Influence of ion shadowing effect on average inter-particle distance in dusty plasma crystals

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Abstract. Average distance between particles of dust in dusty plasma crystals is sensitive to the temperature of neutral atoms in a glow discharge plasma. In some experiments a significant decrease of average inter-particle distance after cooling to low temperatures is observed: the distance at 100 K is up to 4 times less than at 300 K. In this work dusty plasma system is studied by the method of numerical solving of Newton equations which is similar to the method of molecular dynamics. It is shown that the model of dusty plasma interaction including only the Debye potential and electrostatic parabolic trap may be not enough to explain this effect. Adding ion shadowing potential to this model increases the difference between the values of inter-particle distance at 100 and 300 K by 2–3 times. Comparison of theoretical results with experiments of other groups shows that some of the experimental points may be well approximated by this model.

1. Introduction

Macroparticles of dust injected in a plasma acquire a high electric charge due to the different mobility of electrons and ions of plasma. Typical values of the acquired charge ($\sim 10^3$–$10^4 e$, $e = 4.8 \times 10^{-10}$ statC) correspond to a high degree of non-ideality of the dusty plasma system which leads to the appearance of ordered dusty structures [1]. Properties of these structures are mostly defined by the parameters of surrounding plasma while the charged particles influence a plasma themselves. Due to this reason, the problem of counting characteristics of the structures is self-consistent and is of great interest for modern dusty plasma physics. The main difficulties are as follows:

- a proper choice and modification of the interaction potential (usually, the Debye potential is used);
- account of numerous external forces acting on the particles from neutral gas and plasma components (ion drag force, thermophoretic force, ion wake effect, neutral shadowing effect);
- poor understanding of physics of the medium containing the particles of dust (e.g., glow discharge plasma).

One of the possible ways to resolve these problems is to consider the average distance between particles in dusty structures. As in any many-particle system, average inter-particle distance is sensitive to most forces and effects influencing the system. In the recent experiments [2–6],
average inter-particle distance in the dusty structures is measured in the conditions of cooling the system down to cryogenic temperatures in a glow discharge. These results allow analyzing the role of the main forces acting in the system on the basis of suggestions about their dependence upon temperature.

In this work, the significant decrease of average inter-particle distance after cooling the system down to low temperatures in the experiments [2,3,5,6] in a glow discharge is under consideration. In one of the former works [5] it was suggested that this effect is caused by the decrease of the Debye length in plasma. However molecular dynamics (MD) simulations with dusty plasma system show that the Debye potential is not enough to provide such a decrease of distance. Due to this reason, ion shadowing potential is added to the numerical model and its influence is tested. In the second section, the theoretical model used for the MD code is described. In the third section, results for the case accounting ion shadowing potential and not accounting it are both given. In the fourth section, discussion and comparison with experimental results are made. The fifth section is devoted to conclusions.

2. Theoretical model and its justification

2.1. Contents of the model

Method of molecular dynamics is applied to the dusty plasma system by many authors [1, 7]. The model of dusty plasma chosen for this work corresponds to a typical experiment in a glow discharge. The following effects and suggestions are considered for numerical simulations:

- Debye–Hückel interaction potential.

This potential is typically used to describe the interaction of ions and electrons in plasma and is the direct solution of the Poisson’s equation accounting the linearized Boltzmann distribution. Despite the fact the Boltzmann distribution cannot be linearized for highly charged dust particles, this potential is often used for isotropic dusty plasma and shows good agreement with the experiment [8]. The mathematical form used in this work is the following one:

$$\varphi_{ij} = \frac{q}{r_{ij}} \exp \left( - \frac{r_{ij}}{\lambda_D} \right),$$

where $r_{ij}$ is the distance between two particles (numbered $i$ and $j$), $q$ is the particle charge, $\lambda_D$ is the screening length in plasma. The screening length is counted from the standard formula

$$\lambda_D = \sqrt{\frac{kT_i}{4\pi n_i e^2}},$$

where $n_i$ is the concentration of ions, the temperature of ions equals the temperature of neutrals $T_i = T_n$ as it is usually suggested.

- Electrostatic parabolic trap.

Radial electric field appears in the discharge tube in order to equalize the diffusion flows of electrons and ions to the tube walls. It attracts dust particles to the center of the tube and plays the role of a trap. Near the tube axis approximate formula for the trap looks the following way [9]:

$$\varphi_{\text{trap}} = \frac{1}{2} \alpha r_i^2,$$

where $r_i$ is the radius-vector of a particle from the center of the tube and $\alpha$ is given by the formula

$$\alpha = -\frac{1}{r_i} \frac{T_e}{e} \frac{1}{n_i(r_i)} \frac{dn_i}{dr_i},$$

where $T_e$ is the temperature of electrons.
Table 1. Values of parameters of particles, discharge plasma and discharge used in simulations.

| Parameter                        | Value       |
|----------------------------------|-------------|
| Mass \(m\) (g)                  | \(10^{-10}\) |
| Particle radius \(a\) (\(\mu\)m) | 1.5         |
| Electrons temperature \(T_e\) (eV) | 3           |
| Trap parameter \(\alpha\) (SGS units) | 0.045       |
| Tube radius \(R\) (cm)           | 0.8         |
| Step of numerical integration \(\Delta t\) (s) | \(1.8 \times 10^{-4}\) |
| Friction coefficient \(\gamma\) (s\(^{-1}\)) | 3           |

• Friction from the environment.
Dust particles move in a viscous medium consisting mostly of neutral gas atoms. Hence their interaction with the environment is well described by the Langevin equation [7,10–12]. In MD simulations the Langevin thermostat is created by adding the following force to the model:

\[ F_{\text{Lang}} = -m\gamma \ddot{r}_i + \sqrt{\frac{2m\gamma k_B T}{\Delta t}} \dot{h}(t), \]  

where \(m\) is the mass of a particle, \(\gamma\) is the friction coefficient, \(T\) is the temperature of the environment, \(\Delta t\) is the step of numerical integration and \(\dot{h}(t)\) is a normally distributed random value.

• Ion shadowing potential.
Continuous fluxes of ions and electrons flowing in the direction of a particle lead to the appearance of an attracting force between two particles caused by the transfer of momentum by ions to each of them. This can be considered as the radial ion drag force. On large distances it competes with the repulsive electrostatic potential and in certain conditions might even exceed it [13]. The formula used for the description of this potential is as follows [13]:

\[ U_{\text{sh}} \simeq -\frac{1}{3} \sqrt{\frac{2}{\pi}} \frac{q_\text{e} J_i}{r_{ij}} \frac{q_\text{e}}{T_i} \Lambda, \]  

where \(J_i\) is the ion flux counted with the use of the relation \(J_i = \sqrt{8\pi a^2 n_i v_{Ti}(1 + zT_e/T_i)}\), \(z = q_\text{e}/(aT_e)\) is the particle charge in units of \(aT_e/e\), \(a\) is the particle radius, \(\Lambda\) is the modified Coulomb logarithm [14].

Values of the most important parameters for modeling are given in table 1. It is supposed that the temperature of electrons does not change significantly with the decrease of the temperature of neutrals.

In a former work of the authors [6] it is shown that the number of particles in a structure influences the density of a structure similarly for different values of particle charge, screening length in plasma and trap parameter. Due to this reason, two particles are used in all simulations.

2.2. Justification of the model
In the simplified model of a dusty plasma system including only the electrostatic parabolic trap and the Debye potential average inter-particle distance in the structures is defined by three parameters: the charge of a particle \(q\), the screening length in a plasma \(\lambda_D\) and the parameter of a parabolic trap \(\alpha\). These parameters significantly change in the experiments in which dusty plasma is cooled down to low temperatures. Before adding ion shadowing potential into the
Figure 1. Influence of dependence of particle charge upon temperature, trap variation in the course of an experiment and ion shadowing potential on average inter-particle distance decrease. The vertical axis shows the change of average inter-particle distance after consecutive account of different factors. The black line corresponds to the simplified model with constant charge and constant trap. This model is chosen as the reference one (model 1). The red line corresponds to adding the dependence of particle charge on temperature to model 1 (model 2); the green one—to increasing the trap to its maximum counted value and using this value in model 2 (model 3); the blue and the dark-green one—to the account of ion shadowing potential in model 3 at the values of ion concentration $10^9$ (model 4) and $10^{10}$ cm$^{-3}$ (model 5) respectively.

model, influence of these three parameters on average inter-particle distance in cold dusty plasma is tested. A few assumptions about their dependence upon the temperature of neutral atoms are made:

- The charge of a particle decreases at low temperatures due to a decrease of mobility of ions and electrons. The formula for its dependence on temperature is obtained by approximation of data given by Maiorov in [5]:

$$q = -e(a_q + b_q T_n^{0.955}),$$

where $a_q = -195$, $b_q = 1900$ K$^{-0.955}$. In the original work [5] the charge of an isolated dust particle was counted using particle-in-cell simulations for three values of temperature of neutral gas: 4.2, 77 and 300 K. Dusty plasma was considered in the conditions of helium glow discharge which is similar to the model system studied in this work. The formula for our simulations is obtained from three values of charge and might be a rough approximation at other temperatures. However, it reflects the trend of the behavior of the charge at temperatures lower than room one.

- The screening length in a plasma is proportional to the square root of temperature as the Debye length.

- The parameter of a parabolic trap in a dc discharge depends on the temperature of electrons in surrounding plasma which is defined by the product of $pR$ where $p$ is the neutral gas pressure, $R$ is the discharge tube inner radius. In the experiments considered in this work, the range of measured pressures and the diameters of the tubes correspond to the
temperature of electrons lying in the range 2.5–4.0 eV. Trap parameters that are counted using this range of temperatures lie in the range $(4.0–6.0) \times 10^{-2}$ SGS units.

In order to test the influence of each parameter on average inter-particle distance, dependence of the distance upon temperature is included in the model consecutively in serial molecular dynamics simulations. The results of these simulations are presented in figure 1 in the form of relative contribution of each factor to the decrease of average inter-particle distance $(-\Delta r / r_0)$ where $r_0$ is the distance between the particles in the simplified model). The bottom line in the graph derives from the standard model in which the charge of the particle and the trap parameter are supposed to be constant ($q = 3000e$, $\alpha = 4.5 \times 10^{-2}$ SGS units, $n_i = 10^9$ cm$^{-3}$). The only factor that is dependent on the temperature of neutral atoms in this case is the screening length in a plasma. Account of the charge dependence upon temperature leads to the miserable decrease of inter-particle distance at low temperatures. This effect causes only 2% difference in inter-particle distance at low temperatures. Variation of the trap parameter up to the maximum value $6.0 \times 10^{-2}$ SGS units causes further decrease of average inter-particle distance up to 4.5% at low temperatures. However, account of ion shadowing potential drops the distance by 24% at low temperatures at the value of ion concentration $n_i = 10^{10}$ cm$^{-3}$ and by 65% at the value of ion concentration $n_i = 10^{10}$ cm$^{-3}$. While at low concentrations of ions ($\sim 10^8$ cm$^{-3}$) the influence of this force is miserable, at high values of concentration it is to be accounted in the model.

3. Theoretical results
The first group of numerical experiments is conducted using the standard model including only the Debye potential and electrostatic parabolic trap. At the beginning of a numerical simulation, two particles are located at random positions. In the course of 3000–4000 steps of integration they move to their equilibrium positions and in each run $\sim 10000$ more steps are made in order to confirm that the structure is stable. The animation of the structure evolution is watched every time. 50 runs at each value of temperature allow averaging the value of inter-particle distance. The second group of numerical experiments is implemented using the same technical algorithm. The theoretical model for the second group includes the ion shadowing potential.

The results for both groups are given in figure 2. Red lines correspond to the numerical experiments accounting ion shadowing potential, blue lines—to the ones without it. It can be seen that the inter-particle distance dependence on temperature defined only by the Debye potential is almost horizontal. The distance does not change significantly due to a weak change of the Debye length with temperature decrease. At a temperature close to a room one and the ion concentration $n_i = 10^9$ cm$^{-3}$, account of ion shadowing does not cause a noticeable change of inter-particle distance. However when ion concentration is $10^{10}$ cm$^{-3}$, the change of distance is about 20 $\mu$m and can be measured in an experiment. At low temperatures, ion shadowing causes an even higher difference between the two dependencies: 50 and 120 $\mu$m at 70 K respectively.

In the latter case, it is 60% of the original distance.

This result has a qualitative explanation: the ion shadowing force is attractive, it is proportional to the ion density and is inversely proportional to the ion temperature. It grows with temperature decrease and ion concentration increase, attracting particles stronger and lessening the distance between them.

4. Comparison with experimental results
From the results obtained in the previous section, it is clear that the model including only the Debye potential and electrostatic parabolic trap cannot explain a large drop of inter-particle distance in dusty plasma structures at low temperatures. However, it is often observed in laboratory experiments. In the experiment [5] the value of inter-particle distance measured at
Figure 2. Dependence of the distance between particles in dusty plasma structures upon the temperature of neutral atoms. Blue lines correspond to results obtained for the model not accounting ion shadowing potential; red lines—for the one accounting it. Solid lines correspond to the ion concentration $n_i = 10^9$ cm$^{-3}$; dotted lines—$n_i = 10^{10}$ cm$^{-3}$.

Figure 3. Dependence of the distance between particles in dusty plasma structures upon the temperature of neutral atoms. Black line corresponds to numerical simulations, red one—to the experiment [2].

300 K is 500–750 µm and at 77 K is 200–250 µm. The ratio is approximately 3 and is higher than could be provided by the Debye potential. In [6] the inter-distance distance decreases by 2 times when the temperature changes from 300 to 200 K.

In [2] cooling the system from 300 down to 100 K leads to the distance decrease in the center of the structure from 140 to 40 µm—by 3.5 times. The pressure in the experiment is 0.61 Torr. Assuming that it stays constant in the process of cooling and that ionization degree of
plasma does not change at constant current, the dependence of ion concentration on the neutrals temperature is \( n_i = 6 \times 10^9 \times \frac{300}{T_n} \). The value of ion concentration at a room temperature is chosen in order to get the same value of inter-particle distance as in the experiment.

Results of modeling of this situation are presented in figure 3. It can be seen that the drop of inter-particle distance by 3.5 times coincides both in theory and the experiment. The overall behavior of the dependence is different which may be caused by a more significant change of ion concentration in the process of cooling than expected.

5. Conclusions
It is shown that the theoretical model of dusty plasma including the Debye potential and electrostatic parabolic trap is not enough to explain the significant decrease of inter-particle distance in dusty plasma structures at low temperatures. Account of ion shadowing force allows obtaining drops of inter-particle distance by up to 4 times at low temperatures and up to 10% at a room temperature. It means that at high values of ion concentration (\( > 10^9 \) cm\(^{-3}\)) ion shadowing force is to be accounted in theoretical models of dusty plasma. However, ion shadowing force does not explain the form of the dependence of average inter-particle distance on temperature. It is the problem of further research.

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