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Stochastic model applied to plasma-surface interaction's simulation

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Abstract. The kinetic approach of the nonequilibrium distribution functions (contrasted with the both sizes and coordinates) were calculated for liquid thin film islands as well as for gaseous-vacancy defects into lattice (blisters). The model based on Ito-Stratonovich stochastic differential equations solution, was applied to the defects migration and to defects fluctuation stage of cluster formation. The material porosity and lattice strain values were estimated. Computer simulation results such as surface damaging, the structural and phase alternation of state surface transformation can be compared with experiments of impact powerful pulse plasma fluxes of nano- and micro-second duration ionizing radiation.

PACS. 52.40.Hf Plasma-material interactions; boundary layer effects – 52.25.Tx Emission, absorption, and scattering of particles – 52.65.Ff Fokker-Planck and Vlasov equation

1 Introduction

The non-equilibrium phenomena at these fluctuating stage: blistering [1–4], thin covers formations [5–7] is accompanied by adatomic thermo-emission [8], the dusty charged particle influence [11] interacting with plasma fluxes surface, and other physical, chemical, and biological processes accompanied plasma-surface interaction with time scale comparable with the colliding particles mean-free-time and accompanied plasma-surface interaction are interesting for controlled thermonuclear fusion problems, nanotechnology, microelectronics, at space exploration and gas discharges technology problems.

Full kinetic plasma particle-in-cell object-oriented (PIC) code SUR, developed earlier [9–12], gives us an ability to analyze the examined processes diagnostics. Kinetic codes allows us to investigate non-linear processes in plasma over a wide range of physical parameters and makes possible to clarify limits and approximation efficiency level [9]. The object-oriented 3D3V dusty plasma model [11,12] (which was the world's first) has been developed (see [11,12]) and gave evidence that application of an object-oriented approach to dusty or complex plasma simulation [9–12] and plasma-like media (such as defects of lattice [2,13] and surface covered by deposited material [6]) is a very efficient approach. This model solves the problem by means of splitting computer simulation methods. It permits to uniformly describe and solve the enormous number of plasma kinetics problems, including those that are very complicated to describe and solve. Plasma computer simulation code SUR [9,10] has been built using C++ language and it was tested by typical plasma physics problems solution such as Landau damping, two-stream instability, beam-plasma instability, modulation instability and so on.

Plasma computer simulation code the SUR [9,10] has been complimented by plasma-surface interaction processes investigations leading to helium blistering into metal lattice and plasma deposition processes using stochastic analog method [14], which is based on the strict results of the probability analysis of mathematical physics equations, the plasma and rarefied gases kinetic theory, and the theory and practice of the numerical experiment in the non-linear plasma simulation.

The complex plasma model, which underlies the code, includes the following self-consistent parts: particle ... (PIC) method is used for electrons and ions; Poisson equation is solved for self-consistent fields, although external electromagnetic fields are also applicable; the PDPM (particle-dust particle-mesh) method is used for interaction (collision) simulation between plasma particles and dust grains; dust grains are modeled as unique particles with the predefined set of self-consistent parameters (size, charge, mass, momentum, energy and so on); the stochastic analogies of the physical-chemical processes on lattice surface as well as on the dusty grain surface and other.

The insight into dynamics and kinetics of the plasma and gas processes can be extended by more precise determination of the particles distribution function /DF/,

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which are strongly non-equilibrium on the time scale of interest and can be studied numerically by the stochastic analog simulation method (similar to kinetic approach in the both: plasma and dusty plasma). Note that the basic macroscopic media characteristics (so-called distribution function moment) are obtained by averaging the particle velocity (or other) DF. The determination of effects, which are associated with non-equilibrium processes on the sample surface, is resulting from

1. collisions that lead to reaction;
2. the electromagnetic radiation action or particle beam on plasma and on lattice defect formation;
3. adatomic de-excitation radioactive process with internal freedom degree;
4. first and the second orders of phase transitions that take place on the surface (or into crystal lattice subsurface layers) at the fluctuation stage.

Our main goal here is the plasma-like-media simulation and near surface physical processes in kinetic approach without accounting chemical reaction due to collision and without any molecular freedom degree investigation (vibrational, rotational) which (at the beginning) are participated in surface structure transformation. We put forward principally new numerical quasi-linear kinetic model including processes such as: blistering, thin film's island formation, and adatomic thermoemission.

2 Thin films formation

Computer solids surfaces simulation and adatomic clusterization under plasma influence is interesting for thin films preparation and covers the predefined properties. The ions implantation study into near surface layers, interstitial atomic motion and formed clusters migrations from solids to surface is very important for making of self-repair materials and covers.

The thin films formation fluctuation stage is examined in this article. The covers formation and growth can be presented as first-order phase transition, new phase islands consist of deposited atoms of evaporated material predominantly and the small number of implanted atoms which went on surface as the result of diffusion on substrate lattice. Increase (or decrease) of cluster sizes depends on stochastic change of size and fusions of the same clusters. For examined problem solution we used Brownian motion model which has been adapted for flat coordinate configuration, stochastic analogues method [14], and physical processes splitting processes discussed in [6]. The stages separation of clusters sizes formation and clusters migration on the surface is possible because of its processes that have essentially different typical times. Clusters move on solid surface under potentials substrate surface exposure and long-range part of the indirect interaction between uncharged clusters, which in dielectric crystals are the elastic interaction, i.e. indirect interaction through the acoustic phonons; but in metal are the indirect interaction via defect-induced Friedel oscillations in the electron density for the spherical Fermi surface and acoustic phonons [15,16].

When physical processes have been split, kinetics equations looks like following:

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

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

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

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

where $S_\alpha(f_\alpha)$ – vapour source function, vapour DF f_α is Maxwell for temperature is 2500 K, g is the number of atoms in new phase (islands-clusters), $D_g(g,t)$ is the diffusion coefficient in phase space $\{G\}$ of cluster sizes ($\forall\ g \in\{G\}$); $f_r(g,t)$ is the cluster probabilistic distribution function contrasted with its sizes and time, $\Delta\Phi(g,\vec{r},t)$ is the Gibbs energy of cluster formation, M_g is the cluster mass, $f_g(\vec{r},t)$ is the blister space DF contrasted with coordinate $(\vec{r})$, $\vec{r}$ is the position of cluster mass center in orthogonal coordinate system, $x_{\text{left}} \cong 200$, $x_{\text{right}} = 200$, $y_{\text{left}} \cong 200$, $y_{\text{right}} = 200$, x, y are measured in lattice parameters $F_x = -\partial U(x,y)/\partial x$, where $U(x,y)$ is the clusters interaction potential between them through lattice acoustic phonons and electrons in the case of metal lattice. The form of potential is similar to [2–6]. The $D_g(g,t)$ and $\Delta\Phi(g,\vec{r},t)$ are nonlinear functional-coefficients that influencing on clusters sizes. The non-linear Gibbs energy of islands formation includes following parts: difference of chemical potentials of two phases (vapour and liquid), interface tensions of condensate-vapour, condensate-substrate, substrate-vapour, elastic force of lattice and possibility of releases of part of connections in lattice, and cluster locations on surface [6]. The heterogeneous condensation is considered on clusters surfaces. The diffusion functional-coefficient in phase space $\{G\}$ $D_g(g,t)$ depends on adsorption energy, adatomic diffusion activation energy (on surface), adatomic concentration (on surface), system temperature and others. Several clusters can be fused due to inelastic collision, when Brownian clusters motion is realized.

Numerical calculation results in:

1. if islands radiuses are distributed uniformly from 5.31 Å to 17.7 Å at initial time moment, then from 10^{-4} s form of distribution function shows that two most probably radiuses exist. Its first size (∼16 Å) is similar to critical size and corresponds to newly form

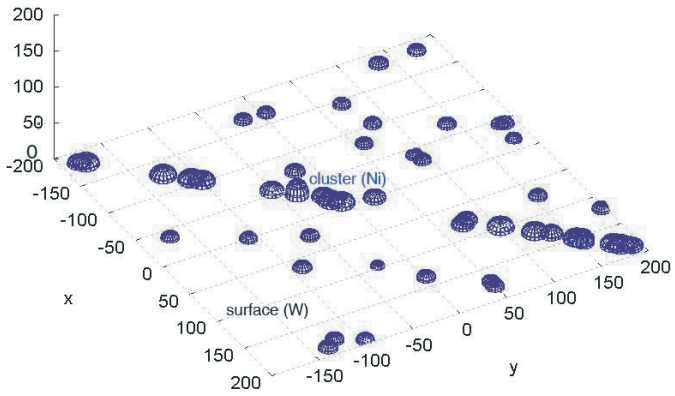

Fig. 1. Clusters dispositions at the end of the fluctuating stage.

clusters, second size (∼61 Å) corresponds to islands which grow at the expense of fusions during calculation;
2. the number of islands placed near linear dislocation is far more than clusters number approximately at 8 times. So, the thin films formation begins on surface defects such as dislocations (Fig. 1);
3. three cover formation stages during fluctuation stage are discovered. The first stage lasts from 0 to 8×10^{-7} s; it is the stage of slow development. The second stage continues from 8×10^{-7} s to 5×10^{-5} s and it is the stage of thin film's quick growth. The third stage lasts from 5×10^{-5} s to 10^{-4} s and it is notable for growth rate deceleration. At that, cover square increases approximately at 11 times with respect to cover square at the initial moment of time;
4. the calculations confirm that cover influence approximately reaches the lattice parameters on depth of 5. At the same time, the strain on surface and near surface layers caused by thin film formation does not exceed the strain caused by blisters development. The strain on the surface connected with cover's growth increases at 21 times during fluctuating stage.

3 Blistering

Blistering is a formation process of lattice defect's gas bubbles (blisters) in the subsurface layer of a solid body irradiated by gas ions flux (with low solubility). We pay attention to the blistering's high-temperature at the nonequilibrium fluctuating stage. The following model was put forward to solve this problem: bubble nucleation and bubble growth/degradation are considered as the first-order phase transition; the bubble nucleus is considered as a Brownian particle with spherical shape and variable mass. The kinetic equations for Brownian particle are partial integral-differential equations similar to the same equations, which were examined in previous part, and are acceptable but complicated for solving. The physical processes of bubble size fluctuation and stochastic motion over the lattice have sufficiently different time scales (the coefficients for dimensionless time variable are $\tau_g \sim 10^{-9}$, $\tau_r \sim 10^{-8}$ s, where τ_g is the duration of cluster formation, τ_r is the same value for Brownian motion). Thus, kinetic equations on a discrete time grid are solved by splitting technique in terms of physical processes, and every stage is represented by its stochastic analogue. Size increasing, migration on lattice, bubbles fusion are examined by computer simulation. Recently we put forward the model of heterogeneous condensation on bubble surface, accounting the difference between chemical potential of two phases: gas particle and vacancy-gaseous bubble, surface tension on bubbles surface, elastic solids lattice reaction in case of weak anisotropic lattice, bubbles position non-equivalence (most likely that bubbles embedded in the lattice point), interaction between bubbles, interaction between bubbles and solid surface as well as bubbles and crystal lattice. The crystal lattice's breaking connections are considered in [1,3,4]. Interaction between bubbles is indirect, through lattice acoustic phonons and Friedel oscillation of electron density [1,4,7]. Bubbles can come to surface and destroy at it. For solving this authors modified Artemiev's method [17]; it is a second-order accuracy method, the solution is stable over the infinite area (according to methods [17] it was developed to solve stochastic differential equations). Used approach allows us to receive following characteristics: bubbles DF contrasted with bubbles size and its position in crystal lattice, mathematical expectation of bubble size and distance from the surface, porosity evaluations of several solids layers and the calculated tensions due to blistering.

Numerical experiments revealed the following regularities of bubbles self-organization into lattice under permanent ion flux influence [5]:

1. blisters chains are formed athwart to incident ions fluxes;
2. bubbles quasi-lattice is observed;
3. blister size can reach 12 Å during fluctuation stage;
4. bubbles size reaches maximum when curve of solid temperature to materials melting temperature is 0.47;
5. the bubbles migration into the surface by means of (under) irradiation if bubble radius is less than 5 Å, in the other cases bubbles stop;
6. the greatest porosity (Fig. 1) and tensions (Fig. 2) are observed on depths of $\sim0.85R_p$ and $\sim0.35R_p$, R_p is middle depth of projection run;
7. DF of bubbles contrasted with bubbles sizes and coordinates in lattice are nonequilibrium;
8. the study of $1/f$-noise spectrum is confirmed the existence of large quantity of bubbles with small sizes and limited number of bubbles with big sizes [3].

4 Thermoemission

This section deals with stochastic simulation of plasma-surface interaction processes such as electron's thermoemission, the same adatomic emission, secondary electrons emission, elastic and inelastic plasma particles's collisions from dusty grains surface's penetrations into dusty grains

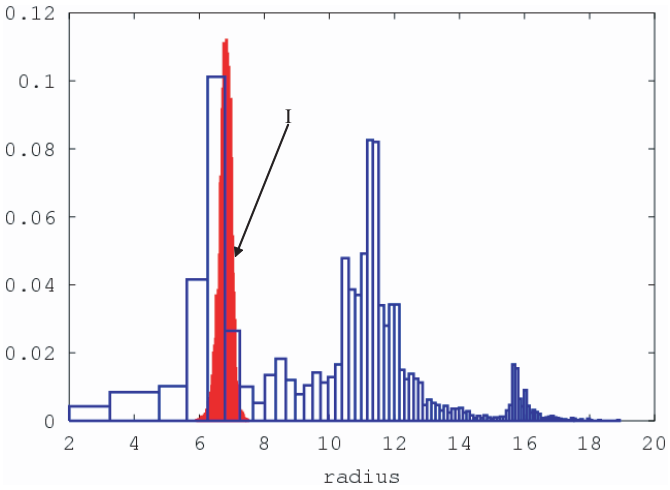

Fig. 2. Clusters distribution function according to radiuses (in Å), the initial state is noted by "I".

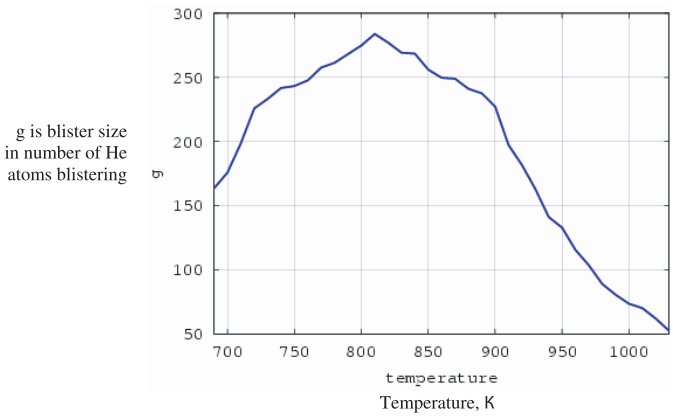

Fig. 3. Dependence from average blister size to different temperatures. The results refer to finish instants of calculation time.

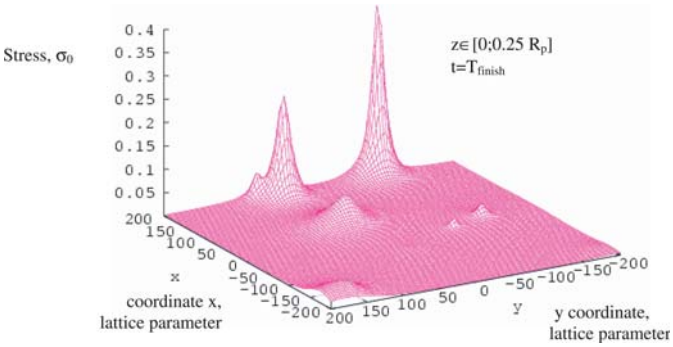

Fig. 4. Strain in depth layer form from $z = 0$ (surface) to $z = 0.25R_p$ at the moment of finishing the fluctuating stage. The z-axis directs into substrate.

and others. The processes lead to plasma pollution by atoms of dusty grains material and change the plasma properties. Special attention here is payed to thermoemission. The model is supplement with self consistent 3D kinetic dusty plasma model [11]. Processes simulation on the dusty grain's surface is based on kinetic theory of Brownian motion model and stochastic analogues methods. The Leontovich equation is associated with the Brownian motion model and Kramers problem. Emission under the ions influence and electrons is described in terms of jump like Markov processes. Thermoemission and adatomic emission from surface are simulated by Wiener stochastic processes, which is associated with Brownian motion model, and which is applied to adatomic interaction with charged dust particle surface with potential U. The equation for electrons thermoemission is:

$$\frac{\partial f}{\partial t} + v_r \frac{\partial f}{\partial r} + \frac{e}{m_e}\frac{\partial U}{\partial r}\frac{\partial f}{\partial v_r} = \gamma \frac{\partial (\vec{v} f)}{\partial \vec{v}} + \frac{\gamma T}{m_e}\frac{\partial^2 f}{\partial \vec{v}^2}$$

where U is modelled as

$$U(r) = \begin{cases} \left(\dfrac{Q}{R_d} - A_{out}\right)\left(1 + \alpha \cos\dfrac{2\pi r}{a}\right), & r \le R_d - a \\ 1.58\dfrac{\dfrac{Q}{R_d} - A_{out}}{1 + \exp\left(\dfrac{3(r - R_d)}{a}\right)}, & R_d - a \le r \le R_d + 2a. \\ \dfrac{Q/R_d}{r}, & r \ge R_d + 2a \end{cases}$$

Here r is distance from dusty grain centre, $\vec{v}$, v_r are electron velocity and its radial component, e, m_e are electrons charge and mass, $\gamma = \gamma(r)$ is damping parameter, R_d, Q are dusty particle's radius and charge, a is lattice parameter, A_{out} is work function for dusty grain's material. The potential $U(r)$ in eV is presented in Figure 5.

To solve kinetic thermoemission's equation the splitting method is used. The kinetic equation's system is solved. The determinate and stochastic parts are separated. The kinetic equation solution for $f(\vec{v}, \vec{r}, t)$ is substituted by two equations solutions for f_1 and f_2 related to each other:

$$\begin{cases} \dfrac{\partial f_1}{\partial t} + v_r \dfrac{\partial f_1}{\partial t} + \dfrac{e}{m_e}\dfrac{\partial U}{\partial r}\dfrac{\partial f_1}{\partial v_r} = 0 \\ f_1(r, v_r, t = t_0) = f(r, v_r, t = t_0) \end{cases}$$

and

$$\begin{cases} \dfrac{\partial f_2}{\partial t} = \gamma \dfrac{\partial (\vec{v} f)}{\partial \vec{v}} + \dfrac{\gamma T}{m_e}\dfrac{\partial^2 f}{\partial \nu^2} \\ f_2(r, v_r, t = t_0) = f_1(r, v_r, t = t_0 + \Delta t) \\ f_2(r, v_r, t = t_0 + \Delta t) = f(r, v_r, t = t_0 + \Delta t) \end{cases}.$$

The first equation of this system is solved using centred explicit second order leap-frog scheme, and the second equation of the system containing stochastic part is replaced to suitable stochastic analogue [14] and solved using modified Artem'ev method [17].

The kinetic approach lets to receive not only particles density leaving the dusty grains surfaces, but also DF on space coordinates and velocities. As a result of numerical experiments the distribution function v_r is received (Fig. 6).

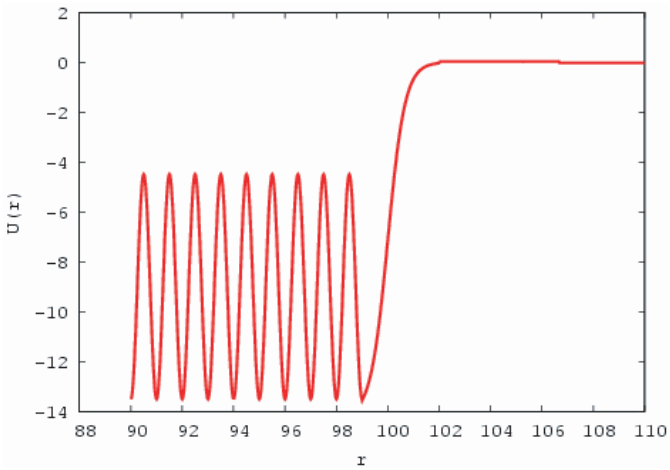

Fig. 5. The $U(r)$ inside and outside of dusty grain is shown, here r is the distance from dusty grain's centre measured in lattice parameters a, $R_d = 100a$.

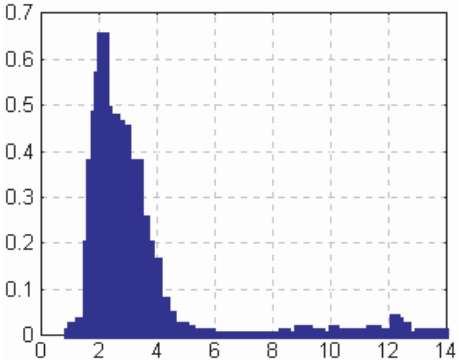

Fig. 6. The distribution functions $f(v_r)$ averaged on scattering angles from radial velocitie's component is shown at the time of finishing the calculation. Here the grain temperature is 1 eV as presented in Figure 6.

The emitted particles from dusty grains change the plasma parameters. Hence their distribution functions are necessary for development of completely selfconsistent 3D kinetic model of dusty plasma and numerical code for simulating the processes in dusty plasma. Formation and development of some maximums on $f(v_r)$ is observed; part of high velocity secondary electrons and typical electron velocity increases when dusty grain temperature increases. The dependence from number of electrons left grain surface to particle temperature is shown in Figure 7.

The dependence (presented in Fig. 7) looks like Richardson-Deshman law in low temperature region, the variances from Richardson-Deshman form in high temperature region concern distribution functions non-stationarity $f(v_r)$ of electrons inside dusty grains.

5 Conclusion

New results on the both: gaseous-vacancy defects in lattice and thin film liquid islands on the surface dynamics

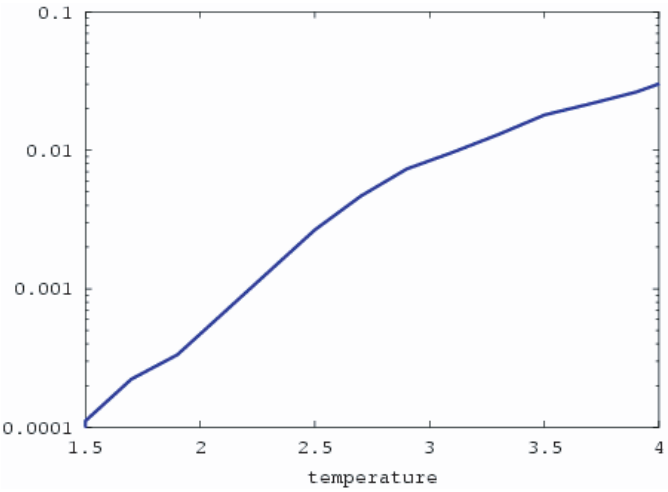

Fig. 7. The ratio logarithm of electrons left grain surface to total electron number is presented in the figure. The particle temperature is measured in eV and shown on (abscissa) Y-axis.

in open systems with nonequilibrium distribution functions are reviewed and demonstrated via computer simulation based on the Ito-Stratonovich stochastic differential equations. It is shown that the fluctuation phase transition's stage (defects growth or degradation) can be investigated as well as its Brownian motion in lattice due to long-range indirect interaction's potential (via lattice acoustic phonons and via Friedel electron's density oscillation). Non-linear effects: average size's dependence of blisters contrasted with sample temperature, the porosity formation layers, the blisters distribution of contrasted with sizes and depth from surface, the strain in depth layers are received. The details of thin film islands dynamics (sizes distribution contrasted with time, formation rate, islands location's dependence from lattice dislocation) are founded. New computer simulation model of adatomic thermoemission was proposed as a contribution to dusty plasma kinetic 3D3V object oriented code SUR.

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Annexe A: Numerical scheme for the method of stochastic analog for blistering simulation

To solve a system of SDE with functional-coefficients, it is required to construct a series expansion for exact Cauchy problem's solution:

$$x(t) = x_0 + \int_0^t H(x(\tau))d\tau + \int_0^t \sigma(x(\tau))dW(\tau), \quad 0 \le t \le T_{fin}.$$

A modified Artemiev's method was used; it is a second-order accuracy method, with infinite stability domain (according to methods developed for SDEs solving) [10]. 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. Using the Stratonovich's form for SDE makes possible to take a standard white noise instead of random function $\xi(t)$, and this simplifies the stochastic integral's calculation procedure for the Wiener process in the numerical method's realization. As a sample, we can take the equation for the bubble size's calculation. For the i trajectory of diffusive Markov's process its value g_{n+1} at the time moment $n+1$ can be calculated through this formula:

$$g^i_{n+1} = g^i_n + \left[I - \frac{h}{2}\frac{\partial H^i_n}{\partial g}\right]^{-1} \times \left[hH^i_n + \sqrt{h}\sigma^i_{ng}\xi_{ng} + \frac{h}{2}\frac{\partial \sigma^i_{ng}}{\partial g}\sigma^i_{ng}\xi^2_{ng}\right],$$

$$H^i_{ng} = -\frac{1}{kT}D^i_g(g_n,t_n)\frac{\partial \Delta\Phi^i(g_n,t_n)}{\partial g_n} - \frac{1}{2}\frac{\partial D^i(g_n,t_n)}{\partial g_n},$$

$$\sigma^i_{ng} = \sqrt{2D^i(g_n,t_n)}.$$

In this method g_n is the SDE system's approximation solution at grid points by time $\{t\}$, h is the time step, I is the unit matrix, ξ_n is the sequence of independent random numbers with a zero expected value and unit dispersion. While modelling the SDE solution on a computer, the values of ξ_n can be calculated by equation $\xi_n = \sqrt{-2\log\alpha_1}\cos(2\pi\alpha_2)$, where α_1 and α_2 are random numbers uniformly distributed in the interval (0, 1).

Annexe B: Brief review of SUR-dust

The Thermoemission model has to be associated with kinetic dusty plasma description. Let us present multidimensional 3D3V object oriented code SUR-Dust [11] which is based on a set of Vlasov-Poisson equations for electron-ion plasma:

$$\frac{\partial f_\alpha}{\partial t} + \vec{v}_\alpha \cdot \frac{\partial f_\alpha}{\partial \vec{r}} + \left(\vec{F}_{ext}(\vec{r}) + e_\alpha \vec{E}(\vec{r})\right)\cdot\frac{\partial f_\alpha}{\partial \vec{v}} = I_\alpha + C_\alpha$$

$$\vec{E}(\vec{r}) = -\nabla\varphi,\ \Delta\varphi = -4\pi\left(\rho_d + \sum_\alpha \rho_\alpha\right),\ \rho_\alpha = e_\alpha\int f_\alpha d\vec{v}$$

which are solved by the PIC method. According to the rule the real number of one species's plasma particles is aggregated in a coarse "modelling" particle with the same e_α/m_α charge/mass ratio (e, m are electron charge and mass) where index $\alpha = e, i$ refers to plasma particles species, while index d refers to dust grains. $f_\alpha = f(\vec{r},\vec{v},t)$ is species's distribution function α in 3D3V phase space coordinates $\vec{r}$ and velocities $\vec{v}$, I_α are volume particles ionization source, C_α is particles source/effluent onto dusty grains surface and ρ_α are its charge density. Due to PIC method, the set of equations for the "modelling" particle will be exactly the same as for an individual plasma particle:

$$\frac{d\vec{r}^{\,i}_\alpha}{dt} = \vec{v}^{\,i}_\alpha,\quad \frac{d\vec{v}^{\,i}_\alpha}{dt} = -\frac{eZ_\alpha}{m_\alpha}\vec{E},\quad \vec{E} = \nabla\varphi.$$

Two spatial scales are used for the force calculation acting on plasma particle ("particle-dust") nearby the dusty grain, and "particle-mesh" if the particle is far from the grain: $\vec{f} = \vec{f}^{lr} + \vec{f}^{sr}$, where $\vec{f}^{sr}$ is the short time scale's force measurement as well as $\vec{f}^{lr}$ is the long time scale's force. In order to calculate the attractive force between the grains we should describe the ions motion near the grain in details. To calculate self-consistent field $\vec{E}(\vec{r})$ and potential φ for dusty plasma the *PDPM* (particle-particle particle-mesh) new algorithm had been developed, which yields a large dividend in accuracy and efficiency of interaction's force. In our model both electrons and ions are represented by rectangular shaped clouds. The number of "macro particles" in calculation is equal to $\sim 10^5$, the grid mesh number $\sim 10^7$ and number of dusty grains (droplets) $\sim 10^2$. The simulating of 3D region is periodic across two coordinates (x and y). Across the third coordinate (axis z): at the top, the region contacts with undisturbed plasma's reservoir, while at the bottom we have partial absorption/rejection from the metal wall, width of plasma layer is $420\lambda_D$ (Debye lengths). The injection into near-electrode plasma's particles volume is realized over the volume or through the surface. Dust charging is due to electron and ions collection from ambient plasma. Here we solve quasi-stationary problem: First, plasma comes to equilibrium with dust grains, and after that, each grain is displaced in the direction of its velocity and so on. The behaviour influence of droplets into plasma flux can be defined by set of individual characteristics of each model's droplet charged. r_d is the equilibrium radius of spherical liquid droplet. For the droplet motion equations one must take into account that its charge, Q_d, momentum $m_d\vec{v}_d$ and temperature T_d which are affected self-consistent with plasma parameters

$$\frac{d\vec{r}_d}{dt} = \vec{v}_d,$$

$$\frac{d(m_d\vec{v}_d)}{dt} = \vec{F}_{ext} + Q_d\vec{E}(\vec{r}_d) + \sum_{e,i}\oint m_\alpha\vec{v}f_\alpha\vec{v}d\vec{S}.$$

The evolution equations of droplet charge and temperature are the follows

$$\frac{dQ_d}{dt} = \sum_{e,i}\oint e f_\alpha\vec{v}d\vec{S},\qquad \frac{dT_d}{dt} = \sum_{e,i}\oint \frac{m_\alpha v^2}{2}f_\alpha\vec{v}d\vec{S}.$$

Here integrals are electron's and ion's momentum of charge and of energy fluxes onto dusty grain's (or droplet's) surface.

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