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A scattering cross-section and ionization equilibrium in dense metal plasmas

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Abstract
The kinetic and thermodynamic properties of non-ideal Al and Cu plasmas were investigated on the basis of pseudopotential models, taking screening and quantum-mechanical effects into account. For investigation of ionization stages, the Saha equations with corrections to non-ideality (lowering of ionization potentials) were used.

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1. Introduction

The present work is devoted to studies of collision processes in a dense aluminum and cupreous plasma consisting of electrons, ions and atoms and including studies of its thermodynamical characteristics. The number density changes in the range of $n_{\text{tot}} = n_e + n_i + n_a = 10^{18}\text{–}10^{22}\,\text{cm}^{-3}$ and the temperature domain is $T = 10^4\text{–}10^6$ K. It is convenient to describe the plasma state with dimensionless parameters which characterize the dimension physical values such as the number density. The coupling parameter Γ characterizes the potential energy of interaction in comparison with the thermal energy: $\Gamma = Ze^2/ak_{\text{B}}T$, where $a = (3/4\pi n)^{1/3}$ is the average distance between the particles. For a weakly coupled plasma, $\Gamma < 1$. The density parameter is the relation of the average distance to the Bohr radius: $r_S = a/a_{\text{B}}$, where a_{B} is the Bohr radius.

2. Interaction models

Various approaches are used for a description of plasma properties with different parameters. In the calculation of thermodynamic functions for a non-ideal plasma, we have difficulties related to the interaction of particles. A pseudopotential model that takes into consideration quantum-mechanical and screening effects was used for the description of interaction between the charged particles in [1]:

$$\Phi_{\mathrm{es}}(r) = \frac{Z_s e^2}{\sqrt{1 - 4\lambda_{ee}^2/r_{\mathrm{D}}^2}} \left(\frac{\mathrm{e}^{-Br}}{r} - \frac{\mathrm{e}^{-Ar}}{r} \right), \tag{1}$$

where $\lambda_{es} = \hbar/(2\pi\mu_{es}k_{\mathrm{B}}T)^{1/2}$ is the de Broglie wavelength, $r_{\mathrm{D}} = \sqrt{k_{\mathrm{B}}T/(4\pi n e^2)}$ is the Debye radius, $B^2 = \frac{1-\sqrt{1-4\lambda_{ee}^2/r_{\mathrm{D}}^2}}{2\lambda_{ee}^2}$, $A^2 = \frac{1+\sqrt{1-4\lambda_{ee}^2/r_{\mathrm{D}}^2}}{2\lambda_{ee}^2}$ and $s = e, i$.

For describing the ion–ion interaction, an effective potential was used:

$$\Phi_{\mathrm{ii}}(r) = \frac{Z_i Z_i e^2}{\sqrt{1 - 4\lambda_{ee}^2/r_{\mathrm{D}}^2}} \left(\frac{\left(1 + \sqrt{1 - 4\lambda_{ee}^2/r_{\mathrm{D}}^2}\right) \mathrm{e}^{-Br}}{r} - \frac{\left(1 - \sqrt{1 - 4\lambda_{ee}^2/r_{\mathrm{D}}^2}\right) \mathrm{e}^{-Ar}}{r} \right). \tag{2}$$

The polarization potential was chosen as the potential of the charge–atom interaction in a partially ionized non-ideal plasma [2]:

$$\Phi_{ea}(r) = -\frac{e^2\alpha_p}{2r^4\left(1 - \lambda_{ee}^2/r_{\mathrm{D}}^2\right)} (\mathrm{e}^{-Br}(1 + Br) - \mathrm{e}^{-Ar}(1 + Ar))^2, \tag{3}$$

where α_p is the polarization of an atom for other elements. It is supposed that diffraction effects are also taken into account when considering atom–electron interactions.

3. Scattering cross-sections

To calculate scattering sections, the method of phase functions has been used [3, 4]; within this method, the Calogero equation has been solved:

$$\frac{\mathrm{d}}{\mathrm{d}r}\delta_l(k, r) = -\frac{1}{k}\frac{2\mu_{\alpha\beta}\Phi_{\alpha\beta}(r)}{\hbar^2}\left[\cos\delta_l^{\alpha\beta}(k, r) \cdot j_l(kr) - \sin\delta_l^{\alpha\beta}(k, r) \cdot n_l(kr)\right]^2, \tag{4}$$

where k is the wave number, l is the orbital moment, $\delta_l^{\alpha\beta}(0) = 0$, $\delta_l^{\alpha\beta}(k) = \lim_{r\to\infty} \delta_l^{\alpha\beta}(k, r)$, $j_l(kr), n_l(kr)$ are the Ricatti–Bessel functions and $\alpha, \beta = e, i, a$.

The total and transport cross-sections of elastic scattering for plasma particles are determined using phase scattering shifts $\delta_l^{\alpha\beta}$ as follows [5]:

$$\begin{aligned} Q_{\alpha\beta}^P(k) &= \frac{4\pi}{k^2}(2l + 1)\sin^2\left(\delta_l^{\alpha\beta}(k)\right), \qquad Q_{\alpha\beta}^F(k) = \sum_{l=0}^{\infty} Q_{\alpha\beta}^P(k), \\ Q_{\alpha\beta}^T &= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(l + 1)\sin^2\left(\delta_l^{\alpha\beta}(k) - \delta_{l+1}^{\alpha\beta}(k)\right). \end{aligned} \tag{5}$$

The results obtained will be applied for calculating transport coefficients, and they have been compared with the results of different authors as in [6, 7].

Figure 1 presents partial and total cross-sections for scattering of an electron at an aluminum atom. One can see that at the partial cross-section of the electron–atomic interaction, there is a pronounced minimum which reminds us of the Ramzauer effect. Such behavior is typical of atoms with a complex structure of an electron shell. Usually, such an anomaly scattering cross-section is manifested at the scattering of slow electrons.

The local minima and maxima at the curves of the transport scattering section (see figure 2), calculated based on the polarization potential (2), can serve as indications of the resonance nature of the interaction. It is obvious that at small wave numbers of an incident

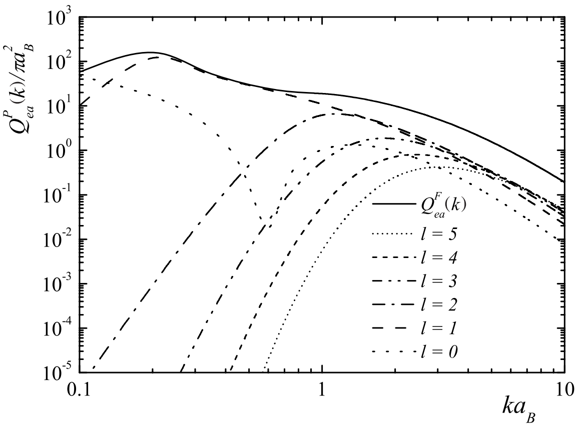

Figure 1. Full and partial cross-sections of an electron on the aluminum atom on the basis (2). System parameters: $\Gamma = 0.7$ and $r_S = 3$.

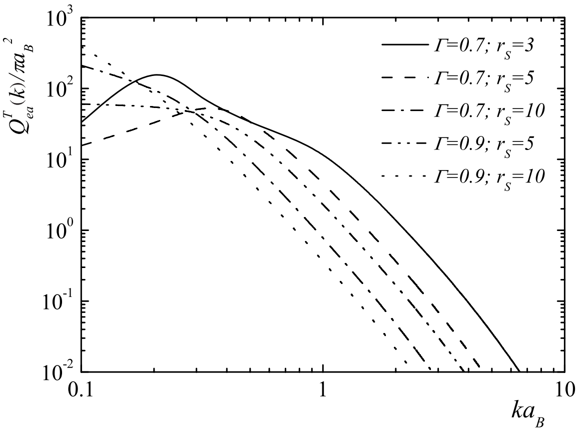

Figure 2. The transport cross-section of an electron on the aluminum atom at different system parameters.

particle with local extrema of the scattering cross-sections, the particle's thermal de Broglie wave is close to the atomic diameter which results in diffraction effects.

Figure 3 shows how the quantum effect of diffraction accounting reflects on the transport cross-section. The values of the scattering cross-section given by pseudopotential (1) are situated lower than the corresponding values for the Debye–Hückel potential.

4. Ionization equilibrium and thermodynamic properties

A partially ionized plasma is a multicomponent system that contains electrons, other ionized ions and atoms. As is known, the interaction of electrons and ions with atoms in a moderately dense plasma results in a decrease of the ionization potential. Finding the number density for any particle type as a function of temperature and density is reduced to determining the possible reactions in the system. In this work, we neglect the formation of molecules and neutral clusters.

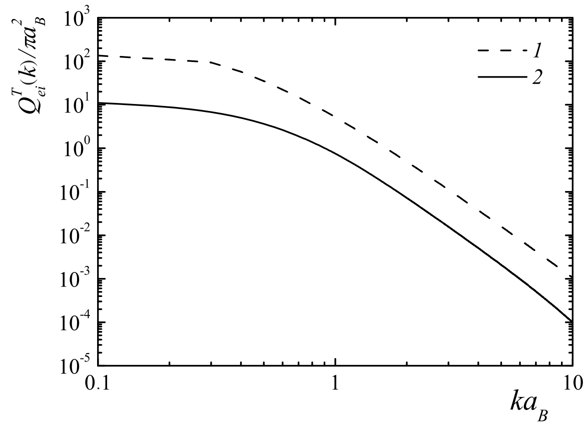

Figure 3. Electron–ion transport cross-section at $\Gamma = 0.9$ and $r_S = 5$. 1—Debye-Hückel potential and 2—pseudopotential (1).

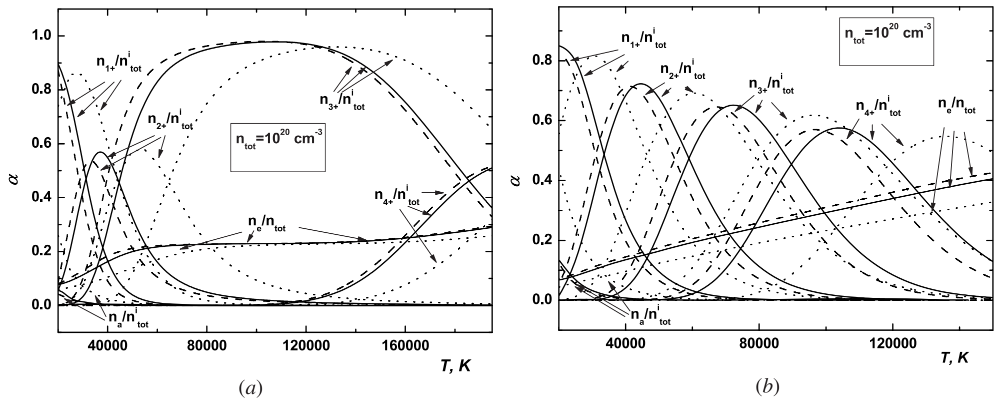

Figure 4. Ionization equilibrium of a plasma: solid lines are the results of the present work; dotted lines describe the ionization equilibrium, calculated without lowering the ionization potential; dashed lines are the Debye approximation. (*a*) For a non-ideal Al plasma and (*b*) for a non-ideal Cu plasma.

The ionization degree is introduced as the ratio of the number of free ions and atoms to the total number of all particles $\alpha_k = n_k^* / n^i_{\text{tot}}$, where $n^i_{\text{tot}} = \sum n_i + n_a$ and $\alpha_e = n_e^*/n_{\text{tot}}$ for electrons.

Let us write down a system of Saha equations [8] for calculations of plasma composition with a maximal ionization rate 5:

$$\begin{aligned} n_0 &= \tfrac{1}{2} n_{1+} \exp\left[\beta\left(\mu_e^{\text{id}} + E_{\text{ion}}^{1+} + \Delta\mu_1\right)\right], \ldots, \\ n_{4+} &= 2 n_{5+} \exp\left[\beta\left(\mu_e^{\text{id}} + E_{\text{ion}}^{5+} + \Delta\mu_5\right)\right], \end{aligned} \tag{6}$$

where $\beta = 1/k_{\text{B}}T$ and values $\Delta\mu_k = \mu_e^{\text{nonid}} + \mu_k^{\text{nonid}} - \mu_{k-1}^{\text{nonid}}$ are corrections for non-ideality to the chemical potentials.

The contribution from polarization [6] was calculated for the interaction of electrons with atoms (2) $\mu^{\text{nonid}}_{\text{eAl,Cu}} = n^0_{\text{Al,Cu}} B^{\text{PP}}$, $B^{\text{PP}} = \int \Phi_{\text{ea}}(r)\, \mathrm{d}^3 r$.

This system of equations was solved numerically based on potentials (1) and (2). Figure 4 presents the curves for relative portions of particles versus temperature for dense

Al and Cu plasmas. As one can see from the figures, such a plasma becomes totally ionized, i.e. consist of ions and electrons. Also, the figure presents comparisons with other theories.

5. Conclusions

The interaction of an electron with an aluminum atom is of resonance nature. Partial sections for scattering of electrons at aluminum atoms show anomaly in section behavior typical of the Ramzauer effect. Additional consideration of particle diffraction in a dense plasma lowers the scattering probability.

Consideration of quantum diffraction effects in interaction at calculation of composition for a dense metal (Al and Cu) plasma results in lower values for the ionization potential compared to those in Debye theory.

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