

INFLUENCE OF THE SIZE DEPENDENCE
OF THE WORK FUNCTION ON THE FREE
ELECTRON CONCENTRATION IN THERMAL DUSTY
PLASMA FORMED BY NANOPARTICLES
OF TUNGSTEN AND HOT INERT GAS

I. I. Fayrushin¹, N. F. Kashapov¹, and A. I. Saifutdinov^{1,2}

¹Kazan Federal University
Kazan 420008 Russia
e-mail: fairushin_ilmaz@mail.ru

²St. Petersburg State University
St. Petersburg 198504, Russia

Taking into account the size dependence of the electron work function, the average concentration of free electrons in thermal plasma dusty plasma formed by nanoparticles of tungsten and hot inert gas has been calculated. It is shown that taking into account the size dependence of the electron work function of tungsten nanoparticles leads to an underestimation of the average concentration of free electrons in thermal plasma. With increasing temperature, this effect is weakened. It is found that with decreasing radius of nanoparticles ranging from 5 to 50 nm, averaged thermal electron concentration in the plasma increases monotonically, the maximum is not observed.

Introduction

Low-temperature plasma containing the particles of the condensed matter is commonly called dusty plasma or plasma with dust condensed dispersed phase. If the pressure of the gas surrounding the dust particles, is close to atmospheric or higher pressure and at temperature from 1500 to 3500 K, the particles may be heated to emit electrons and acquire a certain positive charge [1–5]. Such a system is called the thermal of

dusty plasma (TDP). This kind of plasma occurs in practical applications such as, for example, thermal spray coating application processes, and plasma chemical gas-phase synthesis of the particles, as well as in nature. It should be noted that the TDP can be formed by heating the gas by passing of shock waves in the presence of particulate [6, 7].

There are many experimental and theoretical papers devoted to research of TDP (see, for example, [1, 2, 5–8]). In the recent paper [8], the calculation of TDP conductivity has been carried out. The main objective of this work is to determine the concentration of electrons emitted by particles in the ambient buffer gas. In this paper, it is pointed out that in the calculations, the size dependence of the electron work function of the material particles was not taken into account. However, it should be borne in mind that the inclusion of dimension correction for a work function may affect the final result of calculations of the concentration of free electrons in the TDP. The question of the size dependence of the work function has been extensively studied (see, for example, [9–16]). In [9], it is noted that an increase in the work function with decreasing particle size results in the fact that at a certain radius of particles, the maximum effect of emission of electrons in the hot gas is achieved. This, in turn, leads to the fact that the condensed particles may more efficiently deliver free electrons than the gas phase.

Model Description

In this paper, accounting of the size dependence of the work function in the calculation of the electron density in the heat of dusty plasmas produced by nanoparticles of tungsten and hot inert gas has been carried out. The temperature was set in the range from 3100 to 3500 K.

The following equation was used to take into account the contribution of the size effect in the work function [10–16]

$$I_p(n) = W + \frac{\text{Const}}{n^{1/3}} \quad (1)$$

where $I_p(n)$ is the ionization potential (work function) of the particle, consisting of n atoms and W is the work function of bulk material. Equation (1) was obtained in studies on the size dependence of the work function, which is used in various modifications of the method of

density functional theory. According to theoretical works [10,11,14] and experimental data [12,13,15,16], the constant in Eq. (1) depends on the material. If, following Smirnov [17], one takes as $I_p(1)$ the ionization potential of a single atom, then, for instance, in the case of a tungsten particle of diameter 10 nm (which contains approximately 263 200 atoms), one obtains $I_p(263\,200) = 4.594$ eV. It is seen from this that for such level of precision, the size correction for these particles is 0.054 eV.

To calculate the value of the concentration of free electrons in the TDP, let us use the model which is based on the Poisson–Boltzmann equation for the electric field potential ϕ :

$$\Delta\phi = \frac{q}{\varepsilon\varepsilon_0} n_{e0} \exp\left(\frac{q\phi}{kT}\right) \quad (2)$$

where q is the absolute value of the electron charge; ε is the relative dielectric constant of the gas; ε_0 is the electric constant; k is the Boltzmann constant; and T is the absolute temperature of the TDP. The number density of the thermally emitted electrons near the surface of a particle is determined from the following expression [18,19]:

$$n_{e0} = 2 \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} \exp\left(-\frac{I_p(n)}{kT}\right),$$

this includes the value of $I_p(n)$ which also takes into account the size dependence of the work function.

Since the spherical particles are considered to be of the same radius and to be uniformly distributed in space, Eq. (2) becomes

$$\frac{d^2\phi}{dr^2} + \frac{2}{r} \frac{d\phi}{dr} = \frac{q}{\varepsilon\varepsilon_0} n_{e0} \exp\left(\frac{q\phi}{kT}\right).$$

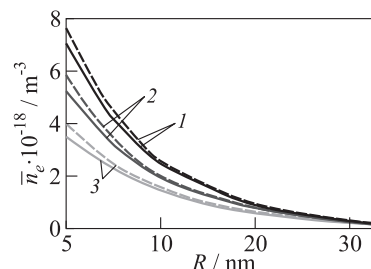
The boundary conditions are specified in the form $\phi(R) = 0$, $\phi'(l) = 0$, and the second condition means electroneutrality area per particle (Wigner–Seitz cell).

Results

Knowing the distribution of potential in terms of the Boltzmann equation, the distribution of the concentration of free electrons in the space

between the particles can be calculated. The figure shows the plots averaged over the volume concentration of free electrons in plasma vs. the radius of the particles at different temperatures. The calculations are performed for tungsten nanoparticles by their mass equal to the plasma concentration of 19.25 g/m^3 . The particle radii were set in the range of 5 to 50 nm. The smaller particles were not considered because in this case, the size dependence of tungsten melting temperature starts to influence [20].

As can be seen from the figure, the account of the size dependence of the electron work function of tungsten nanoparticles leads to not significant underestimation of the concentration of free electrons in the plasma formed by the heat of the dust of these particles and the heated inert gas. When the temperature increases, the relative increase in the concentration of free electrons is reduced. When the particle size decreases, the electron density monotonically increases. Thus, in the tungsten particle radius range between 5 and 50 nm, the maximum concentration of free electrons in the plasma was not observed.



The dependence of the concentration of free electrons in TDP on the radius of the nanoparticles of tungsten at various temperatures: 1 — 3500 K; 2 — 3300; and 3 — 3100 K. Solid curves — the dimensional adjustment is taken into account for work output; and dashed curves — without dimensional amendments

Concluding Remarks

Thus, it was shown that taking into account the size dependence of the electron work of tungsten nanoparticles exit leads to an underestimation of the concentration of free electrons in the TPD formed by these particles and the heated inert gas. In the above range of the free-electron concentration, the maximum particle size is not found in the TDP. This maximum is apparently located in the smaller nanoparti-

cles of tungsten which has to be considered as well as size-dependent melting and vaporization of substance.

Acknowledgments

The reported study was funded by the Russian Foundation for Basic Research, according to the research project No. 16-38-60187 mol_a_dk. The work is performed according to the Russian Government Program of Competitive Growth of Kazan Federal University.

References

1. Fortov, V. E., V. S. Filinov, A. P. Nefedov, O. F. Petrov, A. A. Samaryan, and A. M. Lipaev. 1997. Creation of ordered structures in a classical thermal plasma containing macroparticles: Experiment and computer simulation, *J. Exp. Theor. Phys.* 84:489.
2. Samarian, A. A., O. S. Vaulina, A. P. Nefedov, V. E. Fortov, B. W. James, and O. F. Petrov. 2001. Positively charged particles in dusty plasmas. *Phys. Rev. E* 64:056407.
3. Fortov, V. E., A. G. Khrapak, and I. T. Yakubov. 2004. *Fizika neideal'noy plazmy* [Physics of nonideal plasma]. Moscow: Fizmatlit. 528 p.
4. Fortov, V. E., and G. E. Morfill, eds. 2010. *Complex and dusty plasmas: From laboratory to space*. CRC Press. 440 p.
5. Vishnyakov, V. I. 2012. Charging of dust in thermal collisional plasmas. *Phys. Rev. E* 85:026402.
6. Bityurin, V. A., and N. I. Klyuchnikov. 2011. A conducting macroparticle in dense electronegative gas under thermionic emission. *High Temp.* 49:466.
7. Bityurin, V. A., A. C. Dobrovol'skaya, and N. I. Klyuchnikov. 2013. The shock wave structure in a dense electronegative gas containing conductive particles. *High Temp.* 51:575.
8. Zhukhovitskii, D. I., O. F. Petrov, T. W. Hyde, G. Herdrich, R. Laufer, M. Dropmann, and L. S. Matthews. 2015. Electrical conductivity of the thermal dusty plasma under the conditions of a hybrid plasma environment simulation facility. *New J. Phys.* 17(5):053041.
9. Maltsev, V. M. 1977. *Main characteristics of combustion*. Moscow: Khimiya. 320 p.
10. Wood, D. M. 1981. Classical size dependence of the work function of small metallic spheres. *Phys. Rev. Lett.* 46:749.

11. Van Staveren, M.P.J., H.B. Brom, L.J. de Jongh, and Y. Ishii. 1987. Energetics of charged small metal particles. *Phys. Rev. B* 35:7749.
12. Leopold, D.G., J.H. Ho, and W.C. Lineberger. 1987. Photoelectron spectroscopy of mass-selected metal cluster anions. I. Cu_n^- , $n = 1-10$. *J. Chem. Phys.* 86:1715.
13. Ganteför, G., M. Gausa, K.-H. Meiwes-Broer, and H.O. Lutz. 1988. Ultraviolet photodetachment spectroscopy on jet-cooled metal-cluster anions. *Faraday Discuss. Chem. Soc.* 86:197.
14. Bréchnignac, C., P. Cahuzac, F. Carlier, M. de Frutos, and J. Leygnier. 1990. Alkali-metal clusters as prototypes of metal clusters. *J. Chem. Soc. Faraday Trans.* 86:2525.
15. Gausa, M., G. Ganteför, H. O. Lutz, and K.-H. Meiwes-Broer. 1990. Electronic structure of group III heavy element clusters studied by photoelectron spectroscopy. *Int. J. Mass Spectrom. Ion Proc.* 102:227.
16. Seidl, M., K.H. Meiwes-Broer, and M. Brack. 1991. Finite-size effects in ionization potentials and electron affinities of metal clusters. *J. Chem. Phys.* 95:1295.
17. Smirnov, B.M. 2000. Cluster plasma. *Phys. Usp.* 43:453.
18. Williams, H., J.D. Lewis, and R.M. Hobson. 1961. The influence of thermal ionization processes on the design of a fossil fuelled mhd power generator. *Advances in magnetohydrodynamics*. Sheffield University. 140 p.
19. Sodha, M. S., and S. Guha. 1971. Physics of colloidal plasma. *Adv. Plasma Phys.* 4:219.
20. Borynyak, L. A., and A. P. Chernyshev. 2013. The method of the equivalent sintering temperature calculation. *Metal Working Mater. Sci.* 2(59):39-49.