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Theoretical Electron- Impact Excitation, Ionization and Recombination Rate Coefficients and Level Population Densities for Scandium-Like Ion

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Abstract

Absolute excitation, ionization and recombination rate coefficients for 22 levels have been evaluated from our experimental results at different Plasma temperatures for excited atomic states in Ti II. The corresponding electron densities are determined to calculate the populations of the 22 excited levels belonging to $3d^3$, $3d^24s$ and $3d^24p$, namely for doublet and quartet states. The calculations have been carried out by using the coupled rate simultaneous equations in which the monopole and the quadrupole transitions have been introduced in the calculations in addition to the dipole transitions. A theoretical population model has been developed to study the influence of the different processes that might contribute to the population of the different levels at our plasma parameters. The population densities for the 22 different levels were then derived from these rate coefficients. It is found that, the highest value of the population densities is for the $3d^3$ (^4F) excited level and the lowest value is for the 4p (^2P) excited level.

Introduction

Rate coefficients for ionization, recombination and excitation of highly charged multi-electron atoms by electron collision are needed in many areas of physics [1]. A detailed knowledge of the different rate coefficients is needed in the study of high temperature plasmas [2-4] in astrophysics and in controlled thermal-nuclear fusion research. Only if these and the transition probabilities are known the radiation emitted by a non-equilibrium plasma can be quantitatively described by a theoretical population model. For electron – induced ionization, recombination, excitation and de-excitation, mainly from excited atomic states, a detailed analysis is presented for the dependence of the rate coefficients on electron energy, on the temperature and on the atomic parameters.

In the present work, the absolute electron impact ionization, recombination and excitation rate coefficients of $3d^2 4s$ (^4F, ^2F, ^2D, ^4P, ^2G, ^2P), $3d^3$ (^4F, ^2G, ^4P, ^2P, ^2D, ^2H, ^2F,) and $3d^2 4p$ (^4G, ^4F, ^2F, ^2D, ^4D, ^2G, ^2S, ^4P, ^2P) levels of Ti II were calculated.

Oscillator strengths for allowed and forbidden transitions including relativistic effects in Berit-Pauli approximation were calculated by using Cowan code [5] and also by using Wiese [6] results. The level populations are calculated as a functions of the electron density and the plasma temperature for these 22 different levels. The theory is presented in section 2. Section 3 displays the results of the present calculations. Finally a conclusion is given in the last section.

Theory

Rate Coefficients

We consider the electronic $|p\rangle\,|n\rangle$ and $|p\rangle|\,i\rangle$ transitions in an atom, where p and n are the (effective) principal quantum numbers of initial and final states $|p\rangle$ and $|n\rangle$, and $|i\rangle$ denotes the ion ground state [7]. The following notation is used : E_{pi} and $E_{pn} = E_n - E_p$ are the ionization, excitation (for $E_n > E_p$) and de-excitation ($E_n < E_p$) energies, E_e and E are the incident electron and the energy transfer to the atom respectively.

Ionization Rate

The ionization rate Coefficient is given by [8]:

$$K_{pi} = \frac{9.56\times10^{-6}\left(kT_e\right)^{-1.5}\exp\left(-\varepsilon_{pi}\right)}{\varepsilon_{pi}^{2.33} + 4.38\varepsilon_{pi}^{1.72} + 1.32\varepsilon_{pi}} \quad cm^3 s^{-1} \tag{1}$$

Where, ε_{pi} is the energy transfer ($\varepsilon_{pi} = E_{pi}/kT_e$) and kT_e is expressed in eV.

Recombination Rate

The recombination rate coefficient is given by:

$$K_{ip} = \frac{3.17\times10^{-27}\left(kT_e\right)^{-3}\left(g_p/g_i\right)}{\varepsilon_{pi}^{2.33} + 4.38\varepsilon_{pi}^{1.72} + 1.32\varepsilon_{pi}} \quad cm^6 s^{-1} \tag{2}$$

Where g_p and g_i are the statistical weights of level $|p\rangle$ and of the ion ground state $|i\rangle$.

Excitation Rate

An empirical formula which represents the numerical rate coefficients for excitation rate with energy transfer ε_{pn} is:

$$k_{pn} = \frac{1.6\times10^{-7}\left(kT_e\right)^{0.5}\ \exp\left(-\varepsilon_{pn}\right)}{kT_e\ +\ \Gamma_{pn}}\times\left[A_{pn}\ \ \ln\left(\frac{0.3kT_e}{R}\ +\ \Delta_{\mathrm{pn}}\right)+B_{pn}\right]\quad cm^3S^{-1} \quad (3)$$

where, kT_e is in eV , R (Rydberg energy) in eV and $\varepsilon_{pn} = {E_{pn}}/{kT_e}$.

$$\Gamma_{pn} = R\ \ \ln\left(1+\frac{p^3kT_e}{R}\right)\left[3+11\left(\frac{s}{p}\right)^2\right]\times\left(6+1.6ns+\frac{0.3}{s^2}+0.8\frac{n^{1.5}}{s^{0.5}}\left|s-0.6\right|\right)^{-1}$$

R = 13.595, $p = z_{eff}\times\sqrt{{R}/{E_{pi}}}$, $n = z_{eff}\times\sqrt{{R}/{E_{ni}}}$, $s = \left|n-p\right|$

$$A_{pn} = \left({2R}/{E_{pn}}\right)f_{pn} \quad (4)$$

f_{pn} being the absorption oscillator strength.

$$\Delta_{pn} = \exp\left(-\frac{B_{pn}}{A_{pn}}\right)+\frac{0.06s^2}{np^2}$$

where $B_{pn} = \frac{4R^2}{n^3}\left(\frac{1}{E_{pn}^2}+\frac{4E_{pi}}{3E_{pn}^3}+b_p\frac{E_{pi}^2}{E_{pn}^4}\right)$ and $b_p = \frac{1.4\ln p}{p}-\frac{0.7}{p}-\frac{0.51}{p^2}+\frac{1.16}{p^3}-\frac{0.55}{p^4}$

De-excitation Rate

The de-excitation rate is given by:

$$k_{pn} = \frac{1.6\times10^{-7}\left(kT_e\right)^{0.5}\ {g_n}/{g_p}}{kT_e\ +\Gamma_{np}}\times\left[A_{np}\ \ln\left(\frac{0.3kT_e}{R}+\Delta_{np}\right)+B_{np}\right] \quad (5)$$

where Γ_{np} and Δ_{np} are obtained from Γ_{pn} and Δ_{pn} by interchanging *p* and *n*. g_p and g_n are the statistical weights of level $|p\rangle$ and $|n\rangle$.

Population Densities

Level population can be calculated by solving the steady-state rate equations [9,10]

$$N_j\left[\sum_{i<j}A_{ji}+N_e\left(\sum_{i>j}C_{ji}^d+\sum_{i>j}C_{ji}^e\right)\right] = N_e\left(\sum_{i<j}N_iC_{ij}^e+\sum_{i>j}N_iC_{ij}^d\right)+\sum_{i>j}N_iA_{ij} \quad (6)$$

where N_j is the population of level j , A_{ji} is the spontaneous decay rate from level j to level i (transition probabilities), C^e_{ji} is the electron collisional excitation rate coefficient, C^d_{ji} is the collisional de-excitation rate coefficient.

The population of the j th level is obtained from the identity [9]

$$N_j = \left(\frac{N_j}{N_I}\right)\left(\frac{N_I}{N_T}\right)\left(\frac{N_T}{N_e}\right)N_e \tag{7}$$

where N_I is total number density of all the levels of the ion under consideration , and N_T is the total number density of all ionization stages. Since the populations calculated from Equation (6) are normalized such that [9,10]

$$\sum_{j=1}^{n}\left(\frac{N_j}{N_I}\right) = 1 \tag{8}$$

where n is the number of all the levels of the ion under consideration, the quantity actually obtained from Equation (6) is the fractional or reduced population N_j / N_I . We calculated the population densities and rate coefficients by using the method given by Vriens [8] and by Feldman [9].

Results and Discussion

Excitation, Ionization and Recombination Rate Coefficients

For the evaluation of electron impact ionization, excitation and recombination rates, for excited atomic states in Ti II, the rate coefficients have been evaluated by using an empirical formula which is published by Vriens [8]. The calculations were carried out by using a computer program (CRMO code) [11]. The calculations include all forbidden and allowed transitions that are necessary for the calculations. Therefore, in addition to the dipole transitions we have introduced the monopole and quadrupole transitions in the calculations.

The rate coefficients are determined for $3d^24s$ (^4F, ^2F, ^2D, ^4P, ^2G, ^2P), $3d^3$ (^4F, ^2G, ^4P, ^2P, ^2D, ^2H, ^2F,) and $3d^24p$ (^4G, ^4F, ^2F, ^2D, ^4D, ^2G, ^2S, ^4P, ^2P) excited atomic states in Ti II. The calculations were carried out at different electron densities: 1.67×10^{16} cm^{-3}, 1.81×10^{16} cm^{-3}, 1.63×10^{16} cm^{-3}, 1.40×10^{16} cm^{-3}, 1.20×10^{16} cm^{-3}corresponding to different plasma temperatures: 0.81 eV, 0.85 eV, 0.84 eV, 0.81 eV and 0.80 eV, respectively. The excitation rates for some levels are drawn versus kT in Figs (1-5). These figures show that the excitation rate has its highest value at the highest value of kT_{exc}. The ionization rates are drawn versus kT, for some levels and are shown in Figs (6-10). It is clear from the figures that the ionization rate has its highest value at the highest value of kT.

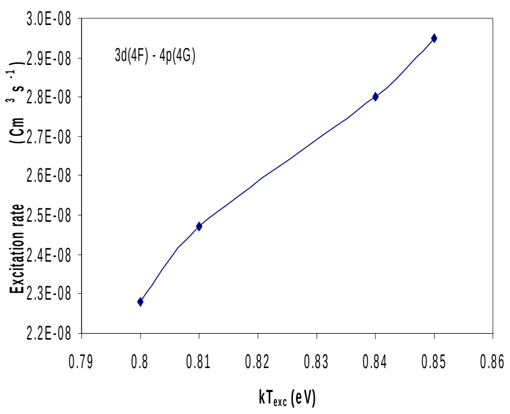

Figure 1: Excitation rate versus excitation temperature for 3d(^{4}F) - 4p(^{4}G) transition.

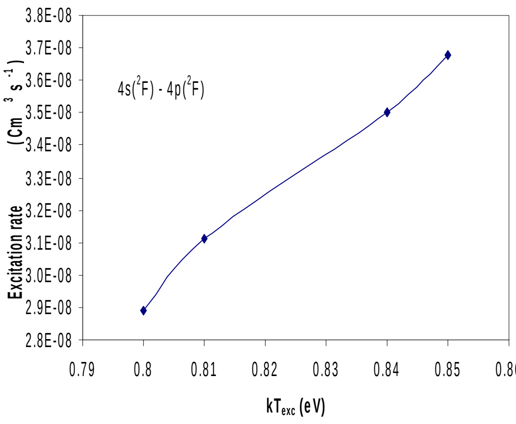

Figure 2: Excitation rate versus excitation temperature for 4s(^{2}F) -4p(^{2}F) transition.

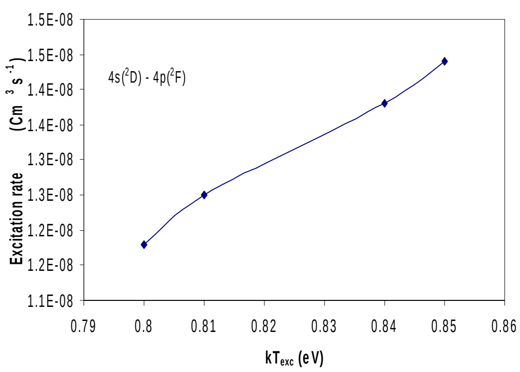

Figure 3: Excitation rate versus excitation temperature for 4s(^{2}D) - 4p(^{2}F) transition.

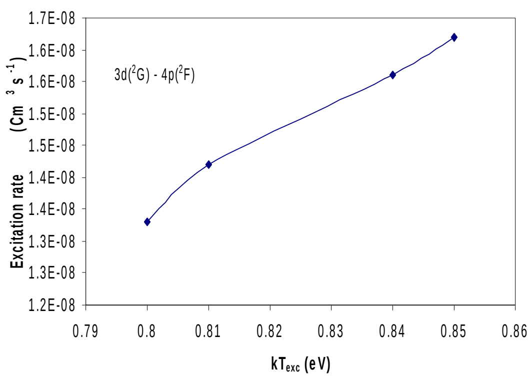

Figure 4: Excitation rate versus excitation temperature for 3d(^{2}G) - 4p(^{2}F) transition.

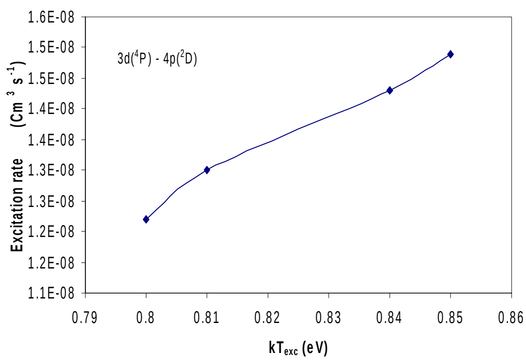

Figure 5: Excitation rate versus excitation temperature for 3d(^{4}P) - 4p(^{2}D) transition.

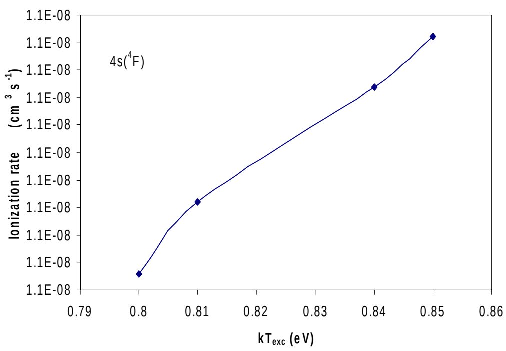

Figure 6: Ionization rate versus excitation temperature for the 4s(^{4}F) level.

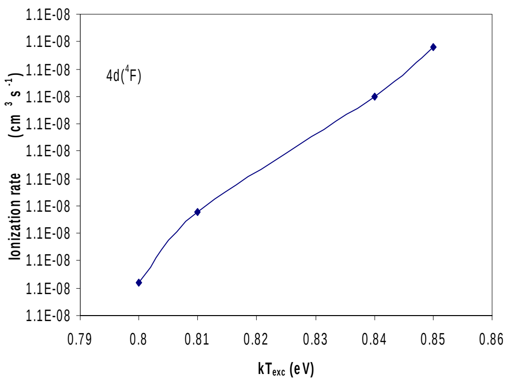

Figure 7: Ionization rate versus excitation temperature for the 4d(^{4}F) level.

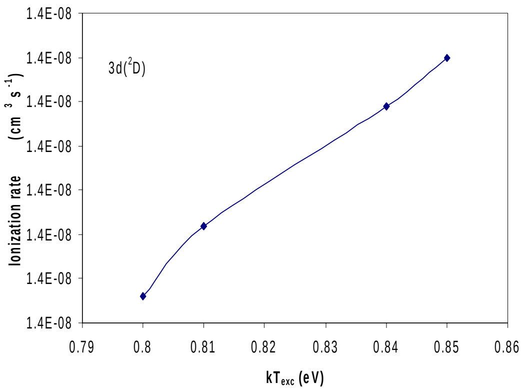

Figure 8: Ionization rate versus excitation temperature for the 3d(^{2}D) level.

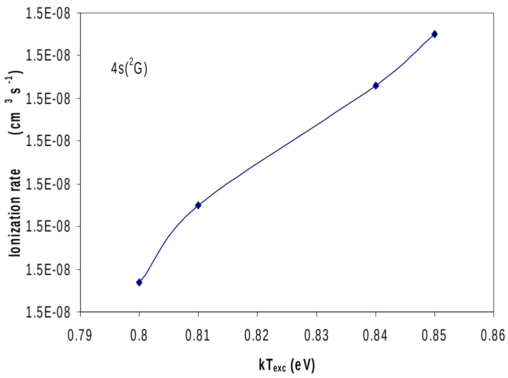

Figure 9: Ionization rate versus excitation temperature for the 4s(^{2}G) level.

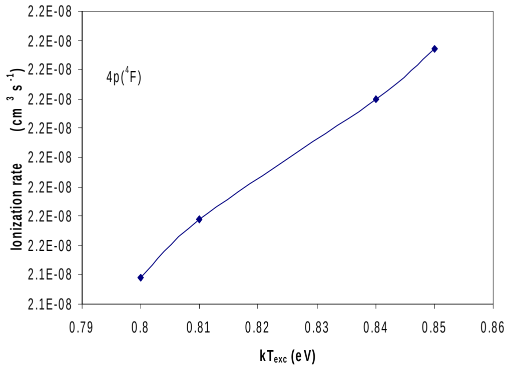

Figure 10: Ionization rate versus excitation temperature for the 4p(^{4}F) level.

Population Density of The Exited Levels

The population density of 22 levels in Ti II namely; 4s(^{4}F), 3d(^{4}F), 4s(^{2}F), 4s(^{2}D), 3d(^{2}G), 3d(^{4}P), 3d(^{2}P), 4s(^{4}P), 3d(^{2}D), 3d(^{2}H), 4s(^{2}G), 4s(^{2}P), 3d(^{2}F), 4p(^{4}G), 4p(^{4}F), 4p(^{2}F), 4p(^{2}D), 4p(^{4}D), 4p(^{2}G), 4p(^{2}S), 4p(^{4}P) and 4p(^{2}P) levels are calculated using the coupled rate equations (5). The levels are calculated at five different plasma temperatures 0.81 eV, 0.85 eV, 0.84 eV, 0.81 eV and 0.80 eV corresponding to electron densities 1.67×10^{16} cm^{-3}, 1.81×10^{16} cm^{-3}, 1.63×10^{16} cm^{-3}, 1.40×10^{16} cm^{-3}, 1.20×10^{16} cm^{-3}. The spontaneous decay rate A(j,i) given in equation (4) is calculated by using Cowan code [5] and by also using Wiese [6] results. To calculate the population densities, the parameters C^e and C^d are substituted into the coupled rate equations explained in section (2). Then, the computer program (CRMO code[11]) is used for solving simultaneous coupled rate equations. The level populations of the various levels of Ti II are listed in table (1).

At our case of low electron densities ($N_e<10^{17}$ cm^{-3}), the population density is directly proportional to the electron density at different plasma temperatures as shown in Figs. (11,12) for 4s(^{4}F) and 3d (^{4}F) levels. The behavior of level populations of the various levels of Ti II can be explained as follows: In general, at our case of low electron densities ($N_e < 10^{17}$ cm^{-3}), the population density is directly proportional to the electron density, where at these electron densities excitation to the upper levels is followed immediately by radiative decay, and collisional mixing of the excited levels can be ignored.

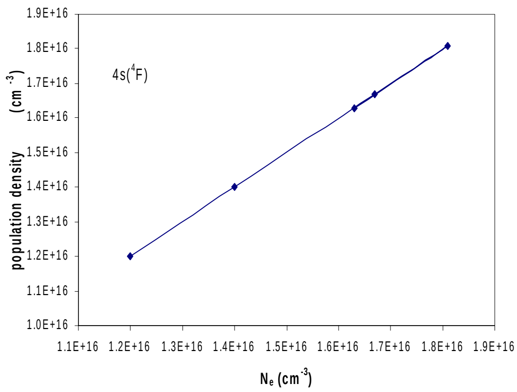

Figure 11: Population density of the 4s(^{4}F) level versus electron density.

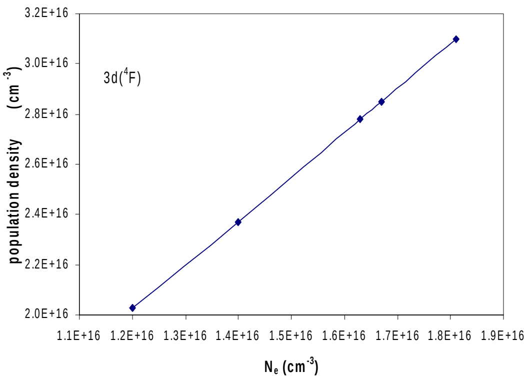

Figure 12: Population density of the 3d (^{4}F) level versus electron density**.**

Table 1: Level population densities (in cm^{-3}) at different excitation temperatures and their corresponding electron densities.

Level	**kT$_e$=0.81 eV N$_e$=1.67E+16 cm^{-3}**	**kT$_e$=0.85 eV N$_e$=1.81E+16 cm^{-3}**	**kT$_e$=0.84 eV N$_e$=1.63E+16 cm^{-3}**	**kT$_e$=0.81 eV N$_e$=1.40E+16 cm^{-3}**	**kT$_e$=0.80 eV N$_e$=1.20E+16 cm^{-3}**
4s(^{4}F)	1.67E+16	1.81E+16	1.63E+16	1.40E+16	1.20E+16
3d(^{4}F)	2.83E+16	3.10E+16	2.78E+16	2.37E+16	2.03E+16
4s(^{2}F)	1.23E+16	1.38E+16	1.23E+16	1.04E+16	8.74E+15
4s(^{2}D)	6.56E+15	7.55E+15	6.68E+15	5.51E+15	4.60E+15
3d(^{2}G)	1.03E+16	1.20E+16	1.05E+16	8.68E+15	7.22E+15
3d(^{4}P)	3.96E+15	4.57E+15	4.04E+15	3.32E+15	2.77E+15
3d(^{2}P)	1.84E+15	2.13E+15	1.88E+15	1.55E+15	1.28E+15
4s(^{4}P)	5.40E+15	6.26E+15	5.53E+15	4.53E+15	3.76E+15
3d(^{2}D)	2.41E+15	2.85E+15	2.50E+15	2.03E+15	1.67E+15
3d(^{2}H)	6.00E+15	7.10E+15	6.22E+15	5.04E+15	4.15E+15
4s(^{2}G)	4.04E+15	4.85E+15	4.24E+15	3.40E+15	2.77E+15
4s(^{2}P)	6.65E+14	8.10E+14	7.02E+14	5.60E+14	4.55E+14
3d(^{2}F)	1.36E+15	1.70E+15	1.47E+15	1.15E+15	9.18E+14
4p(^{4}G)	4.24E+14	5.62E+14	4.77E+14	3.57E+14	2.78E+14
4p(^{4}F)	2.19E+14	2.92E+14	2.47E+14	1.84E+14	1.43E+14
4p(^{2}F)	2.69E+14	3.60E+14	3.05E+14	2.26E+14	1.75E+14
4p(^{2}D)	1.86E+14	2.50E+14	2.11E+14	1.56E+14	1.21E+14
4p(^{4}D)	1.67E+14	2.26E+14	1.91E+14	1.41E+14	1.10E+14
4p(^{2}G)	1.69E+14	2.31E+14	1.94E+14	1.42E+14	1.10E+14
4p(^{2}S)	2.71E+13	3.77E+13	3.16E+13	2.28E+13	1.73E+13
4p(^{4}P)	3.90E+13	5.62E+13	4.65E+13	3.29E+13	2.50E+13
4p(^{2}P)	7.89E+12	1.16E+13	9.56E+12	6.65E+12	4.93E+12

Conclusions

The ionization, recombination and excitation rates are determined for 22 levels in Ti II. The population density for each level is calculated and it is found that the highest value of the population density is for the $3d^3(^4F)$ excited level and the lowest value is for the $4p(^2P)$ excited level.

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