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ELECTRON ENERGY DISTRIBUTION FUNCTION IN THE COLLISIONAL-RADIATIVE MODEL OF ARGON PLASMA[1]

J. VLČEK[2], Plzeň

A numerical solution method for the Boltzmann equation has been developed to obtain the electron energy distribution function in nonequilibrium argon plasma characterized by a set of measurable quantities (T_e, T_a, T_i, n_e and n_1) which are in accordance with the usual input parameters of the collisional-radiative models.

ФУНКЦИЯ РАСПРЕДЕЛЕНИЯ ЭНЕРГИИ ЭЛЕКТРОНОВ В УДАРНО-РАДИАЦИОННОЙ МОДЕЛИ АРГОННОЙ ПЛАЗМЫ

В работе описан метод численного решения уравнения Больцмана, который развит с целью получения функции распределения энергии электронов в неравновесной аргонной плазме, характеризуемой набором измеримых величин (T_e, T_a, T_i, n_e и n_1). Эти величины совпадают с обычными входными параметрами ударно-радиационной модели плазмы.

I. INTRODUCTION

One of the important assumptions made in almost all extensive studies based on the realistic collisional-radiative (CR) models (see, e. g., Ref. [1—4]) is the use of the Maxwellian electron energy distribution function.

However, it has been shown by many authors that this assumption is unjustified for a wide range of physically interesting conditions in various gases.

Distribution functions in argon plasma have been calculated, e. g., by Winkler [5], Judd [6], Smits and Prins [7], Morgan and Vriens [8] and Ferreira and Ricard [9].

Our objective was to develop a numerical method allowing the solution of the Boltzmann equation for the electron energy distribution function under various

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[2] Department of Physics, Institute of Mechanical and Electrical Engineering, Nejedlého sady 14, 306 14 PLZEŇ, Czechoslovakia

nonequilibrium conditions in argon plasma characterized by a set of measurable quantities, such as the electron temperature T_e, the atom temperature T_a, the ion temperature T_i, the electron number density n_e and the ground state atom population n_1, which are in accordance with the usual input parameters of the rate equations of the CR models.

A substantial feature of the method used is a consistent calculation of the electric field strength E corresponding to the chosen set of the input parameters.

II. THE BOLTZMANN EQUATION

Assuming the electron velocity distribution to be slightly anisotropic in velocity space, the only component of the electron energy distribution function to appear in the rate coefficients of the CR model is the isotropic one $f(u)$ where $u = \epsilon/kT_e$ (ϵ is the electron energy and k is the Boltzmann constant).

For a stationary and homogeneous monoatomic gas plasma $f(u)$ is given by the equation [10—13]:

$$\frac{\mathrm{d}}{\mathrm{d}u}\left[H(u)\frac{\mathrm{d}f(u)}{\mathrm{d}u} + G(u)\,f(u)\right] = C_{IN}(u) \tag{1}$$

where

$$H(u) = \frac{e^2E^2u}{3\sum\limits_{h.p.} n_h Q_{eh}^{(m)}(u)\,(kT_e)^2} + \sum_{h.p.} 2\frac{m_e}{m_h} n_h Q_{eh}^{(m)}(u)\frac{T_h}{T_e}u^2 + 3n_e\overline{Q_{ee}}A_1(u)$$

and

$$G(u) = \sum_{h.p.} 2\frac{m_e}{m_h} n_h Q_{eh}^{(m)}(u)\,u^2 + 3\,n_e\overline{Q_{ee}}A_2(u).$$

Here, e is the electron charge, m_e and m_h are the electron and heavy particle (i.e. argon atoms and singly ionized ions Ar_+ with the number density $n_i = n_e$) mass, respectively, n_h and T_h are their number density and temperature, respectively. $Q_{eh}^{(m)}(u)$ is the electron-heavy particle momentum transfer cross section. In the case of atoms $Q_{ea}^{(m)}(u)$ was approximated [13] by a formula giving a reasonable fit to the experimental data of Massey and Burhop [14]. For $Q_{ei}^{(m)}(u)$ there holds:

$$Q_{ei}^{(m)}(u) = \pi\left(\frac{e^2}{4\pi\varepsilon_0 kT_e u}\right)^2 \ln\left[\frac{12\pi(\varepsilon_0 kT_e)^{3/2}}{n_e^{1/2}e^3}\right]$$

where ε_0 is the vacuum permittivity. The energy averaged cross section for the electron-electron scattering can be written as:

$$\bar{Q}_{ee} = 6\pi\left(\frac{e^2}{12\pi\varepsilon_0 kT_e}\right)^2 \ln\left[\frac{12\pi(\varepsilon_0 kT_e)^{3/2}}{n_e^{1/2}e^3}\right].$$

The integral functions $A_1(u)$ and $A_2(u)$ are defined by the relations:

$$A_1(u) = \frac{4\pi}{3}\left(\frac{2kT_e}{m_e}\right)^{3/2}\left[\int_0^u u^{3/2} f(u)\,\mathrm{d}u + u^{3/2}\int_u^\infty f(u)\,\mathrm{d}u\right] \tag{2}$$

and

$$A_2(u) = 2\pi\left(\frac{2kT_e}{m_e}\right)^{3/2}\int_0^u u^{1/2} f(u)\,\mathrm{d}u. \tag{3}$$

The basic equation (1) was linearized by using an approximation consisting in the replacement of the function $f(u)$ by the corresponding Maxwellian function $f_M(u)$ in expressions (2) and (3). This approach causes only slight inaccuracies in our results for $f(u)$ because the quantities $A_1(u)$ and $A_2(u)$ are weakly dependent on the course of the function $f(u)$, especially in its high-energy tail (see Ref. [7] and [15]). Furthermore, according to Winkler [5], who calculated the distribution function in argon plasmas without any approximations of the above mentioned integrals, the deviations between the low-energy parts of the functions $f(u)$ and $f_M(u)$ tend rapidly to zero with a growing effect of the electron-electron scattering.

The operator $C_{IN}(u)$ includes generally all terms referring to various types of the possible inelastic processes. Their influence on the distribution function is investigated in Ref. [13].

This study proves that only the terms corresponding to the collisional excitations from the ground state of the atom to the two lowest excited effective levels ($n = 2$ and $n = 3$) and the collisional ionization of the ground state need to be considered under the usual conditions in equation (1). It should be noted that the effective levels denoted by $n = 2$ and $n = 3$, each containing resonance and metastable states, consist of $^3P_1$ and $^3P_2$ levels and $^1P_1$ and $^3P_0$ levels, respectively.

Equation (1) can then be rewritten in the form:

$$\frac{\mathrm{d}}{\mathrm{d}u}\left[H(u)\frac{\mathrm{d}f(u)}{\mathrm{d}u} + G(u)\,f(u)\right] = n_1 u M(u)\,f(u) \tag{4}$$

where $M(u) = 0$ for $u \leq u_{12}$
and

$$M(u) = \sigma_{12}(u) + \sigma_{13}(u) + \sigma_1(u) \text{ for } u > u_{12}.$$

The formulas for the cross sections $\sigma_{12}(u)$, $\sigma_{13}(u)$ and $\sigma_1(u)$ referring to the processes mentioned above are taken from Ref. [4]; u_{12} is the dimensionless excitation energy of the level $n = 2$.

The normalization condition for $f(u)$ is expressed as:

$$2\pi\left(\frac{2kT_e}{m_e}\right)^{3/2}\int_0^\infty u^{1/2} f(u)\,\mathrm{d}u = 1. \tag{5}$$

III. NUMERICAL SOLUTION

III.1. The elastic region

For $u \leq u_{12}$ we obtain [13] the solution of equation [4] in the form:

$$f(u) = NI(u) \tag{6}$$

where

$$I(u) = J(u)\left\{1 + \left[G(0) - H(0)\right]\int_0^u \frac{\mathrm{d}y}{H(y)J(y)}\right\},$$

$$J(u) = \exp\left[-\int_0^u \frac{G(x)}{H(x)}\mathrm{d}x\right]$$

and for the constant N it follows from condition (5):

$$N = \left(\frac{m_e}{2kT_e}\right)^{3/2}\frac{1}{2\pi}\frac{1}{\int_0^\infty u^{1/2}I(u)\,\mathrm{d}u}. \tag{7}$$

The value of the electric field strength E corresponding to the chosen set of input parameters was determined numerically by means of the equation defining the electron temperature:

$$\frac{3}{2}kT_e = \bar{\epsilon}$$

where $\bar{\epsilon}$ is the mean electron energy. This relation can be rewritten as:

$$\frac{\int_0^\infty u^{3/2}I(u)\,\mathrm{d}u}{\int_0^\infty u^{1/2}I(u)\,\mathrm{d}u} = \frac{3}{2}. \tag{8}$$

The values of E and N are calculated in two different ways for all cases investigated.

The first one is suitable when the high-energy tail of $f(u)$ falls off very rapidly with respect to $f_M(u)$. Then it follows that

$$N = \left(\frac{m_e}{2kT_e}\right)^{3/2}\frac{1}{2\pi}\frac{1}{\int_0^{u_{12}} u^{1/2}I(u)\,\mathrm{d}u} \tag{7a}$$

and

$$\frac{\int_0^{u_{12}} u^{3/2}I(u)\,\mathrm{d}u}{\int_0^{u_{12}} u^{1/2}I(u)\,\mathrm{d}u} = \frac{3}{2}. \tag{8a}$$

The second approach eliminating the premature cut off of the calculated integrals is used with the highest values of the ionization degree in which case especially formula (8a) fails. For this reason the above relations were modified:

$$N = \left(\frac{m_e}{2\pi kT_e}\right)^{3/2}\frac{\int_0^{u_{12}} u^{1/2}e^{-u}\,\mathrm{d}u}{\int_0^{u_{12}} u^{1/2}I(u)\,\mathrm{d}u} \tag{7b}$$

and

$$\frac{\int_0^{u_{12}} u^{3/2}I(u)\,\mathrm{d}u + u_{12}^{3/2}I(u_{12})}{\int_0^{u_{12}} u^{1/2}I(u)\,\mathrm{d}u} = \frac{3}{2}. \tag{8b}$$

III.2. The inelastic region

For $u > u_{12}$ equation (4) can be transformed [13] to the form which is appropriate for the numerical solution

$$f(u) = f(u_{12})\exp\left\{-\int_{u_{12}}^u \frac{G(x)}{H(x)}\mathrm{d}x - \int_{u_{12}}^u \left[\frac{1}{H(x)f(x)}\times \times\int_x^\infty n_1 y M(y) f(y)\,\mathrm{d}y\right]\mathrm{d}x\right\} \tag{9}$$

where $f(u_{12})$ is given by the relation (6) for $u = u_{12}$. The iterative procedure suggested for the solution of equation (9) is similar to that developed by Sherman [16] who neglected the effect of the electron-electron scattering.

IV. RESULTS

In Fig. 1 and 2 we give the numerical results for the ratio $f(u)/f_M(u)$ obtained for the following input parameters characterizing typical nonequilibrium argon plasmas: $n_1 = 1.61 \times 10^{17}$ cm^{-3}, $T_e = 10\,000$ K and $T_e = 30\,000$ K, $T_a = T_i = 300$ K and $T_a = T_i = 1000$ K and 10^8 cm$^{-3} \leq n_e \leq 10^{14}$ cm^{-3}.

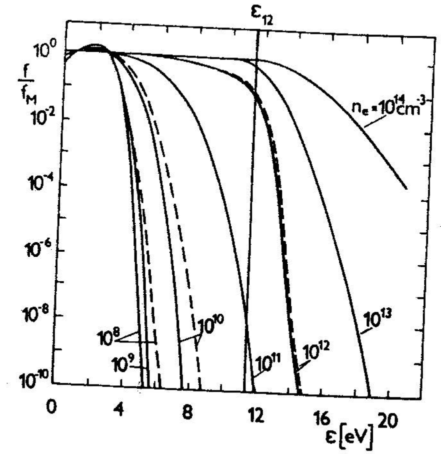

Fig. 1. Electron distribution function normalized on a Maxwellian at the electron temperature $T_e = 10\,000$ K as a function of electron energy. Solid curves: $T_a = T_i = 300$ K, dashed curves: $T_a = T_i = 1000$ K; $n_1 = 1.61 \times 10^{17}$ cm^{-3}.

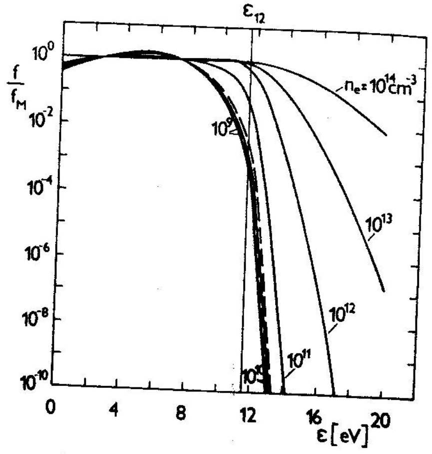

Fig. 2. Electron distribution function normalized on a Maxwellian at the electron temperature $T_e = 30\,000$ K as a function of electron energy. Solid curves: $T_a = T_i = 300$ K, dashed curves: $T_a = T_i = 1000$ K; $n_1 = 1.61 \times 10^{17}$ cm^{-3}.

V. CONCLUSIONS

From our numerical results it follows:

i) The assumption of the Maxwellian distribution function usually found in the extensive studies based on the CR models is unjustified under the conditions considered.

ii) The body of the distribution function is nearly Maxwellian for the ionization degree $n_e/n_1 > 5 \times 10^{-5}$ for all cases investigated. This information may be valuable in formulating the basic equations of the CR model [10], in the application of the two-electron group model [8], in electron temperature probe measurements and in the treatment of electron collisions with excited states in kinetic modelling studies.

iii) For lower values of T_e and low values of n_e it is impossible to neglect the heavy particle temperature term in the Boltzmann equation as most authors do.

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