SIMULATION OF NANOPARTICLE DEPOSITION FROM PLASMAS ON SOLID SURFACE

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In this paper a computer simulation of depositing nanoparticles from rarefied plasma on a solid substrate, which is at a floating potential, is carried out. In our model, we used the equation of cold hydrodynamics for ions, the equilibrium distribution of Boltzmann for electrons, and the particle in cell method for modeling nanoparticles. Dust particles are charged by electron and ion currents, which are described in accordance with the orbit-limited motion approach. Calculations were performed for various radii of nanoparticles, their concentrations and directed velocities in the unperturbed plasma. The results of the simulation show that, at a sufficiently large size of nanoparticles in the area of the sheath, a dust cloud, whose position changes in time, is formed. This leads to the formation of a minimum of the potential of the electric field and to the change in the structure of the sheath. The modification of the sheath by nanoparticles results in reflection and oscillation of the particles, which causes not stationary flow of nanoparticles onto the substrate.

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INTRODUCTION

Nowadays, plasmas are widely used for production and coating of nanoparticles in the including large-scale plasma-based production of single walled carbon nanotubes and integration of plasma-grown silicon single-crystalline nanoparticles in nanoelectronic and solar cell devices [1, 2]. Controlled deposition and structural incorporation of such nanoparticles will make deterministic fabrication of nanostructured films with predictable properties a reality in the near future. Moreover, to create such a technology it is important to understand the dynamics of nanoparticles in the sheath that separates the plasma from the solid wall. Movement of nanoparticles in the sheath is governed by a number of forces unique to a low-temperature plasma and is extremely sensitive to the nanoparticle charge and mass. The nanoparticle charge is usually negative in the plasma bulk, but near negative substrates can be positive, since in this region the electron density is much smaller than the ion density. In this case, the electrostatic repulsion changes to attraction and the nanoparticles can deposit on the substrate. On the other hand, at a high density of nanoparticles, their charge can significantly affect the structure of the sheath. In this case, it is necessary to take into account the mutual influence of nanoparticles and the electric field in the sheath.

In this article, using numerical simulation we compute the nanoparticle fluxes onto solid surface, which is at a floating potential.

1. MODEL AND SIMULATION METHOD

We consider the solid substrate, which interacts with plasma and assume that it is under floating potential. On the boundary of the plasma and the substrate has formed a sheath. We have a stream of nanoparticles with radius r_d onto this substrate from the side of unperturbed plasma. The concentration of atoms is negligible, so collisions of particles with neutrals are neglected. In addition, we neglected the collisions of ions with electrons.

To describe the potential of a self-consistent electric field, we used the Poisson equation:

$$\frac{d^2\varphi}{dx^2} = -\frac{1}{\varepsilon_0} e\left(n_i - n_e\right) + q_d n_d \, , \tag{1}$$

where n_i, n_e, n_d are the densities of ions, electrons and dust particles, q_d is the charge of dust particle.

Ions are described by the equations of cold hydrodynamics

$$\frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial x} = -\frac{e}{m_i} \cdot \frac{\partial \varphi}{\partial x}, \tag{2}$$

$$\frac{\partial n_i}{\partial t} + \frac{\partial \left(v_i n_i\right)}{\partial x} = -\frac{I_i}{e} n_d \, , \tag{3}$$

where v_i, e, m_i are ion hydrodynamic velocity, charge and mass. We take in account the recombination of ions on dust particles surfaces in the continuity equation (3). Ion current I_i on dust particles is described approximate formula in accordance with OML theory [3]

$$I_i = \pi r_d{}^2 e n_i \cdot \left(\frac{8kT_i}{\pi m_i} + v_i{}^2\right)^{1/2} \cdot \left[1 - \left(\frac{e q_d}{r_d\left(kT_i + \frac{m_i v_i{}^2}{2}\right)}\right)\right]. \tag{4}$$

Density of the electrons satisfies the Boltzmann distribution

$$n_e = n_0 \exp\left(\frac{e\varphi}{kT_e}\right), \tag{5}$$

where n_0 is electron density in unperturbed plasma far from the solid wall, T_e is the electron temperature, which is assumed to be constant in the sheath.

The boundary conditions for Poisson equation are given in the form: at $x = 0$ $E = \sigma_w$ and at $x = \infty$ $E = 0$. Here $E = -\partial\varphi/\partial x$ is electric field, σ_w is surface charge density on the solid wall, which is defined by equation

$$\frac{d\sigma_w}{dt} = e\left(n_i v_i - n_e\sqrt{\frac{8kT_e}{\pi m_e}}\right).$$

As boundary conditions for equations (2), (3) are given: $n_i = n_0$ and $v_i = 0$ at $x = \infty$.

For the simulation of the nanoparticles we use PIC method [4]. According this method the dust component is modeled by a set of macroparticleseach of whichis a set of nanoparticles with roughly identical coordinates and velocities. The motion of macroparticlesis described by equations

$$\begin{gathered} \frac{dx_{di}}{dt} = u_{di}, \\ M_d\frac{du_{di}}{dt} = Q_{di}E(x_{di}). \end{gathered} \qquad (6)$$

Here x_{di}, u_{di}, M_d and Q_{di} are the spatial coordinate, velocity, mass and charge of themacroparticles, $E(x_{di})$ is an electric field at the point where the macroparticle is located. The charge of the macroparticle is determined from the equation

$$\frac{dQ_d}{dt} = \left(I_i + I_e\right)N_s, \qquad (7)$$

where $I_e = -\pi r_d^{\,2} \cdot e \cdot \left(\frac{8kT_e}{\pi m_e}\right)^{1/2} \cdot n_e \cdot \exp\left(\frac{eq_d}{r_d kT_e}\right)$ is the electron current on the nanoparticle, N_s is the number of nanoparticles grouped in a macroparticle.

The algorithm for solving the problem looks like this. To solve equations (2), (3), we introduce a difference grid in the modeling domain anduse the finite difference method, namely the Lax-Wendroff scheme [5]. On the same difference grid, we calculate the charge density of the dust component, which is taken into account in the Poisson equation when calculating the electric field potential.

2. RESULTS AND DISCUSSION

The calculations were performed for different radii of nanoparticles r_d , their concentration n_{d0} and flow velocity v_{d0} at the boundary of the sheath. Fig. 1 shows the spatial distributions of nanoparticles charge density for different times after the nanoparticles injection for the case $r_d = 10\ nm$, $v_{d0} = 0.2 \cdot c_{is}$, $n_{d0} = 0.05 \cdot n_0$ (a) and for the case $r_d = 2\ nm$, $v_{d0} = 0.2 \cdot c_{is}$, $n_{d0} = 0.05 \cdot n_0$ (b). It is seen thatin the case of large dust particles in the region of the sheath a peak of charge of the dust component is formed, whose position varies in time.This causes the formation of an electric potential minimum in the region of the peak of the negative charge (Fig. 2). In the case of small dust particles, compression of the dust component is not observed. During the motion of the dust stream through the sheath, oscillations of the charge form on its front.With time, distribution of the charge density of the dust component becomes stationary and homogeneous. In this case, the formation of dense clouds of nanoparticles is not observed.

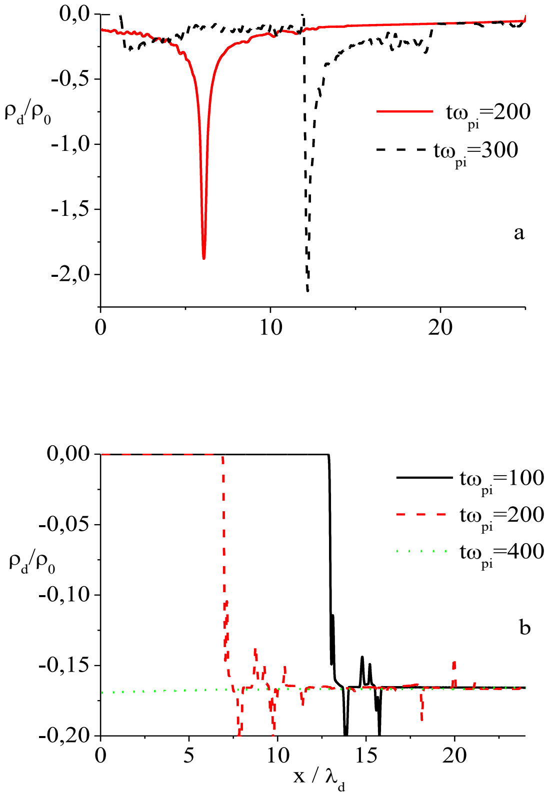

Fig. 1. Spatial dust charge density distributions at different times after nanoparticles injection

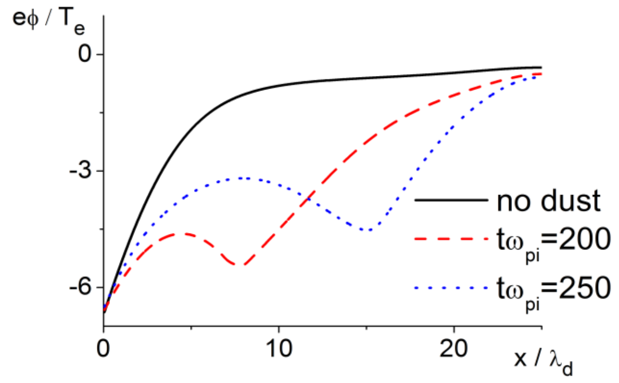

Fig. 2. Spatial electric potential distributions at different times after nanoparticles injection

Fig. 3 shows coordinates of some dust particles as function of time. The selected dust particles are injected into the sheath at different moments of time. The first dust particle is decelerated slight in the sheath and getto thewall, but the other dust particles are reflected from negative peaks of dust charge and leave the modeling area in the direction of the unperturbed plasma. Modification of the sheath by nanoparticles leads to a discontinuous flow of nanoparticles over time onto the substrate: there is no flow to the substrate in some time intervals (Fig. 4).This phenomenon resembles the instability of Bursian, which is observed in a flat diode, when the current exceeds a certain limiting value.

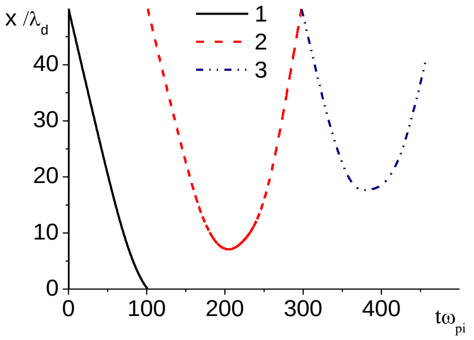

Fig. 3. Spatial coordinates of nanoparticles as functions of time

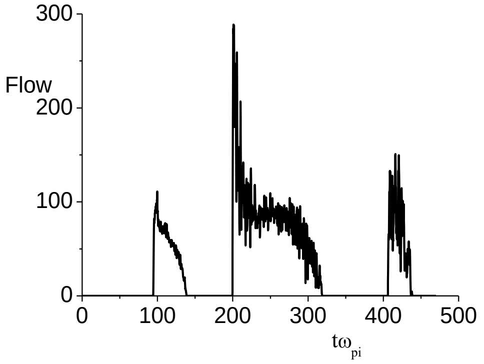

Fig. 4. The flow of nanoparticles onto the substrate as functions of time

CONCLUSIONS

We studied the process of nanoparticles deposition on the substrate. The changed structure of the sheath by charged nanoparticles leads to reflection and vibrations of some particles, which causes an inhomogeneous flow of nanoparticles onto the substrate.

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МОДЕЛИРОВАНИЕ ОСАЖДЕНИЯ НАНОЧАСТИЦ ИЗ ПЛАЗМЫ НА ТВЕРДУЮ ПОВЕРХНОСТЬ

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Проводится компьютерное моделирование осаждения наночастиц с разреженной плазмы на твердую подложку, которая находится при плавающем потенциале. В нашей модели мы использовали уравнения холодной гидродинамики для ионов, равновесное распределение Больцмана для электронов и метод частиц в ячейках для моделирования пылевой компоненты. Пылевые частицы заряжаются электронным и ионным токами, которые описываются в приближении ограниченного орбитального движения. Расчеты проводились для различных радиусов наночастиц, их концентраций и направленных скоростей в невозмущенной плазме. Результаты моделирования показывают, что при достаточно больших размерах наночастиц в области приэлектродного слоя образуется сгусток пыли, положение которого изменяется во времени. Это приводит к образованию минимума потенциала электрического поля и к изменению структуры приэлектродного слоя. Модификация приэлектродного слоя наночастицами приводит к отражению и колебаниям частиц, влечет за собой нестационарность их потока на подложку.

МОДЕЛЮВАННЯ ОСАДЖЕННЯ НАНОЧАСТИНОК З ПЛАЗМИ НА ТВЕРДУ ПОВЕРХНЮ

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Проводиться комп'ютерне моделювання осадження наночастинок з розрідженої плазми на тверду підкладку, яка знаходиться при плаваючому потенціалі. У нашій моделі ми використовували рівняння холодної гідродинаміки для іонів, рівноважний розподіл Больцмана для електронів та метод частинок у комірках для моделювання пилової компоненти. Пилові частинки заряджаються електронним та іонним струмами, які описуються в наближенні обмеженого орбітального руху. Розрахунки проводилися для різних радіусів наночастинок, їх концентрацій та направлених швидкостей в незбуреній плазмі. Результати моделювання показують, що при досить великих розмірах наночастинок в області приелектродного шару утворюється згусток пилу, положення якого змінюється в часі. Це призводить до утворення мінімуму потенціалу електричного поля і до зміни структури приелектродного шару. Модифікація приелектродного шару наночастинками призводить до відбиття і коливань частинок, що спричиняє нестаціонарність їх потоку на підкладку.