ON THE INFLUENCE OF ZIRCONIUM AND TANTALUM IMPURITIES ON THE TRANSPORT PROPERTIES OF MULTICOMPONENT THERMAL PLASMA

P.V. Porytskyy, L.M. Sviata

Institute for Nuclear Research, Kyiv, Ukraine
E-mails: lsvjat@kinr.kiev.ua, poryts@kinr.kiev.ua

The influence of zirconium and tantalum impurities on the transport properties of multicomponent thermal plasma is considered in the ambient atmosphere of argon and air. The calculations are carried out on the base of Grad's method, and it is shown that a small amount of metal causes the essential changes in the values of transport coefficients in comparison with the cases of pure gaseous mixtures. It is revealed that the influence of the Ramsauer effect on transport properties can be neutralized by additions of metal into ambient argon.

PACS: 52.25.Fi, 52.25.Vy, 52.25.Ya, 52.27.Cm, 52.77.Fv, 52.50.Nr, 52.80.Mg

INTRODUCTION

Zirconium and tantalum are known to be widely used in nuclear technology and devices for nuclear power plants. The improvements of nuclear material technology are connected with using of plasma devices and industrial electronic plants. At operation the process of erosion leads to the evaporation of the metal impurities into the discharge region that causes the change of plasma properties.

The improvement in controlling plasma processing needs for accurate numerical modeling. Transport properties are indispensable input data for the modeling. At weakly ionization the Lorentzian theory is suitable to calculate the properties of multicomponent thermal plasma [1]. But at increasing of ionization processes a number of collision processes are known to be included into consideration. Because of that it is the many processes are needed to take into account in the calculation procedure.

In this paper, the transport coefficients for multicomponent plasma with zirconium and tantalum impurities are calculated on the base of the Grad's method [2, 3]. It is shown that the impurities have an influence on the transport properties of thermal plasma.

1. METHOD OF CALCULATION

It should be noted that the present state of the theory of gas mixtures, as well as multicomponent plasma, is characterized by the lack of a unified approach to the description of transport processes. The reason for this is a very complex nature of dependencies of the properties of gas mixtures and plasma on the properties of pure gases and concentrations of the components.

The calculations are carried out at assumption of local thermodynamic equilibrium. The following species have been taken into account for argon-based mixtures: e^-, Ar, Ar^+, Me, Me^+, Me^{2+}, Me_2, Me_2^+, and others analogous mixtures. In turn, for air-based mixtures the following species had used that's are e^-, N_2, O_2, NO, N, O, N^+, O^+, NO^+, N_2^+, O_2^+, Me, Me^+, Me^{2+}, Me_2, Me_2^+. The plasma composition has shown on Fig. 1 for the case of mixture of air with tantalum.

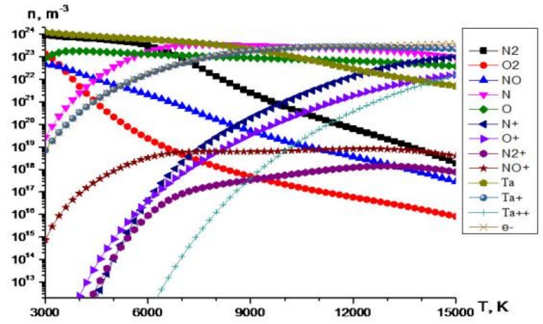

Fig. 1. Plasma composition for mixture of air with tantalum (molar parts 99:1). Others species are negligible small

The knowledge of plasma composition allows us to calculate the transport coefficients for certain plasma mixture. Thus, the coefficient of thermal conductivity is calculated as the sum

$$\lambda = \lambda_h + \lambda_e + \lambda_{\text{int}} + \lambda_{ri} + \lambda_{rd} \ , \qquad (1)$$

where λ_h is the translational thermal conductivity of heavy particles, λ_e is the thermal conductivity of electrons, λ_{int} is the thermal conductivity due to the transfer among the internal degrees of freedom, λ_{ri} is the reactive thermal conductivity due to ionization, λ_{rd} is the reactive thermal conductivity due to dissociation.

In turn, the coefficient of viscosity is calculated as the sum of additions from heavy particle η_h and electrons η_e:

$$\eta = \eta_h + \eta_e \ . \qquad (2)$$

It should be underlined that, now, the Grad's method of moments [2, 3] is an unique alternative in spite of the most developed Chapman-Enskog' method [4-8] to solve the kinetic Boltzmann equation. Both the methods are based on the formalism of Chapman-Cowling kinetic integrals

$$\Omega_{\alpha\beta}^{lr} = \left(\frac{kT}{2\pi\mu_{\alpha\beta}}\right)^{1/2} \int_0^\infty \varsigma^{2r+3} e^{-\varsigma^2} Q_{\alpha\beta}^{(l)}(\varsigma)\, d\varsigma \quad , \qquad (3)$$

where k is Boltzmann constant, T is temperature, $\mu_{\alpha\beta}$ is a reduced mass of collided species of α and β, $\varsigma = \left(\mu_{\alpha\beta}/2kT\right)^{1/2} g$, g is the relative velocity, and transport cross-section of order l is determined as

$$Q_{\alpha\beta}^{l}(g) = 2\pi \int_0^\pi \sigma_{\alpha\beta}(g,\chi)\left(1-\cos^l \chi\right) \sin\chi\, d\chi \; ,$$

where χ is scattering angle, $\sigma_{\alpha\beta}(g,\chi)$ is differential scattering cross-section.

In the 13-moments (13M) approximation of the Grad's method the translational transport coefficients are calculated as the sum of effective coefficients for each species

$$\eta_h = \sum_\alpha \eta_{h\alpha} \; , \qquad (4)$$

$$\lambda_h = \sum_\alpha \lambda_{h\alpha} \; . \qquad (5)$$

The effective coefficients are calculated on the base of combination of the Chapman-Cowling integrals (3).

The studies of electronic transport coefficients are known to need using of higher approximations. In that way for electronic viscosity, electrical conductivity σ, and electronic conductivity one can be write [3], respectively,

$$\eta_e = \frac{5}{2} n_e^2 \left(2\pi m_e kT\right)^{1/2} \frac{|p'|}{|p|} , \qquad (6)$$

$$\sigma = \frac{3}{2} n_e^2 e^2 \left(\frac{2\pi}{m_e kT}\right)^{1/2} \frac{|q'|}{|q|} , \qquad (7)$$

$$\lambda_e = \frac{75}{8} n_e^2 \left(\frac{2\pi kT}{m_e}\right)^{1/2} \frac{|q''|}{|q'|} \; . \qquad (8)$$

Here m_e is the mass of electron, n_e is electronic density, the elements of determinants p^{nk} and q^{nk} are the functions of the above pointed Chapman-Cowling integrals. Script “ ‘ ” denotes the absence of elements with indexes 0 and 1 (see for details [3-8]).

Others coefficients are calculated according to the Lorentzian theory [2].

2. RESULTS AND DISCUSSION

The results of calculations of transport coefficients are shown in Figs. 2-7. The obtained values are in a good agreement with the data obtained by Chapman-Enskog method (Figs. 3, 4).

One can see that the properties of multicomponent plasma have a pronounced non-monotone character with sharp pikes in certain temperature and pressure ranges. The pikes are appeared due to the dissociation, ionization and from others effects connected with metal impurities. Thus, the viscosity peaks (see Fig. 7) are caused by the minor additions of ions in gases at weakly ionization.

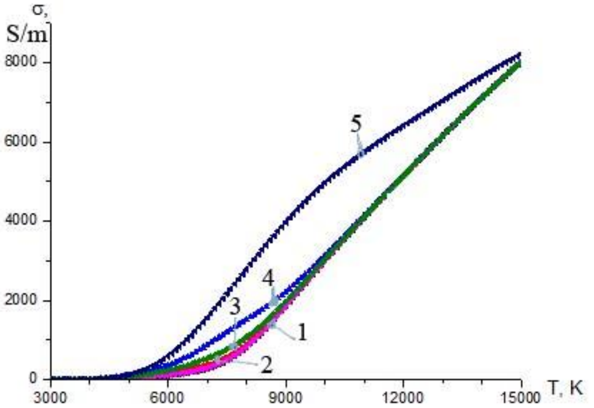

Fig. 2. Electrical conductivity of thermal plasma (p =1 atm) for pure air and the equimolar mixtures of air with tantalum. Curves 1 – air (this work calculations); 2 – air-Ta (99.9:0.1); 3 – air-Ta (95:5); 4 – air-Ta (90:10); 5 – air-Ta (50:50)

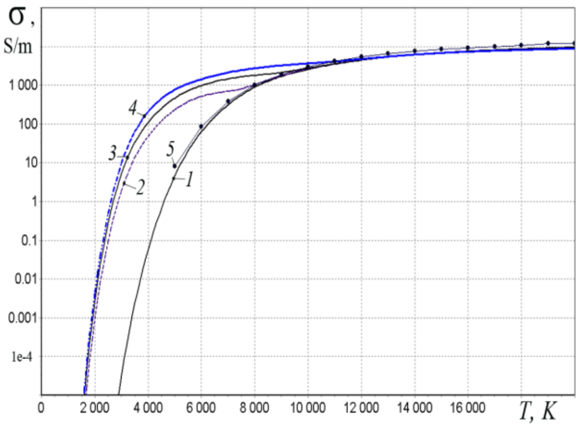

Fig. 3. Electrical conductivity of thermal plasma (p =1 atm) for pure argon and the equimolar mixtures of argon with zirconium. Curves 1 – Ar (this work calculations); 2 – Ar-Zr (99.9:0.1); 3 – Ar-Zr (95:5); 4 – Ar-Zr (90:10); 5 – Ar (data from [8])

It should be noted that under scattering of electrons on argon the Ramsauer effect takes place that is determined the properties of pure argon. However this influence can be neutralized by metal additions in plasma.

Also, one can see that the appearance of zirconium or tantalum impurities causes the essential changing of transport properties with comparison to the case of pure argon or air, respectively. That is needed to take into account under studies of discharges with zirconium or tantalum electrodes.

The peculiarity of the Grad' method is that the values have the same dimensions at all of stages in calculation procedure due to the control of calculation procedure may be improved.

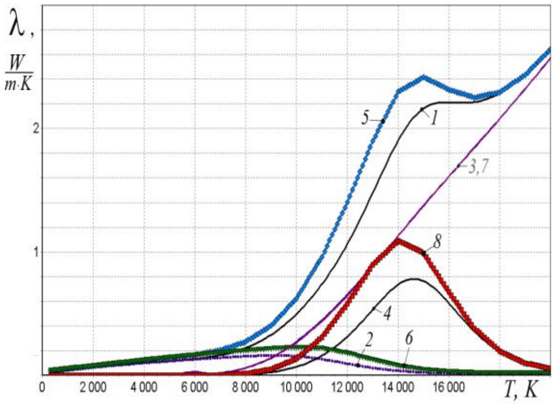

Fig. 4. Thermal conductivity of thermal plasma for pure argon (p =1 atm). Curves 1, 5 are total conductivities; 2, 6 are gaseous ones; 3,7 are electronic ones; 4, 8 are ionization ones. Curves 1, 2, 3, 4 are presented calculations; 5, 6, 7, 8 are the data from [8]

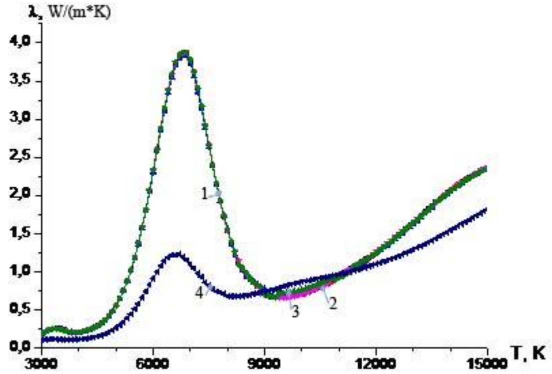

Fig. 5. Thermal conductivity of thermal plasma (p =1 atm) for pure air the equimolar mixtures of air with tantalum. Curves 1 – air (this work calculations); 2 – air-Ta (99.9:0.1); 3 – air-Ta (99:1); 4 – air-Ta (50:50)

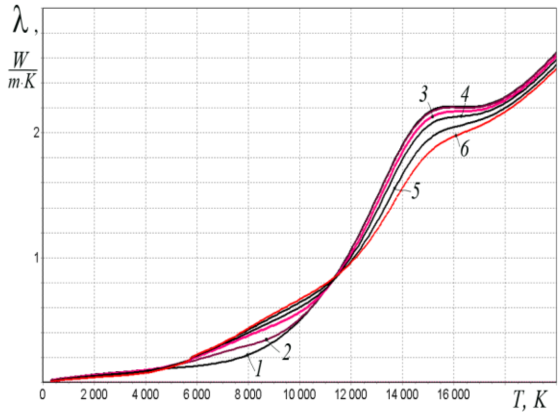

Fig. 6. Thermal conductivity of thermal plasma (p =1 atm) for pure argon and the equimolar mixtures of argon with zirconium. Curves 1 – Ar (this work calculations); 2 – Ar-Zr (99.9:0.1); 3 – Ar-Zr (95:5); 4 – Ar-Zr (90:10); 5 – Ar-Zr (80:20); 6 – Ar-Zr (70:30)

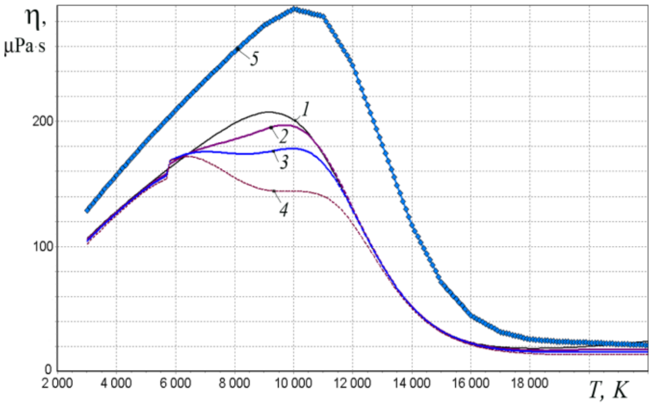

Fig. 7. Viscosity of thermal plasma (p =1 atm) for pure argon and the equimolar mixtures of argon with zirconium. Curves 1 – Ar (this work calculations); 2 – Ar-Zr (95:5); 3 – Ar-Zr (90:10); 4 – Ar-Zr (80:20); 5 – Ar (data from [8])

CONCLUSIONS

Thus, a small amount of zirconium or tantalum causes the essential changes in the values of transport coefficients of thermal plasma in comparison with the cases of pure argon or air, respectively.

The calculations of transport properties on the base of Grad's method have a good agreement with the recent calculations based on Chapman-Enskog method.

The influence of the Ramsauer effect on the transport coefficients can be neutralized by metal additions in plasma.

REFERENCES

1. P. Porytsky, I. Krivtsun, V. Demchenko, U. Reisgen, O. Mokrov, A. Zabirov. On the application of the theory of Lorentzian plasma to calculation of transport properties of multicomponent arc plasmas // *European Phys. Journ. D*. 2010, v. 57, № 1, p.77-85.

2. H. Grad. On the kinetic theory of rarefied gases // *Comm. Pure and Appl. Math*. 1949, v. 2, p. 331-407.

3. V.M. Zhdanov. *Transport Processes in Multicomponent Plasma*. NY: "Taylor and Francis", 2002.

4. S. Chapman, T.G. Cowling. *The mathematical Theory of Nonuniform Gases* / 3rd ed. Cambridge: "Cambbrige University Press", 1970.

5. J.H. Ferziger, H.G. Kaper. *Mathematical theory of transport processes in gases*. North-Holland: "Amsterdam", 1972.

6. R.S. Devoto. Transport properties of Ionized Monatomic Gases // *Phys. Fluids*. 1966, v. 9, № 6, p. 1230-1240.

7. R.S. Devoto. Simplified Expressions for the Transport Properties of Ionized Monatomic Gases // *Phys.Fluids*. 1967, v. 10, № 10, p. 2105-2112.

8. R.S. Devoto. Transport coefficients of ionized argon // *Phys. Fluids*. 1973, v. 16, № 5, p. 2105-2112.

Article received 23.09.2018

О ВЛИЯНИИ ПРИМЕСЕЙ ЦИРКОНИЯ И ТАНТАЛА НА ТРАНСПОРТНЫЕ СВОЙСТВА МНОГОКОМПОНЕНТНОЙ ТЕРМИЧЕСКОЙ ПЛАЗМЫ

П.В. Порицкий, Л.М. Свята

Рассмотрено влияние примесей циркония и тантала на транспортные свойства многокомпонентной термической плазмы в атмосфере смесей аргона и воздуха. Проведенные расчеты основывались на методе моментов Грэда. Показано, что незначительное количество примесей металла может существенно изменить величины транспортных коэффициентов в сравнении со случаем чистого аргона или воздуха. Показана возможность нейтрализации влияния эффекта Рамзауэра на свойства плазмы путем добавки металлических примесей.

ПРО ВПЛИВ ДОМІШОК ЦИРКОНІЮ ТА ТАНТАЛУ НА ТРАНСПОРТНІ ВЛАСТИВОСТІ БАГАТОКОМПОНЕНТНОЇ ТЕРМІЧНОЇ ПЛАЗМИ

П.В. Порицький, Л.М. Свята

Розглянуто вплив домішок цирконію та танталу на транспортні властивості багатокомпонентної термічної плазми в атмосфері сумішей аргону та повітря. Проведені розрахунки ґрунтувалися на методі моментів Ґреда. Показано, що невелика кількість металевих домішок може суттєво змінити величини транспортних коефіцієнтів порівняно із випадком чистого аргону або повітря. Висвітлено можливість нейтралізації впливу ефекту Рамзауера на властивості плазми шляхом додавання металевих домішок.