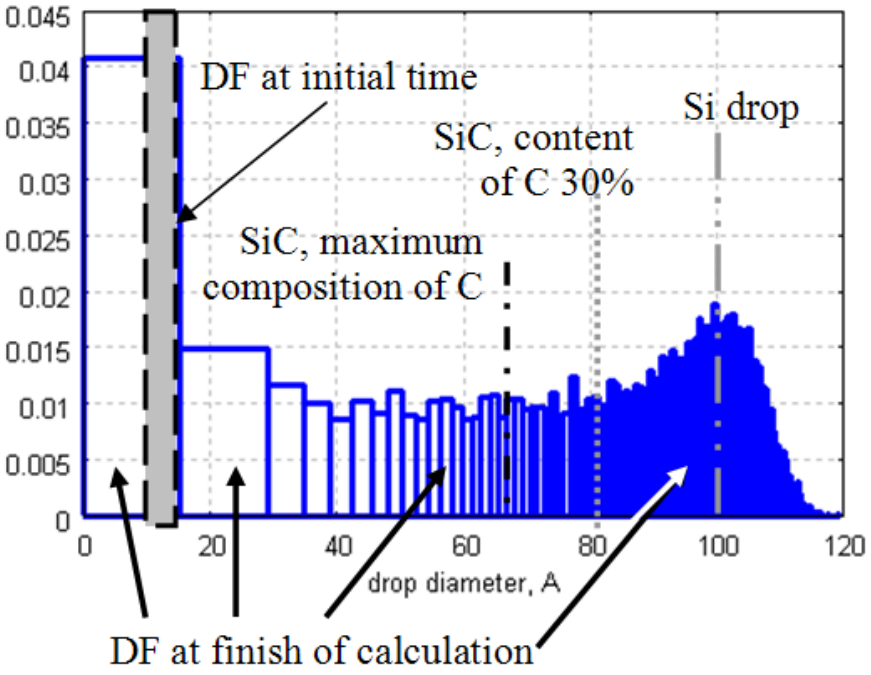

Fig. 24 DF of *Si* charged drops at finish of fluctuation stage (10^{-4} s) is presented (black lines). Light grey color of histogram corresponds to initial value of *Si* drops.

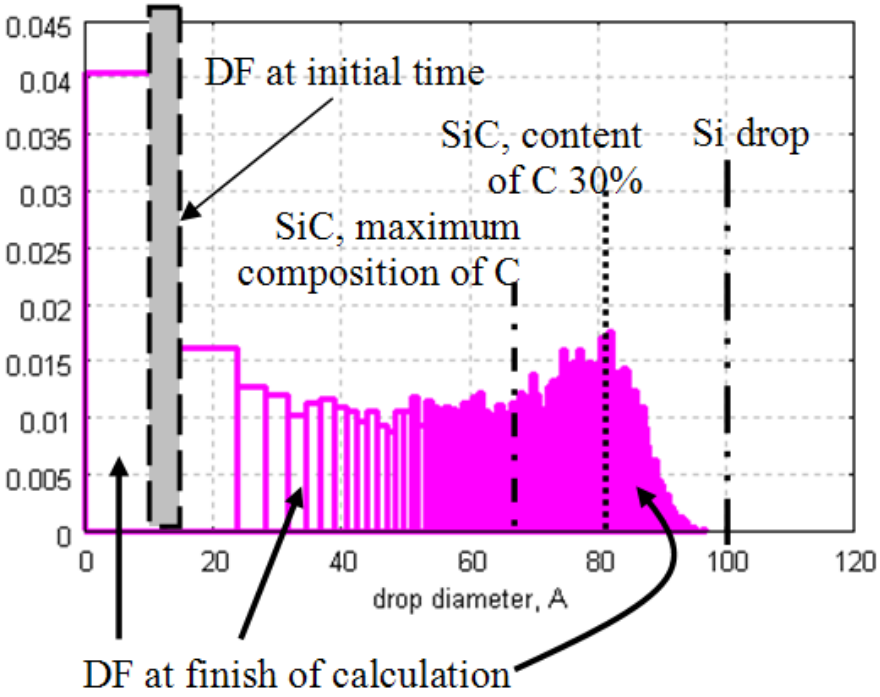

Fig. 25 DF of charged drops at finish of fluctuation stage (10^{-4} s) in model with change of chemical composition is presented (black lines). Gradual change of drops compositions from *Si* to *SiC* (composition of C corresponding of 30% of chemical composition) takes place due to joining carbon. Light grey color of histogram corresponds to initial value of *Si* drops.

As can see from Fig. 23-25 maximum diameter of charged melted drops is observed for *Si* drops, diameters of charged melted drops decrease with increase of *C* composition with *SiC* drops. Saturation by *C* of *SiC* drops leads to change of Gibbs energy and decrease of most probable *SiC* drops size.

Fig. 26 corresponds of solid state of *SiC* clusters. Remind that instantaneous cooling, neutralization and clusterization with polytypic discrimination are assumed, drops segmentation and sputtering of its part are not taken into account during precipitation on *Si(100)*. So, substrate temperature is 1200 K. Others parameters of numerical experiment are as follows: the *Si* substrate size is $2.3 \cdot 10^3 \times 2.3 \cdot 10^3$ A, the initial density of adatoms is 10^{14} cm^{-2}, 10^6 trajectories were used in the calculations, the algorithm step is $\tau_{alg} \approx 10^{-8}$ s, and the fluctuation stage duration is $10^4 \cdot \tau_{alg}$. DF of charged melted drops with carbon composition of 30% relative to maximum *C* composition in *SiC* are initial data for calculation of *SiC* nuclei development on substrate surface. Composition of solid *SiC* on *Si(100)* is supposed not variable. As can see from Fig. 26 nuclei of hexagonal polytype have maximum sizes and minimum dispersion of sizes, at the same time as amorphous nuclei have maximum dispersion of sizes. In accordance with [40] DF of *SiC* from its height can be considered as roughness of substrate surface.

Thermal change of polytypic composition (correlation between amorphous nuclei, *3C-SiC* and hexagonal nuclei) of thin film coordinates with [41]. Part of amorphous nuclei decreases when temperature increases, part of hexagonal nuclei increases with temperature increase.

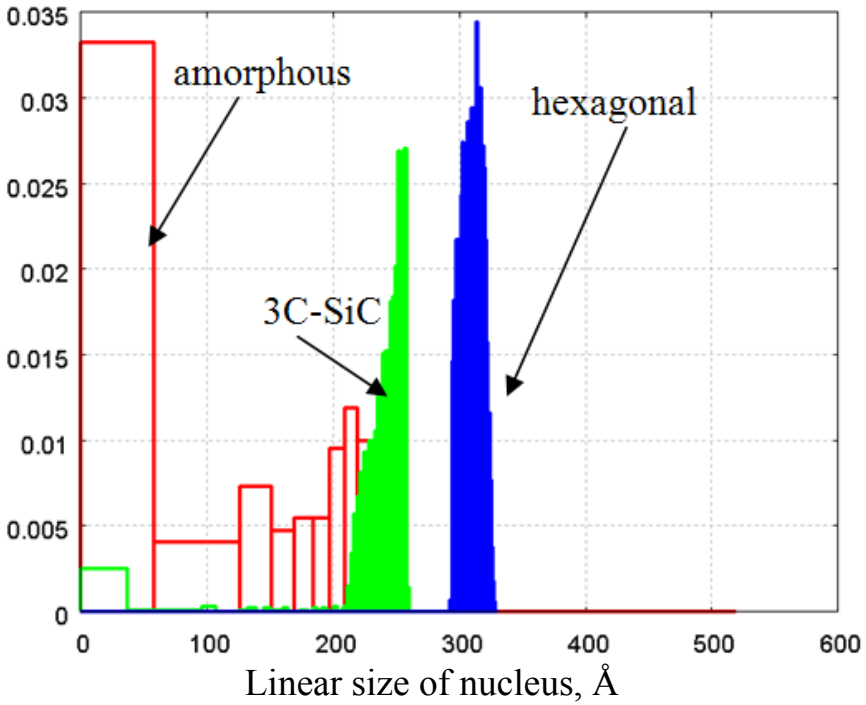

Fig. 26 DF of silicon carbide on a substrate of *Si(100)* with a carbon composition of 30% relative to its maximum composition in SiC is presented. Black color corresponds to hexagonal nuclei, light grey – *3C-SiC* nuclei, dark grey – amorphous nuclei.

8 Conclusion

The fundamental aspects of first-order phase transition (nucleation) are non-steady-state process of cluster formation at the fluctuation stage and Brownian motion of clusters due to long-range self-consistent potentials of its interaction which are taken into account during simulation of *SiC* nuclei development on *Si(100)* surface.

The Gibbs free energy cluster formation and alternating-sign long-range potentials for cluster indirect interaction are taken into account as aspects of self-organization of the open plasma-like media.

The quasilinear kinetic equations (Fokker–Planck– Komogorov and Einstein–Smolukhovskii equation) are transformed into system of interconnected SDEs with functional coefficients which is solved using modified by authors Artem'ev method (stable and effective). This method is based on the strict results of probability analysis using the mathematical-physics equation, i.e. the solved set of Ito–Stratonovich SDEs which are related to the kinetic equations.

We assume that formation of charged clusters and evolution of their size (clustering) is to be described by kinetic distribution function versus sizes. Taking into account of change *SiC* compositions during fluctuation stage (10^{-4} s) leads to change of most probable drops size, which decreases with increase of composition of *C* in *SiC*. C composition in SiC influences in most probable sizes of different SiC polytypes (amorphous, *3C-SiC*, hexagonal), with *C* composition increases most probable sizes decrease.

The ratio of different polytypes of crystals nuclei *SiC* and nuclei without a dedicated internal structure (amorphous nuclei) on the substrate of *Si(100)* indicates the degree of completion of the process of carbidization, i.e. on the carbon composition in carbide silicon.

Thermal change of polytypic composition (correlation between amorphous nuclei, *3C-SiC* and hexagonal nuclei) of thin film in our experiments had been compared with [40]. Results of stochastic simulation coincide with main regularity of experiments [40]. Stochastic simulation results are following: part of amorphous nuclei decreases when temperature increases, part of hexagonal nuclei increases with temperature increase.

Nuclei of hexagonal polytype have maximum sizes and minimum dispersion of sizes, at the same time as amorphous nuclei have maximum dispersion of sizes.

Parameter of the order of the phase transition and its dependence on the fluctuating and the correlating instabilities of the process are analyzed in all variants of the

model of phase transition kinetics (formation islands of thin films, porosity in the metal mirrors, formation of defects in the materials of the controlled fusion, the crystallization of metal, germanium and silicon carbide) [13-15,21,27,41-44].

In addition, stochastic simulation allows:

- ✓ to find blister distribution versus sizes and layer depth;
- ✓ to find porous layers and its depths from surface under irradiation. Layers with maximum porosity is locate near surface *Mo*/*Si* or on it. Maximum of porosity migrate to *Mo/Si* surface with increase temperature ;
- ✓ to find effect of long-size defects structures formation perpendicular to irradiating stream and along irradiating stream;
- ✓ long-size defects structures don't format when the irradiation dose is 10^{15} cm^{-2}. Long-size defects structures are observed if irradiation dose is 10^{16} cm^{-2};
- ✓ lengths of long-size structure defects, which locate perpendicular to Xe^+ flow, and which located along Xe^+ flow, increase with increase of irradiation dose;
- ✓ length of structures perpendicular to irradiating stream (along boundary *Mo/Si*) reaches 60 nm, its width reaches 10 nm;
- ✓ length of structures along irradiating stream (perpendicular to boundary *Mo/Si*) reaches 35 nm, its width reaches 10 nm;
- ✓ pressure in such structure can reach $10^9 \div 10^{12}$ Pa, it can ensure development of cracking of substrate;
- ✓ dependence of lengths of nucleus of long-size structure defects, which located along Xe^+ flow, from temperature are non-linear and has maximum which temperature is ≈0,53 fusion temperature of *Si*;
- ✓ to determine tension gradient corresponding long-size defects structure formation;
- ✓ to find possibility of *Mo* layer peeling with dose equal or more 10^{16} cm^{-2};
- ✓ to find microroughness of *Mo/Si* surface;
- ✓ to detect nanowhiskars formation with *Mo* catalysis;
- ✓ to estimate degradation of multilayer structures due to thermal cycling;
- ✓ to define efficiency of carbon implantation into pores walls and filling of pores by *SiC*.

9 Acknowledgements

Author is grateful to V.D. Levchenko, T.V. Levchenko and T.A. Averina for fruitful discussion on mathematical aspects of model. This work is partially supported by

grants RFBR 09-01-00798 and 11-01-00282, the Department of Mathematics of the Russian Academy of Sciences (prog. no. 3.5).

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Подписано в печать 17.01.2012. Формат 60x84/16. Усл. печ. л. 2,3. Тираж 59 экз. Заказ 2.
ИПМ им.М.В.Келдыша РАН. 125047, Москва, Миусская пл., 4.