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Model of Melting (Crystallization) Process of the Condensed Disperse Phase in the Smoky Plasmas

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Abstract. The paper presents an analysis of the causes of a formation of spatial ordered grain structures in a smoky plasma. We are modeling the process of melting (crystallization) of a condensed phase in this environment taking into account the screened electrostatic interaction and the diffusion-drift force. We discuss an influence of the charge on the melting temperatures.

INTRODUCTION

Smoky plasma is a special type of the plasma with a condensed dispersed phase and differs from the widespread gas-discharge dust plasma by the presence of grains emitting electrons, the coalitional character of the interaction, and the multimode grain size distribution. The peculiarity of the processes in the smoky plasma is also that the grains are formed directly in the plasma. As a result, the condensed phase can be represented by three fractions of grains with average dimensions of 10 nm, 0.1 μm and more than 1 μm. This significantly complicates the processes of interphase and interparticle interaction. That is why in the smoky plasma, in contrast to the "plasma crystals" of dusty plasma, the spatial ordered grain structures which have been observed for the first time in the combustion products of metalized compositions with a readily ionizable admixture of cesium atoms are observed [1]. An analysis of the causes of the formation of ordered grain structures in smoky plasma was carried out much later in [2]. It was found that the formation of spatially ordered structures in the smoky plasma occurs as a result of the action of electrostatic and diffusion-drift forces. Moreover, the diffusion-drift force arises from the anisotropy of the degree of ionization of the plasma around the grain. An interesting feature of the smoky plasma obtained in a gas-dispersed metalized flame is the detected electroacoustic vibrations of alumina particles [3], as well as the presence of negatively charged grains in a thermionic plasma [4]. The obtained data indicate a sufficiently strong interaction of charged condensed grains in the smoky plasma, which stimulates the study of the critical conditions for the melting and crystallization of ordered structures of the condensed phase. At the same time, such studies have not been conducted so far.

The results of modeling the process of melting (crystallization) of a condensed phase in a smoky plasma are presented, taking into account the screened electrostatic interaction [5] and the diffusion-drift force caused by anisotropy of the degree of ionization in the vicinity of the grains in gas phase.

It is assumed that in the plasma the ordered structures of the charged grains of the same charge are formed in the case when the Coulomb repulsion forces are balanced by the diffusion-drift interaction forces. However, this is not enough to determine the conditions for the melting (crystallization) of grains formations. In a weakly ionized plasma, the charges of aluminum oxide grains do not exceed several charges of an electron, and therefore in ordered structures the distances between particles are larger than the Debye screening length. In this case, the energy of interaction between grains is much less than their energy of chaotic thermal motion.

The latter made it possible to assume that the conditions for the melting (crystallization) of the condensed phase occur when the grains approach a distance such that the interaction between them in the ordered structures is much greater than the energy of the chaotic thermal motion. Another condition for melting (crystallization) is to assume the relation between the oscillations amplitude of the grains and the lattice constant of the "crystal." In the crystalline state, the lattice constant is much larger than the amplitude of the oscillations.

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RESULTS

To determine the conditions of melting (crystallization) in a smoky plasma, phenomenological criteria are considered: 1. Lindemann's criterion is the ratio of the mean square displacement of a grain to the average interparticle distance; 2. Criterion Hansen and Verlet; 3. Loewen's dynamic criterion of crystallization [6,7].

The Lindemann's criterion (X_L) is defined as the ratio of the oscillation amplitude of a solid grain (plasma component) to the distance between the centers of the nearest plasma particles [7].

$$X_L = \left(\frac{\langle r^2 \rangle_E}{C^2} \right)^{1/2} \approx 0.133 - 0.186 \tag{1}$$

The numerical value of the Lindemann's criterion is characteristic for systems with the Coulomb interaction. The value $X_L = 0.186$ is characteristic of one component plasma. This plasma state corresponds to the coupling parameter $\Gamma = 178$ (if we measure the distance in units of the Wigner–Seitz radius (R_w). The value $X_L = 0.133$ is characteristic of the model of hard spheres (HS) — the Lenard–Jones system.

The determination of the amplitude of the oscillations of solid grains in a plasma is carried out taking into account the Einstein frequency of oscillations of plasma grains [6]:

$$\langle r^2 \rangle_E = \frac{3h^2 T}{m_p k \theta_E^2 f_y}, \tag{2}$$

where $\theta_E = h\upsilon / k$ — Einstein's temperature, h and k — the Planck and Boltzmann constants respectively; T — plasma temperature, m_p — mass of the grain; f_y — is a function that takes into account the deviation from the linear dependence of the amplitude of the vibration of plasma grains on the plasma temperature at low temperatures and varies within the limits $0 < f_y \leq 1$. The value of the function f_y is determined by the formula [5]:

$$f_y = \left(\frac{2}{y} \right) \left[\frac{1 - \exp(-y)}{1 + \exp(-y)} \right] ; y = \theta_E / T \ . \tag{3}$$

At high temperatures $T >> \theta_E$, the function f_y=1. The distance between the centers of the nearest particles in the plasma is determined as follows:

$$c = \left(6\eta / \pi n_\delta \right)^{1/3}. \tag{4}$$

Formula (4) is written for regular packing with a coordination number of 12. In this case, $\eta \approx 0.74$. In formula (4), n_p is the concentration of grains in the condensed phase, m^{-3}.

It should be noted that in such a record formula (4) is valid for a compacted. At the same time, a solid particle (aggregate) in a plasma should be considered as a regular fractal. Solid particles (aggregates) in a plasma, in general, are randomly distributed in space. Consequently, the correct use of formula (4) requires knowledge of the fractal characteristics in the plasma. Such characteristics are the fractal dimension and the distribution function of particles (aggregates) in size. Formula (4) for evaluating the melting processes of plasma crystals can be considered as the first rough approximation.

The oscillation frequency of the unit is determined by the formula [3]:

$$\upsilon = \sqrt{\frac{4\pi Q^2 n_p}{m_p}} \ . \tag{5}$$

Here, $Q = eZ$ is the grains' average charge, where e is elementary charge, Z is charge number.

The oscillation frequency of aggregates in a plasma can also be calculated by the formula:

$$\upsilon = 2\sqrt{\frac{\mu}{m_p}}, \tag{6}$$

$$\mu = \frac{Q^2}{c^3 D^2} \exp\left(\frac{r_p - c}{D} \right) \left(c^2 + 2D^2 + 2cD \right), \tag{7}$$

where (7), c is the lattice constant, r_p is the radius of the aggregate, and D is the Debye screening length.

Formulas (1–5) can be used to describe the state of the plasma on the melting line. We will assume that the concentration of particles (aggregates) in a plasma can be determined by the formula: $n_p = (6\eta/\pi)d^{-3}$. It should be noted that the calculation of the concentration of particles in the plasma according to this formula can be carried out only with the constraints stipulated for formula (4).

On the basis of the formulas given above, we can write down the condition for the existence of a plasma on the melting line:

$$n_p = \left[\frac{3}{4\pi}\left(\frac{\pi}{6\eta}\right)^{2/3}\frac{kT}{X_L^2 Q^2}\right]^3, \quad (8)$$

$$Q = \left[\frac{3}{4\pi}\left(\frac{\pi}{6\eta}\right)^{2/3}\frac{kT}{n_p^{1/3} X_L^2}\right]^{1/2}. \quad (9)$$

Formulas (8) and (9) are used as the defining parameter of the Lindemann's criterion.

The conditions for the existence of a plasma on the melting line can also be determined on the basis of the plasma nonideality criterion:

$$Q = \left[\Gamma(\kappa)\left(\frac{4}{3}\pi n_p\right)^{-\frac{1}{3}} kT\right]^{\frac{1}{2}}. \quad (10)$$

The melting point of the crystal (plasma) is determined as follows:

$$kT_m = X_L^2 \frac{m}{3}\left(\frac{ck\theta_E}{h}\right)^2. \quad (11)$$

From the formula (9) we obtain:

$$kT_m = \frac{4\pi}{3}\left[\frac{6\eta}{\pi}\right]^{\frac{2}{3}} X_L^2 Q^2 n_p^{\frac{1}{3}}. \quad (12)$$

We consider the conditions for the existence of a plasma on the melting line in the example of a thermal plasma — the condensed phase is represented by submicron smoke particles Al_2O_3 of spherical shape with an effective diameter of 1 μm. The temperature of the condensed phase is equal to T = 2300 K [2]. For particles of this diameter, the particle concentration in the crystalline phase, determined by the formula $n_p = (6\eta/\pi)d^{-3}$, is $10^{18} m^{-3}$. We choose, as a first approximation, the values of the criterion X_L, the intermediate intervals from the interval indicated in formula (1). In this case, the average charge of a particle (aggregate) calculated in accordance with formula (9), in units of elementary charge varies within Z = 1000–4000.

In deriving formula (9), the oscillation frequency of the particle (aggregate) was calculated from formula (5). For comparison, the oscillation frequency of a particle (aggregate) was calculated using formulas (6) and (7). When calculating by formula (7) for the plasma crystal condition, the exponential term, in a good approximation, can be taken equal to unity. The calculation of the oscillation frequency of a particle (aggregate) according to formulas (6) and (7) differs from the value obtained by formula (5) by 15 %. This is due to the fact that the lattice constant in formula (7) is defined for a regular lattice, not a fractal lattice. The values of particle charge number Z = 3–3460 are obtained in this case.

Determination of the melting point is carried out according to formulas (11) and (12) for the following plasma parameters: Z = 1000–4000; $n_p = 10^{18} m^{-3}$; $m_p = 1.67 \times 10^{-14} kg$.

Fig. 1 shows the melting surface for these parameters. It is seen that in the region of small values of the density of the solid phase, the effect of the charge on the critical melting temperature is linear.

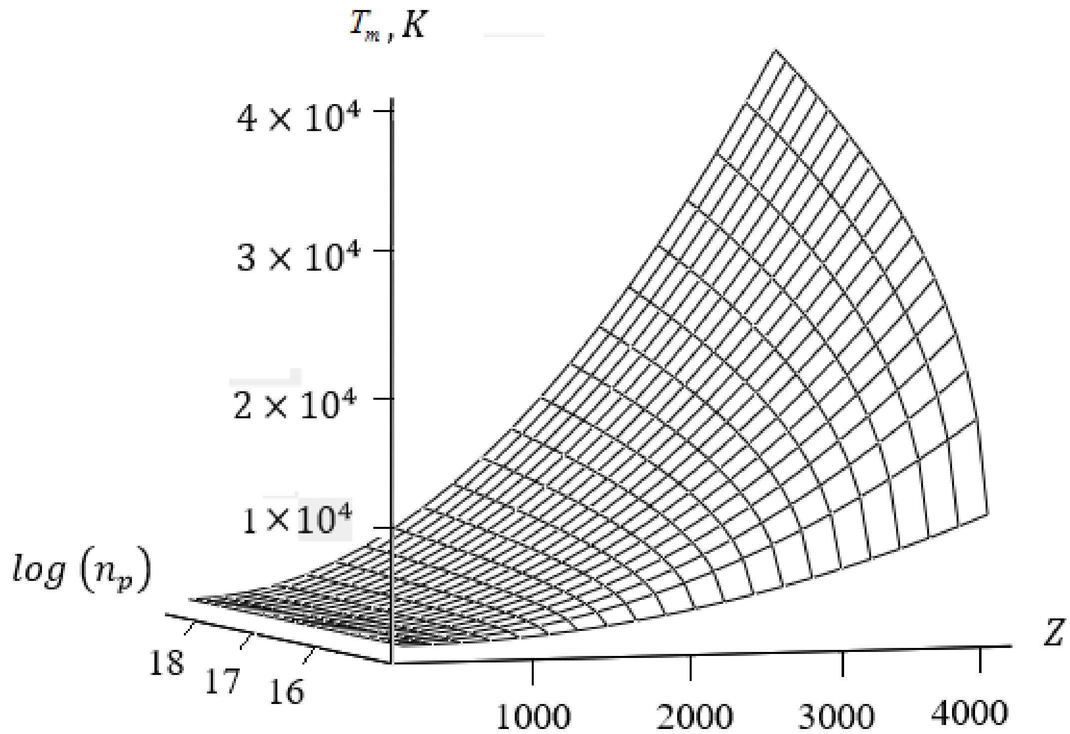

FIGURE 1. Melting surface for: $Z = 1000–4000$; $n_p = 10^{18}$ m^{-3}; $m_p = 1.67\times10^{-14}$ kg.

CONCLUSION

The melting point (T_m) in the parametric representation (Z, n_p) can be described by a surface whose height is close to zero value in the region of low densities and monotonically increases with increasing parameters (Z, n_p). In the region of low density values, the charge practically does not affect the melting temperature. Such a slight change in the melting point is observed almost to the density value of $n_p = 5\times10^{18}$ m^{-3}. In the region of high density values, the influence of charge on the melting temperature increases substantially and nonlinearly.

The main question of using the phenomenological criteria for determining the conditions of the phase transition is the role of size effects: how correct is the plasma crystal interpretation in the macroscopic approximation.

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