VIII International Conference

Plasma Physics and Plasma Technology

Contributed papers

Volume I

Minsk, Belarus,
September 14 – 18, 2015

Institue of Physics
National Academy of Sciences of Belarus

COMPUTER ANALYSIS OF TRANSPORT, OPTICAL AND THERMODYNAMIC PROPERTIES OF PLASMA

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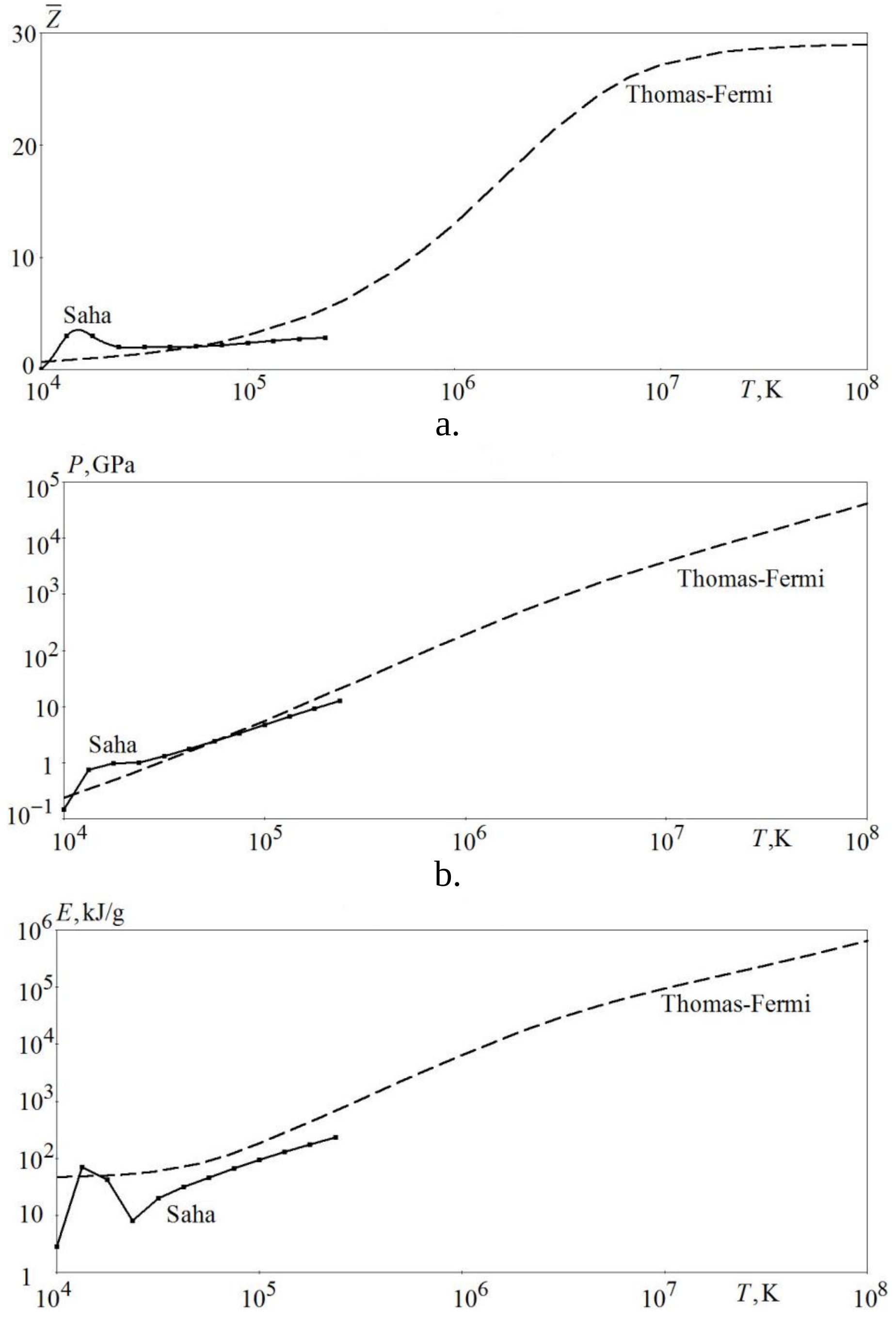
Introduction.

The analysis of plasma thermodynamics is necessary for plasma technologies, astrophysical simulations, calculations of the atmospheric entry and high energy density systems such as fusion devices. The pressure, the specific internal energy, the specific entropy, the thermal conductivity, the electrical conductivity, absorption coefficients have been investigated in a wide range of temperatures and densities. These parameters have been obtained by joining the results of the finite temperature Thomas-Fermi model (Thomas-Fermi model) /1, 2/ and ionization equilibrium model (Saha model) /2, 3/.

Magneto-inertial fusion requires consideration of the magnetic field up to 10^4 T to plasma processes /4–6/. Authors have developed the computational code TERMAG (ThERmodynamic properties of ionized gases mixture in the MAGnetic field) based on the Thomas-Fermi model /7, 8/. This computer code demonstrates quantitatively correct results at temperatures $T > 10^5$ K, because of the applicability of the Thomas-Fermi model for this temperature range /2, 9/. Method of calculation of plasma thermodynamic functions on the basis of the Thomas-Fermi model described in /1, 2, 10/. The plasma at lower temperatures is described by Saha-Boltzmann equations (Saha model). Numerical model for Saha-Boltzmann is shown /1, 3, 10, 11/. Methods of calculation the optical and transport properties are presented in /1, 12/.

Calculation results.

Fig. shows the ionization degree $\overline{Z}$, the full pressure P (the pressure of electrons and ions), the internal energy per unit mass E depending on the temperature T for copper with the density $\rho = 0.105$ g/cm^3.



a.

b.

c.

Fig. The temperature dependence T of the degree of ionization (a.), pressure (b.), specific internal energy (c.) for Cu with the density $\rho = 0.105$ g/cm^3 calculated by the Saha (solid line) and the Thomas-Fermi (dotted line) models

The difference between the Saha model and the Thomas-Fermi model at temperature $T \sim 10^4$ K is evidential because the thermodynamic functions obtained by the Thomas-Fermi model are inaccurate in the temperature range 10^3–$5 \cdot 10^4$ /8/. The results show good agreement for both models at temperature $T \sim 10^5$ K. That is convenient for joining solutions. The difference in results for

$T > 10^5$ K can be explained that the Saha model reaches its limit of the applicability area /8, 11/.

It has been proposed to analyze the validity of the Saha model using the ratio of the ion core volume V^* (the ion core is the nucleus and surrounding inner-shell electrons) to the atomic cell volume V as a criterion in the Ref. /2/. Here $V^* = \frac{4}{3}\pi r^{*3}$, r^* is the ion core radius, $V = 1/n$, n is the concentration of atoms and ions. The parameter $\chi = V^*/V$ describes the limit of applicability of the Saha model. One can use this model when $0.01 < \chi < 1$. The Thomas-Fermi model is applicable at $0.1 < \chi < 1$ (the applicability of the Thomas-Fermi model was evaluated by the amplitude of the ion core oscillations /2/). The criterion of joining the solutions is the parameter χ.

The following expression for the free energy is

$$F(T,V) = \frac{\chi_0}{\chi_0 + \chi(T,V)} F_{Saha}(T,V) + \frac{\chi(T,V)}{\chi_0 + \chi(T,V)} F_{TF}(T,V), \qquad (1)$$

where F_{Saha}, F_{TF} are the free energy which is calculated by Saha and the Thomas-Fermi models respectively, $\chi_0=0.1$. Other thermodynamic functions can be obtained from $F(T, V)$ by differentiation with respect to T and V.

Ion core radius r^* is the coordinate r function, that is corresponding to the minimal radial electron density $4\pi r^2 \rho(r)$. It can be evaluated by the Thomas-Fermi model /1/.

At the same time, the electron density $\rho(r)$ is determined by the Thomas-Fermi potential $\phi(r)$:

$$\rho(r) = \frac{(2 \cdot T)^{3/2}}{2 \cdot \pi^2} I_{1/2}\left(\frac{\phi(r) + \mu}{T}\right), \qquad (2)$$

where T is the temperature, $I_{1/2}$ is the Fermi-Dirac function, $\mu = \mu(\phi(r_0))$ is the chemical potential. All values are in atomic units.

The following table shows the values of the parameter χ obtained by the Thomas-Fermi model for nitrogen. This table shows that χ is proportional to the density ρ, and T^{-1}.

Table. Values of the parameter χ for nitrogen

T, K / ρ, g/cm^3	10^{-7}	10^{-5}	10^{-3}	1	10	10^3
10^6	~ 0	~ 0	1 %	90%	75%	~100%
10^7	~ 0	~ 0	~ 0	4%	16%	~100%
10^8	~ 0	~ 0	~ 0	~ 0	0.1%	~100%

Conclusions.

The numerical simulation is done for thermodynamic functions (the pressure P, the specific internal energy E) and the degree of ionization $\overline{Z}$ for copper plasma. Computational code TERMAG is used for evaluation the thermodynamic properties and the numerical solution for Saha-Boltzmann equations.

The solutions obtained by the Thomas-Fermi and Saha models one can be join using the ratio of the ion core volume to the atomic cell volume. Test results for this ratio for nitrogen are presented. Such data will be used for the construction of the wide range equations of state.

Acknowledgements. This work was supported by the Ministry of Education and Science of the Russian Federation (Project № 13.79.2014/K).

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