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Ionization Equilibrium and Composition of a Dense Partially Ionized Metal Plasma

T.S. Ramazanov[1], **M.T. Gabdullin**[1]*, **K.N. Dzhumagulova**[1], and **R. Redmer**[2]

[1] IETP, al-Farabi Kazakh National University, 96a Tole bi Str., Almaty 050012, Kazakhstan
[2] Institute of Physics, University of Rostock, D-18051, Rostock, Germany

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In the present work we determine the ionization equilibrium of dense tungsten, aluminum and iron plasmas by solving the Saha equations with corrections due to non-ideality. The lowering of the ionization potentials is calculated on the basis of effective potentials by taking screening and quantum effects into account.

1 Introduction

In this work effective potentials are applied to describe the interactions between the particles in the plasma. The composition of dense plasmas $(Al, Fe$ and $W)$ is determined that consist of electrons, ions and atoms.

The number density varies in the range $n_e = 10^{18} - 10^{23}\ cm^{-3}$ and the temperature domain considered here is T_e=10^4-10^6 K . It is convenient to characterize the plasma state with dimensionless parameters which follow from the plasma parameters (number) density and temperature. The coupling parameter measures the potential energy of the interactions between the heavy particles (ions) relative to their thermal energy: $\Gamma = (Ze)^2/ak_BT$, where $a = (3/4\pi n)^{1/3}$ is the average distance between the particles. This parameter is varies in the range $\Gamma = 0.1 - 1$. It is a weakly nonideal plasma. The electron density parameter is the average distance in units of the Bohr radius: $r_s = a/a_B$, with $a_B = h^2/m_e e^2$. This parameter varies in the range $r_s = 2 - 20$. The degeneracy parameter $\Theta = k_BT/E_F$ for the electrons measures the ratio of their thermal energy $k_B\ T$ and the Fermi energy E_F. The condition $\Theta \leq 1$ corresponds to the state of weak and intermediate degeneracy. In the Fig. 1. is presented the range of the investigating plasma.

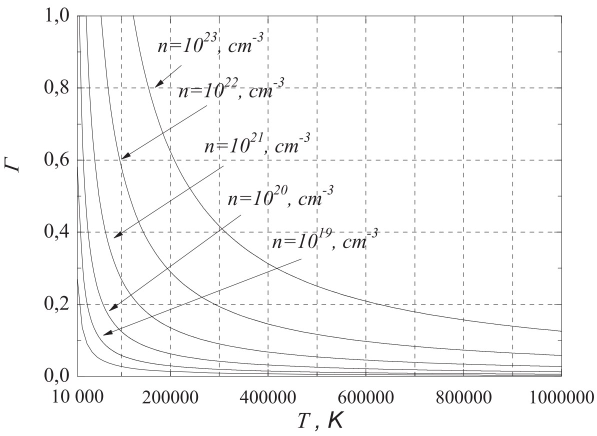

Fig. 1 Region of investigation.

* Corresponding author: e-mail:gabdullin@physics.kz, Phone: 007 7272 924988, Fax: 007 7272 924988

2 Interaction models

On the basis of the method of the dielectric function an effective potential that takes into consideration quantum-mechanical and screening effects was derived for the description of the interaction between the charged particles in [1]:

$$\Phi_{es}(r) = \frac{Ze^2}{\sqrt{1-4\lambda_{es}^2/r_D^2}}\left(\frac{e^{-Br}}{r} - \frac{e^{-Ar}}{r}\right), \tag{1}$$

where $s = e, i$, $\lambda_{es} = \hbar/\sqrt{2\pi\mu_{es}k_BT}$ is the de Broglie wavelength, μ_{es} is the reduced mass of e-s pair, $r_D = \sqrt{k_BT/4\pi\, n_e e^2}$ the Debye radius, and coefficients

$$B^2 = \frac{1-\sqrt{1-4\lambda_{\alpha\beta}^2/r_D^2}}{2\lambda_{\alpha\beta}^2}, \qquad A^2 = \frac{1+\sqrt{1-4\lambda_{\alpha\beta}^2/r_D^2}}{2\lambda_{\alpha\beta}^2} \tag{2}$$

An effective potential was used to describe the ion–ion interaction [2]:

$$\Phi_{ii}(r) = \frac{Z_iZ_ie^2}{\sqrt{1-4\lambda_{ee}^2/r_D^2}}\left(\left(\frac{1}{2}+\frac{1}{2}\sqrt{1-4\lambda_{ee}^2/r_D^2}\right)\frac{e^{-Br}}{r} - \left(\frac{1}{2}-\frac{1}{2}\sqrt{1-4\lambda_{ee}^2/r_D^2}\right)\frac{e^{-Ar}}{r}\right), \tag{3}$$

Interaction between a charge and an atom in plasma is basically caused by effects of polarization and is of short range character. The polarization potential was chosen as the potential of the charge–atom interaction in a partially ionized plasma [3]:

$$\Phi_{sa}(r) = \frac{e^2\alpha_P}{2r^4\sqrt{1-4\lambda_{ee}^2/r_D^2}}\left(e^{-Br}(1+Br) - e^{-Ar}(1+Ar)\right), \tag{4}$$

where α_P is the polarization of an atom. It is supposed that diffraction effects are also taken into account in considerations of atom-electron interactions. All effective potentials can be used when $\lambda_{ei} < r_D/2$.

3 Ionization equilibrium and composition of dense semiclassical plasma

For the determination of the composition of partially ionized plasma we use the chemical model assumes that the plasma consists of electrons, ions and atoms [4,5]. Within the limits of chemical picture the following ionization processes take place in such dense plasma for Al, Fe and W:

$$\begin{array}{lll} Al \rightleftarrows Al^{1+} + e; & Al^{1+} \rightleftarrows Al^{2+} + e; \quad ..., & Al^{10+} \rightleftarrows Al^{11+} + e; \\ Fe \rightleftarrows Fe^{1+} + e; & Fe^{1+} \rightleftarrows Fe^{2+} + e; \quad ..., & Fe^{10+} \rightleftarrows Fe^{11+} + e; \\ W \rightleftarrows W^{1+} + e; & W^{1+} \rightleftarrows W^{2+} + e; & W^{2+} \rightleftarrows W^{3+} + e. \end{array} \tag{5}$$

The system of Saha equations for the calculation of the plasma composition for other elements (Fe, Al, W) with maximal ionization state k can then be written in the following form:

$$\begin{array}{l} n_0 = \frac{g_0}{g_{1+}} n_{1+} \exp\left[\beta(\mu_e^{id} + E_{ion}^{1+} + \Delta\mu_1)\right] \\ n_{1+} = \frac{g_{1+}}{g_{2+}} n_{2+} \exp\left[\beta(\mu_e^{id} + E_{ion}^{2+} + \Delta\mu_2)\right] \\ \qquad .... \\ n_{(k-1)+} = \frac{g_{(k-1)+}}{g_{k+}} n_{k+} \exp\left[\beta(\mu_e^{id} + E_{ion}^{k+} + \Delta\mu_{k+})\right], \end{array} \tag{6}$$

where $\beta = 1/k_BT$. The values $\Delta\mu_k = \mu_e^{nonid} + \mu_k^{nonid} - \mu_{k-1}^{nonid}$ are corrections due to the non-ideality of the plasma, which were calculated on the basis of the effective interaction potentials (1)-(4).

In order to solve the system of Saha equations, we have to consider two further equations, conservation of the number of nuclei and charge neutrality in system:

$$\sum_{k=1} n_k + n_0 = const, \quad \sum_{k=1} kn_k = n_e. \tag{7}$$

The contribution from the polarization of neutral atoms "a" $= Al, Fe, W$ was calculated via the linearized virial coefficient for the interaction of electrons with atoms (4):

$$\mu_{ea}^{nonid} = n_a^0 B^{PP}, B^{PP} = \int \Phi_{ea}(r)\, d^3r. \tag{8}$$

Introducing the ionized coefficient as the ratio of the number of free electrons, ions and atoms to the total number of nuclei $n_i + n_0$ in system:

$$\alpha_e = \frac{n_e}{(n_0 + n_i)}, \quad \alpha_{k+} = \frac{n_{k+}}{(n_0 + n_i)} \quad . \tag{9}$$

Based on this formalism we have calculated the composition of dense Al, Fe and W plasmas.

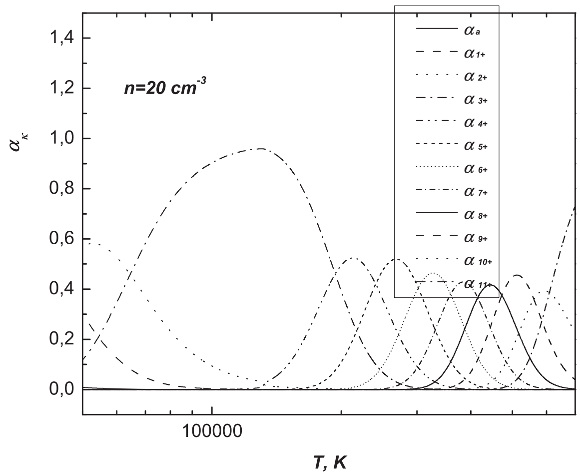

Fig. 2 Composition of non-ideal Al plasma at a constant density of $n = 10^{20}, cm^{-3}$ as function of temperature.

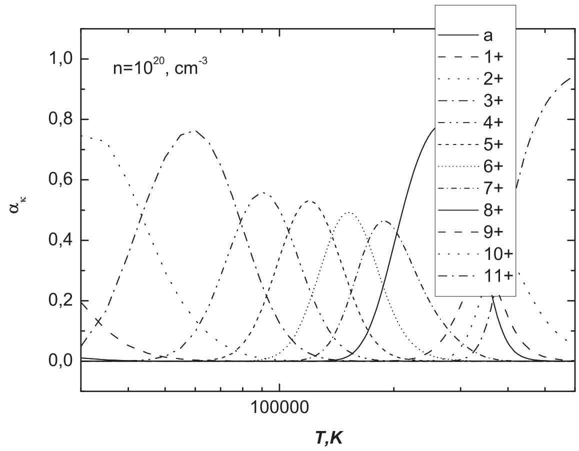

Fig. 3 Composition of non-ideal Fe plasma at a constant density of $n = 10^{20}, cm^{-3}$ as function of temperature.

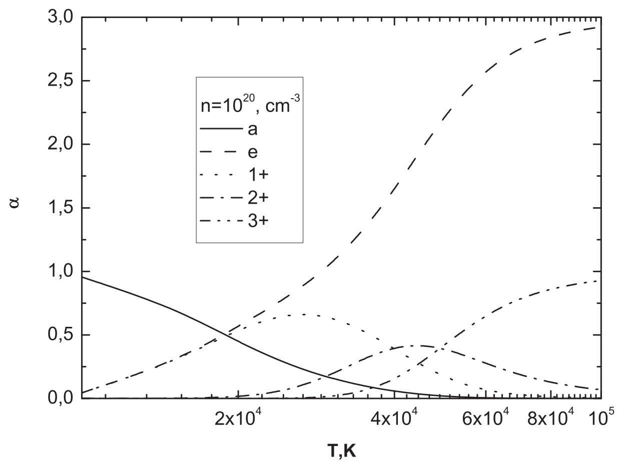

Fig. 4 Composition of non-ideal W plasma at a constant density of $n = 10^{20}, cm^{-3}$ as function of temperature.

We have solved the system of equations (5)-(9) numerically and present the results in Figs. 2-4. Fig. 2 present the curves for the relative fractions of particles versus the temperature for dense Al plasma at $n = 10^{20} cm^{-3}$ with maximal ionization state 11. The plasma composition of Fe is presented in Fig. 3 at $n = 10^{20} cm^{-3}$ with maximal ionization state 11 . The plasma composition of W is presented in Fig. 4 at $n = 10^{20} cm^{-3}$ with maximal ionization state 3 .

4 Conclusion

On the basis of our results we can conclude that the pseudopotential model that takes into account quantum diffraction as well as screening effects can be used for an efficient calculation of the plasma composition in a wide region of densities and temperatures.

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