

The Modern Information Technologies and Visualization Methods for Analysis of Computer Simulation Results for Complex Plasma

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Abstract. In this paper we present a software package based on modern information technologies that allows rapid analysis and visualization of the properties of complex plasmas. The properties of plasma are simulated by two means. First of all, we have applied the molecular dynamics simulation method which numerically solves the equations of motions for plasma particles. Secondly, we calculate microscopic properties of plasma by using the Boltzmann equation with additional relations, initial and boundary conditions.

AMS subject classifications: 68N19, 68U20, 68U35

Key words: Molecular dynamics simulation method, modern information technology, software package, program software.

1 Introduction

Scientific visualization is becoming a key ingredient of research, development, and discoveries in numerous fields of science and technology. Scientific visualization systems help not only to represent the results of calculations, but also to integrate and analyze the results of calculations and experiments accumulated earlier [1,2].

At the present time the study of the complex plasma properties is not only of fundamental interest, but it also has various important technological applications. It is known that as a result of computer simulation we obtain many complicated graphical dependencies. During design engineering of real technological projects it is necessary to imagine

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complicated processes in complex plasma. In this connection the role of visualization methods for analysis of processes in complex plasma is important.

In the present work two types of plasmas have been considered: in the first part the semiclassical dense plasma with a density of particles $10^{21} - 10^{24} \text{cm}^{-3}$ and temperature $10^4 - 5 \cdot 10^5 \text{K}$ is discussed. In the second part the dusty plasma with electron and ion densities $n_i \approx n_e \sim 10^7 - 10^9 \text{cm}^{-3}$, and the density of dust particles may vary in a wide range $n_d \sim (10^3 - 10^8) \text{cm}^{-3}$ which arises in the DC and RF gas discharges is studied. Such plasma occurs in many natural phenomena, laboratory facilities, and the implementation of various technological processes. In both cases the plasma is strongly coupled (non-ideal), i.e. when the electrostatic interaction energy of the particles is comparable to their average thermal energy. It means that in order to determine physical properties of plasma different approximation theories, in particular, the perturbation theory could not be applied due to the absence of a small parameter in the system. In this connection, the computer simulation methods of the plasma properties based on numerical solutions of the equations of motions for the particles (MD method), Boltzmann equation, etc. are widely used. The difference between these methods from each other is that in the first case, for simulation of microscopic and transport properties of the plasma it is necessary to know the interaction potential between particles in the system, in the second one the collision integrals are needed in terms of the corresponding scattering cross sections of the plasma particles. The application of these methods imposes definite limitations, in particular, we investigate the semiclassical plasma which consists of classical ions and degenerate electrons. It is supposed for applying of the Boltzmann model the background plasma is sufficiently rarefied, therefore, it is possible to use the known model particle scattering cross sections of the system. In addition, there are specified limitations relating to the applicability of interaction models between plasma particles, which are discussed in detail in [3–5].

We have developed the program software "PLASMA" using object-oriented programming environment Delphi7 and graphics library OpenGL, which includes two large software packages: "Simulation of properties of two-component plasma on the basis of molecular dynamics method" and "Characteristics of discharge and dusty plasma in DC glow discharge".

The first information system includes the program software allowing the investigation of two-component plasma on the basis of computer methods of molecular dynamics and visually track the movement of the particles. The second information system includes the program software allowing obtaining the values of axial and radial distributions of dusty plasma parameters in discharge tube at different parameters on the basis of the Boltzmann equation.

The program package includes system, instrumental and applied software. The choice of programming language was based on such criteria as the rate of the application development, the possibility of building a friendly and reliable interface, the possibility of including databases by means of language itself, for realization process simulation functions, widened mathematical apparatus, effective compilation, availability of the system

of software and compilers development. Methods of realization of multi-level model of graphical interfaces are very diverse and more less oriented to hardware and operational platforms.

The package gives the possibility to set the parameters and to monitor the process of calculations. The results are displayed in the course of calculations, both in the form of graphs and tables and this allows the user to interrupt the program in case of any deviations. The created software is a convenient and reliable means for the investigation of dusty plasma properties.

The proposed software packages can be used by engineers during construction and testing special experimental setups where the dusty plasma and some ordered structures are formed.

2 Method of molecular dynamics: Pair correlation distribution functions

The method of molecular dynamics is used to calculate the properties of multi-particle systems, where each particle moves according to classical equations of motions. The MD allows obtaining both statistical and dynamic characteristics. In MD method the movement of the system along the trajectory in phase space occurs deterministically, i.e. the problem is to solve the equations of motions for the systems of many particles.

The equations of motions for each particle are the following one:

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i; \quad (2.1a)$$

$$\frac{d\vec{v}_i}{dt} = \frac{1}{m_i} \vec{F}_i, \quad (2.1b)$$

where $\vec{F}_i = -\sum_{j \neq i=1}^N \text{grad}\Phi(r_{ij})$ is the force acting on the particle i from the other particles, Φ_{ij} is the interaction potential energy between particles i and j .

There are various algorithms of solution of N particles motion equations systems by the method of particle dynamics. The program realization of these is carried out into software package enabling to choice the method of motion equation integration as well as enabling to get information on each of the methods. The choice of algorithm and time step depends on the parameters of simulated plasma. This is caused primarily by the correctness of plasma simulation (conservation of the energy of the whole system in the process of simulation) and minimization of computing time. There are following algorithms for coordinate and velocity calculation: Rahman predictor-convector, Verlet, Beeman etc.

In simulation of dense non-ideal plasmas Beeman's algorithm for integration of equations of motion was used. The solution of the system Eq. (2.1) allowed obtaining series of coordinates and velocities in various moments of time. Corresponding statistical processing of these data allows receiving the information on structural properties of the system.

It should be noted that different methods such as Rahman, Verlet, Beeman etc., are applied for integration of the equations of motions. The applying efficiency of one or another methods depends on many parameters (the initial and boundary conditions, integration step, own state of system, etc.) when computer modeling of physical properties for a real system. It is known [6, 7] that molecular dynamics study of the Coulomb systems, in particular, ionic solutions, liquid metals shows the tendency to nonconservation of total energy obtained on the basis of the Verlet scheme. This problem can be solved by applying of high accuracy Beeman's method. As it is noted in [6, 7] the MD study based on the Beeman scheme permitted to conserve of total energy of the system with accuracy of 0,01% during computer simulation. The similar situation occurs at MD studying of strongly coupled (dense) plasma at definite parameters, in this connection, the Beeman method has been used in the present work. The high accuracy of the Beeman's scheme is ensured by accurate approximation of particle coordinates and velocities according to expansion in the Taylor series up to Δt^5 . The dependencies of total energy on the basis of the two different integration methods for a dense semiclassical plasma are shown in Fig. 1. One can see the Beeman scheme ensures satisfactory conservation of total energy due to small relative fluctuations.

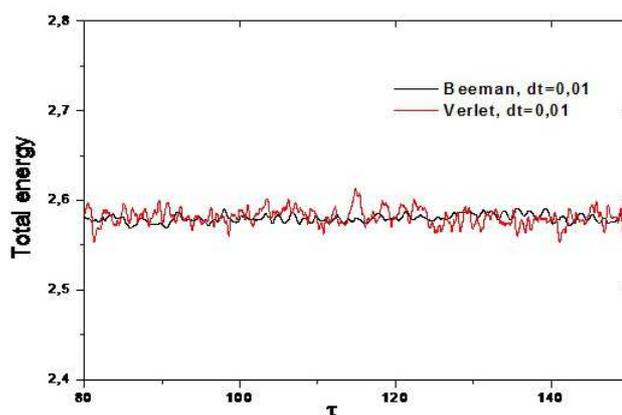


Figure 1: The total energy of the system. The black curve is calculation based on the Beeman scheme and the red curve is the result based on using the Verlet scheme.

In this work we have used the periodic boundary conditions. The time dependence of average potential energy of the system is usually called as control card of computer simulation. This dependence (see Fig. 2) can be conventionally divided into two parts. The first part ($0 < t < 35$) indicates the nonequilibrium state and the second one ($35 < t < 150$) is responsible for the equilibrium state of the system. Initial coordinates and velocities of particles are randomly chosen according to uniform distribution. At thermodynamic limit when the physical system reaches the equilibrium state this distribution is transformed to the Gaussian.

It is known, that the full information on the structural and thermodynamic properties of systems may be obtained using the functions of particles distribution of the given

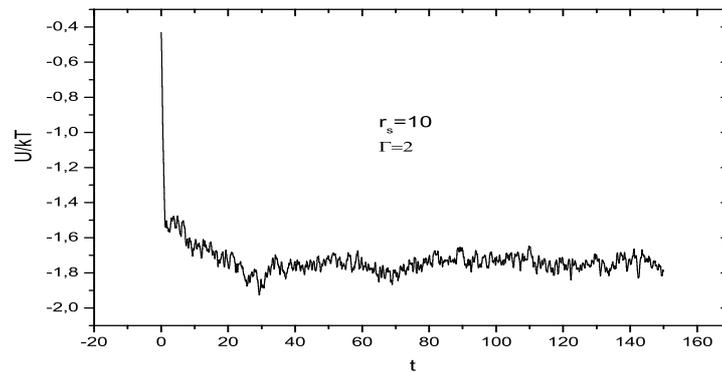


Figure 2: The control card of MD simulation for a dense plasma.

system. The pair distribution correlation function $F(\vec{r}_1, \vec{r}_2)$ determines the probability of finding of the first particle in point \vec{r}_1 and the second one – in point \vec{r}_2 . In the case of isotropic system the pair distribution correlation function depends only on the distance between the particles and is called radial distribution function $g(r)$. The behavior of distribution function depends on the interaction potential of particles. Where the interaction potential of particles vanishes (at large distances) we observe non-correlated distribution. The probability of particles finding at definite distance is generally considered with regard to non-correlated distribution, consequently the radial distribution is supposed to tend to one with the increase in inter-particle distance.

The calculation of radial distribution function proceeds in the following way. For each particle the space around this particle is divided into spherical layers with the thickness Δr from 0 to $L/2$ and the number of particles in each layer is counted. The obtained data for all particles of the given configuration are averaged. Radial distribution function is calculated using the following formula:

$$g(r) = \frac{\nu}{4\pi r^2} \cdot \frac{\Delta \bar{N}(r)}{\Delta r}, \quad (2.2)$$

where $\nu = 1/n$.

3 Software package simulation of two-component plasma properties on the basis of the method of molecular dynamics

In this work the program application includes the program software allowing the investigation of two-component plasma on the basis of computer molecular dynamics methods and visually tracks the movement of the particles. The maximum amount of particles that can be handled by the interface can reach thousands.

On the basis of the mentioned algorithms described software in Delphi 7 was developed. For the visual observation of particles movement a graphic interface OPENGL was

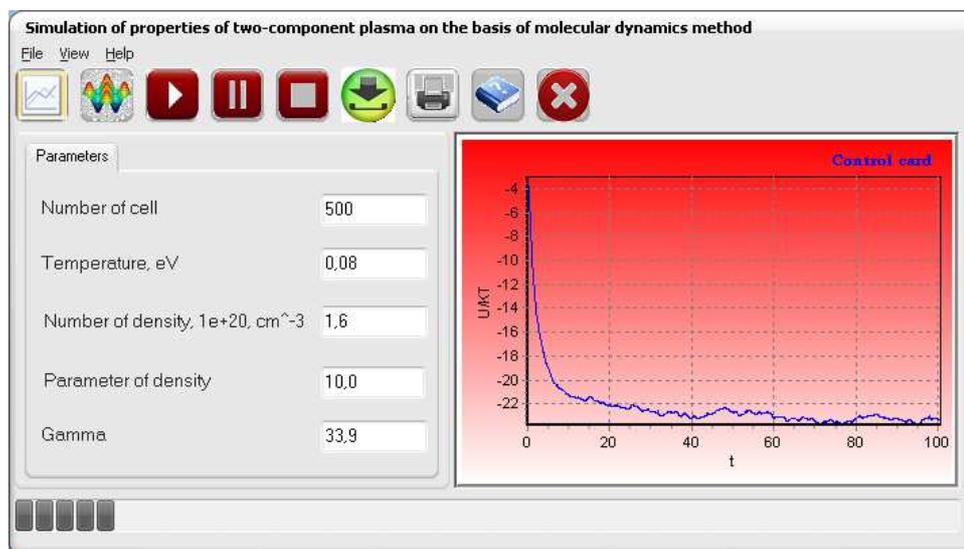


Figure 3: The view of the control card of MD simulation for a given density and temperature of the weakly coupled plasma.

developed. The spatio-temporal dependencies of physical quantities for complex plasma are obtained. Such important processes as a crystallization, phase transition and formation of ordered structures are observed by proposed software. In Fig. 3 the interface of this program is shown. The software allows the user to set the parameters of the task, to control the procedure of calculations.

The results are displayed in the course of calculation both in the form of a chart and in the form of a visualization, thus permitting the user to stop  the calculations pressing the button when any deviations are found. The button  transforms the software into the mode of visual observation of particles motion in the cell. There is the panel "Options" at the left of the software. It displays constant parameters, as well as the data calculated by the system itself. Buttons   are used to obtain the control card of MD simulation, the pair correlation functions and visualization of motion of the particles with periodic boundary conditions.

The view of the control card of MD simulation for a given density and temperature of the two-component plasma is shown in Fig. 3. It may be seen that energy tends to some mean value characterizing the output of the system to a stationary state.

4 Visual observation of particles movement

Visualization is an essential part of the process of numerical modeling, providing analysis and correct interpretation of the results of calculations, as well as further work with the computational model [8].

The special information system for visualization is constructed on the basis of the OPENGL. In the regime of visual observation of particles movement pressing this button  we can enter the values of parameters (Fig. 4). The button  allows changing the scale of the assigned sites of the graphic.

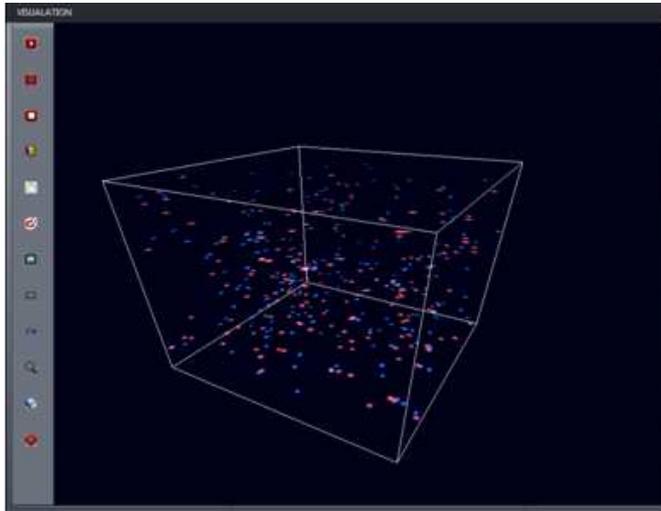


Figure 4: Program of visual observation of particles movement.

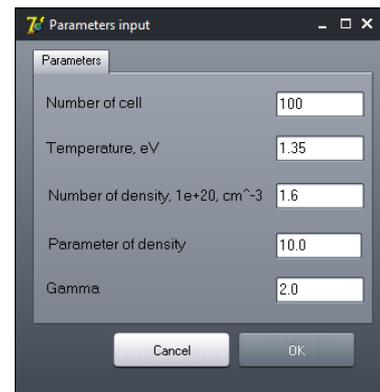


Figure 5: Parameters input.

In Fig. 5 one can see the window for entering the parameters of two-component plasma in the regime of visualization.

In this work such important processes as gas-phase regime, liquid-phase regime and the process of formation of ordered structures may be observed using this proposed software.

The pair correlation distribution functions for various states of plasma are presented in Figs. 6-8. At parameters corresponding to weakly coupled regime we can see that there is no any order in the system and the pair correlation distribution functions for gas-phase state have a monotonic character.

At parameters corresponding to liquid-phase regime we can see a local order in the system (see Fig. 7). At strongly coupled regime a weak thermal movement of particles is observed and one can see oscillation of particles at the equilibrium point.

5 Solving the Boltzmann equation to obtain characteristics of buffer (background) and dusty plasma in DC glow discharge

Dusty or complex plasma is the ionized gas consisting neutrals, ions, electrons, and negatively charged (usually) particles of micron and submicron size. Dust particles can be found in space (e.g., in interstellar clouds, in comet tails or planetary rings) or in different

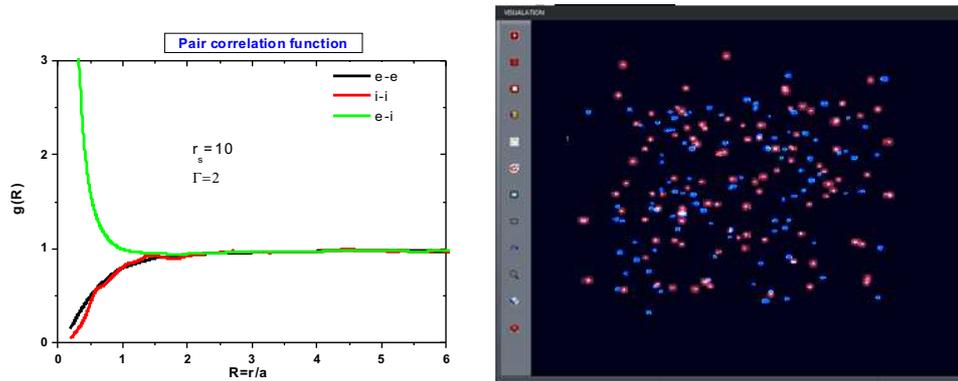


Figure 6: Pair distribution correlation functions and particles movement in weakly coupled regime.

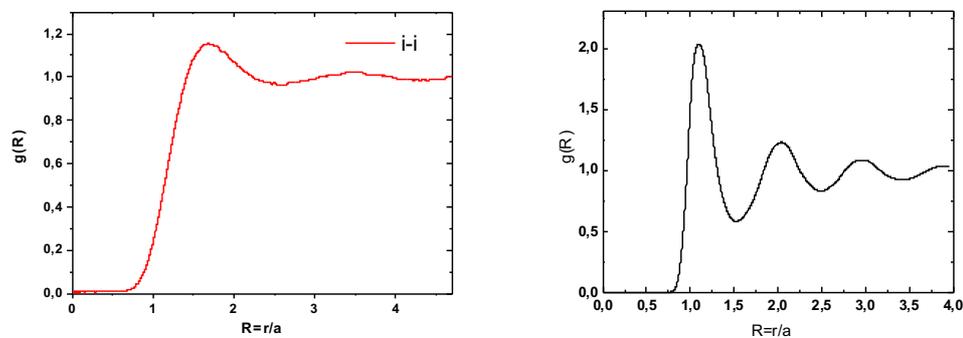


Figure 7: Pair distribution correlation functions in liquid-phase and strongly coupled states.

kinds of technical processes (e.g., plasmachemical reactions used for etching or depositing of thin films, in nuclear fusion reactors, etc.).

In recent years there is a great interest in simulation of electron kinetics in low-temperature plasma, due to numerous technological applications. It is the numerical simulation that gives accurate and complete information about the characteristics of gas-discharge plasma, which is necessary for understanding and interpreting the properties of dust structures in plasma. Dusty plasma structures were found at the following cases of dc glow and RF discharges. The pressures of gases $p = 0,1-0,4$ Torr and currents $I = 0.3-3mA$, temperature of buffer plasma particles $T_i \ll T_e \sim 1 \div 9 eV$, densities of particles $n_{i(e)} \sim (10^8 \div 10^9) cm^{-3}$ gas densities $n_g \sim (10^{14} \div 10^{16}) cm^{-3}$. The parameters of dust particles: radius $a_d \sim (1 \div 10) \mu m$; charge $Z_d \sim (10^2 \div 10^5) e$; density $n_d \sim (10^3 \div 10^6) cm^{-3}$. Under laboratory conditions, dusty plasma in a positive column of DC glow discharge or in radio-frequency (RF) discharges in low-pressure noble gases most of all are performed at such plasma parameters, which are presented below [9–14].

The study of the spatiotemporal evolution of electrons in non-equilibrium collision-dominated plasmas under the action of an electric field represents a widespread interest.

There are a great number of technological applications such as plasma-chemical processing in discharges, the film deposition and surface modification, the production of plasma light sources and gas-discharge lasers, and so on, where the non-equilibrium plasmas of low-pressure glow discharges are used.

In many papers on the study of dusty plasma in the gas discharge at low gas pressure it is assumed that the plasma electrons have a Maxwellian distribution with a temperature which is determined from probe measurements [15]. Druyvesteyn distribution is sometimes used as an alternative model which does not lead to a significant difference in the characteristics of dusty plasmas [16]. But it is well known that Maxwell and Druyvesteyn distributions are significantly different from the actual distributions of the electron energy in the gas discharge, because in a self-discharge, a significant contribution to the electron velocity distribution is made by the ionization and recombination processes.

The charging process of individual dust particles will be considered using the Orbital motion limited theory (OML theory). The charge of a dust particle is defined by equality of ionic and electronic fluxes from the environmental plasma to the particle surface: $I_e + I_i = 0$. In nonequilibrium plasma of gas discharge, the ionic and electronic fluxes towards the particle surface are described by the following formulas:

$$I_e = -e \sqrt{\frac{2}{m_e}} \int_{-e\varphi_s}^{\infty} \sigma_{cap,e}(\varepsilon) f_0(\varepsilon) \varepsilon d\varepsilon; \quad (5.1a)$$

$$I_i = e \int_0^{\infty} \sigma_{cap,i}(V) F_i(V) V d^3 \vec{V}, \quad (5.1b)$$

where $f_0(\varepsilon)$ is the isotropic part of the energy distribution function for electrons (far away from a dust particle), $F_i(V)$ is the ion velocity distribution function. According to OML theory, the electron and ion capture cross sections by a dust particle are as follows:

$$\sigma_{cap,e}(\varepsilon) = \pi r_0^2 \left(1 - \frac{|e\varphi(r_0)|}{\varepsilon} \right), \quad \varepsilon > |e\varphi(r_0)|; \quad (5.2a)$$

$$\sigma_{cap,e}(\varepsilon) = 0, \quad \varepsilon < |e\varphi(r_0)|, \quad (5.2b)$$

$$\sigma_{cap,i}(V) = \pi r_0^2 \left(1 + \frac{2|e\varphi(r_0)|}{MV^2} \right), \quad (5.2c)$$

where $\varepsilon = m_e v^2 / 2$ is the electron kinetic energy. We also assume that the velocity distribution function for ions produces the ion temperature T_i and has the average drift velocity $\vec{V}_i = \mu_i \vec{E}$ (μ_i is the ion mobility coefficient).

For the description of the stratification in the positive column of a glow discharge the Boltzmann kinetic equation for the electron energy distribution function $F(r, \vec{v})$ was used:

$$\frac{\partial F}{\partial t} + \vec{v} \frac{\partial F}{\partial \vec{r}} - \frac{e}{m_e} \vec{E} \frac{\partial F}{\partial \vec{v}} = S_t(F), \quad (5.3)$$

where S_t is the total integral of collisions, e is the charge of an electron and m_e is the electron mass.

For a low electric field along the z -axis, we can use the assumption about slight anisotropy of EEDF, so the EEDF can be expanded through Legendre polynomials and take only two first terms of polynomial (two-term approximation):

$$f\left(\varepsilon, \frac{v_z}{v}\right) = \frac{1}{2\pi} \frac{1}{(2/m_e)^{3/2}} \left[f_0(\varepsilon) + f_1(\varepsilon) \frac{v_z}{v} \right], \quad (5.4)$$

where f_0 is isotropic and f_1 is anisotropic part of EEDF. Taking expressions (5.3)-(5.4) and performing integration by angles, we can obtain the Boltzmann equations for both parts (isotropic and anisotropic) of EEDF:

$$\begin{aligned} \frac{1}{3}\varepsilon \frac{\partial f_1}{\partial z} - \frac{eE(z)}{3} \frac{\partial(\varepsilon f_1)}{\partial \varepsilon} = \frac{\partial}{\partial \varepsilon} \left[2 \frac{m_e}{M} \varepsilon^2 N_g Q^{el}(\varepsilon) f_0 \right] - \sum_k \varepsilon N_g Q_k^{in}(\varepsilon) f_0 \\ + \sum_k (\varepsilon + \varepsilon_k^{in}) N_g Q_k^{in}(\varepsilon + \varepsilon_k^{in}) f_0(\varepsilon + \varepsilon_k^{in}, z), \end{aligned} \quad (5.5a)$$

$$\frac{\partial f_0}{\partial z} - eE(z) \frac{\partial f_0}{\partial \varepsilon} + H(\varepsilon) f_1 = 0, \quad (5.5b)$$

where, z is the distance between cathode and anode, ε is kinetic energy of electrons, $E(z)$ is the electric field, $Q^{el}(\varepsilon)$ and $Q_k^{in}(\varepsilon)$ are cross sections for elastic and inelastic processes, $H(\varepsilon) = N_g Q^{el}(\varepsilon) + \sum_k N_g Q_k^{in}(\varepsilon)$.

Function $f_0(z, \varepsilon)$ allows determining electronic density n_e , temperature of electrons. If EEDF is known, we may determine various macroscopic properties of electrons by means of integrating the energy distribution function. In particular, the distribution of density and electron temperature in the positive column has the following form:

$$n_e = \int_0^\infty f_0(z, \varepsilon) \sqrt{\varepsilon} d\varepsilon; \quad (5.6a)$$

$$T_e = \frac{2}{3} \frac{1}{n_e} \int_0^\infty \varepsilon^{3/2} f_0(z, \varepsilon) d\varepsilon, \quad (5.6b)$$

In order to determine the distribution of the ion density and electric field the model of the drift-diffusion equation was used. The distribution of the ion density $n_i(z, t)$ was calculated using non-stationary drift-diffusion equation of continuity

$$\frac{\partial n_i(z, t)}{\partial t} + \frac{\partial}{\partial z} \left(n_i(z, t) \mu_i E(z, t) - D_i \frac{\partial n_i(z, t)}{\partial z} \right) = 0, \quad (5.7)$$

where μ_i , D_i -coefficient of mobility and diffusion of ions, respectively.

The electric field in the positive column of a glow discharge is determined according to the distribution of ion and electron components of the plasma and in a self-consistent way using the Poisson equation:

$$-\frac{\partial^2 \phi(z, t)}{\partial z^2} = 4\pi e_0 [n_i(z, t) - n_e(z)], \quad E(z, t) = -\frac{\partial \phi(z, t)}{\partial z}. \quad (5.8)$$

Eqs. (5.5a), (5.7)-(5.8) form a complete system of equations for determination three unknown plasma parameters $n_e(z)$, $n_i(z,t)$ and $E(z,t)$. The system of equations was calculated numerically by the method of iteration. The first approximation to the distribution function $f_0^0(z,\varepsilon)$ was obtained by solving Eq. (5.5a) with the corresponding boundary conditions for an arbitrary electric field distribution $E^0(z)$, which was usually taken to be uniform $E^0(z) = const$. At this step, the electron density distribution $n_e(z)$ is obtained by integrating the EEDF. Then the time-dependent problem (5.7)-(5.8) was calculated until reaching of full convergence, i.e. the final calculated ion density distribution satisfies the stationary continuity equation (5.7). The Poisson equation (5.8) for $\varphi(z,t)$ was solved with the help of matrix factorization method. Thus, for a given iteration, the distributions $n_e(z)$, $n_i(z,t)$ and $E(z,t)$ were obtained. At the next iteration, (5.5a) was solved in a new distribution of electric field, and a new electron density distribution, which differs from the previous one, was obtained. Then the iteration process was repeated. For the convergence of the solution, about 30-50 of iterations were necessary depending on the reduced electric field. The final distribution of the axial electric field did not depend on the choice of the initial electric field distribution $E^0(z)$.

6 Software package "Characteristics of discharge and dusty plasma in DC glow discharge"

On the basis of the described model, developed the software, which includes two packages: "Axial distributions of dusty plasma parameters" and "Radial distributions of dusty plasma parameters". In Fig. 8 the interface of this program is shown. The software allows the user to set the parameters of the task, to display the results in the course of calculation both in the form of a chart and in the form of a table.

In the course of simulation of axial distributions of dusty plasma parameters we may obtain a three-dimensional graph of distribution functions of electrons, temperature and density distribution of electrons and charge of dusty particles. In the upper part there is a panel "Parameters of discharge". Here we may assign the pressure of gas, temperature of ions, discharge current density, and initial electric field, which can be controlled by user. As well as clicking on a button "Table" it is possible to obtain the corresponding values of the results in a table and store the data.

In Fig. 9 the spatial distribution of EEDF in argon at $p = 0.17$ Torr in averaged electric field $E_0 = 4V/cm$ is presented. Fig. 9 shows the dependence of the isotropic part of EEDF in $(\varepsilon - z)$ coordinate. It is seen that as the distance to the anode decreases, the peaks of the EEDF are periodically displaced to higher kinetic energies due to electron energy gain in the electric field. It is seen that the modulation of electric field is strongly affects the 3-dimensional form of isotropic part of EEDF. Using spatial two-dimensional distribution of EEDF we may determine the temperature of electrons, the number of density of electrons and the charge of the tested particle in various points of a discharge tube. The temperature of electrons and the number of density of electrons

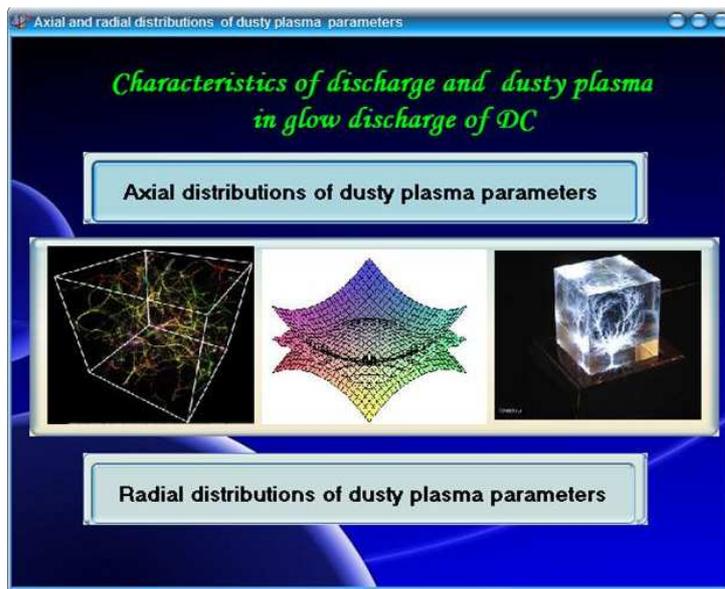


Figure 8: The interface of software package.

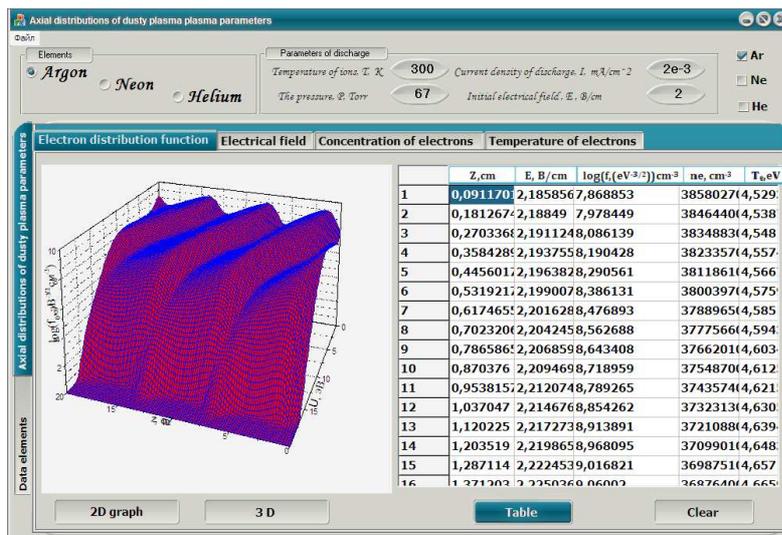


Figure 9: Three-dimensional graph of distribution functions of electrons.

in the discharge tube are shown in Fig. 10. In the radial distribution of the electron temperature in contrast to the electron density distribution, there are areas of non-monotonic for some values of the axial coordinate. This may be due to the fact that the electron energy distribution is highly heterogeneous and excesses. From the figures it is shown that the electron temperature has a hump on the periphery of the tube. This fact can be

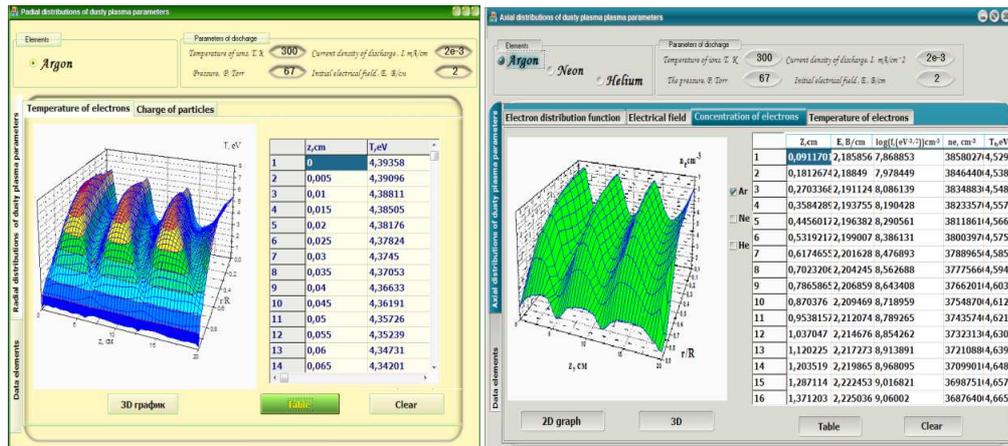


Figure 10: The temperature and the number density of electrons in the discharge tube.

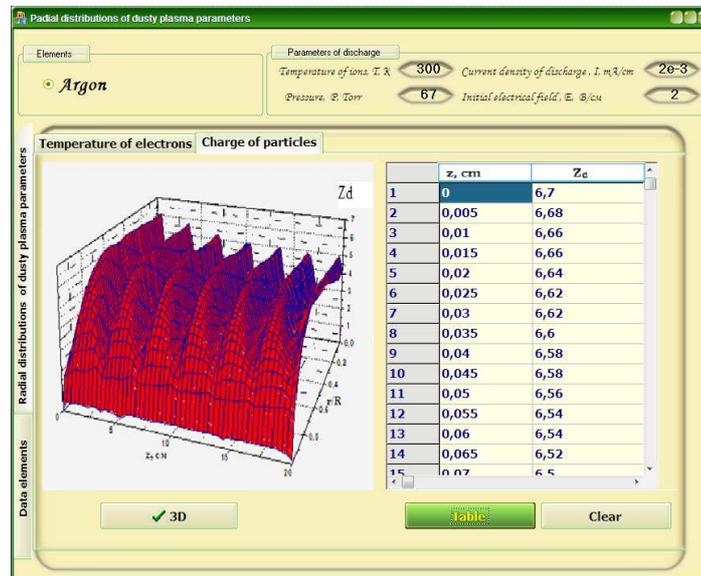


Figure 11: The radial distribution functions of dusty particles charge in 3D view.

interpreted as follows Electrons are heated due to the large values of the radial field at the reaching of the tube wall.

The charge of a single dust particle Z_d introduced into plasma was calculated from the OML theory with account for non-equilibrium EEDF. The radial distribution function of the charge of the test particle is given in Fig. 11. It is seen that there are areas in the strata in which the charge of the dust particles increases with the distance from the center of the tube. It can be concluded that with increasing distance from the tube axis, the peaks in the distribution of the surface potential of the dust particles move towards the anode.

7 Conclusion

We have developed the program software allowing the investigation of two-component plasma properties and visually track the movement of the particles. Also we have developed the second package allowing investigate the axial and radial distributions of dusty plasma parameters using self-consistent kinetic model. The spatio-temporal dependencies of physical quantities for complex plasma are obtained. Such important processes as a crystallization, phase transition and formation of ordered structures are observed by proposed software.

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