The Influence of Hot Electrons on the Calculation of Ionization Rates

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Abstract- Electron-Impact Ionization (EII) is considered one of the most important ionization methods in dynamic systems, in which elements and ions are suddenly exposed to energetic electrons. In many plasma types, it has been observed that some electrons (hot) are governed by a non-Maxwellian energy distribution. This study illustrates the effects of a non-Maxwellian distribution on beryllium and Be^{+2} emission lines and their effective ionization rate coefficients. The focus on beryllium as an impacted material by electron flux aimed to evaluate the EII rates for Be and generate the corresponding datasets needed for Be^{+2} data analysis. An interaction cross-section was generated using the Flexible Atomic Code (FAC) and used in the estimation of the EII distribution energy functions to estimate the ionization rates for a non-Maxwellian distribution. The use of non-Maxwellian energy distributions for different fractions of hot electrons showed the sensitivity of these rates to the fraction of hot electrons and the forms of the electron energy distribution. The results were in good agreement with those found in the literature.

Keywords-Electron-Impact Ionization (EII); FAC; distribution function; non-Maxwellian distribution; cross-sections

I. Introduction

In plasma physics, considerable efforts are deployed to apprehend the emission of electrons during atomic ionization collisions under experimental and numerical perspectives. Electron Impact Ionization (EII) is important in dynamic systems where ions are immediately exposed to energetic electrons [1]. Such incidents may be encountered in solar flares, supernova remnants, and merging clusters of galaxies [2, 3]. EII has attracted considerable interest in the study of the distribution of the charge state of nonthermal electrons in plasma, where the high-energy tail includes a large population of electrons residing above the EII rate. Consequently, EII is important to model astrophysical systems including non-thermal distributions [4]. Determining the spatial distribution of hot electrons in plasma is very crucial as they affect radiation production, energy balance, and plasma dynamics [5, 6]. These electrons may cause considerable energy losses and negatively impact the plasma's stability and control.

In plasma physics and nuclear fusion, non-Maxwellian distributions and hot electrons relate to plasma sources and their evolution. Besides that, they are necessary to assess the radiative properties of a broad range of plasma sources. Beryllium (Be) was used in the ITER fusion reactor project to cover the inner surface of the first wall as a plasma-facing material because of its unique physical property to contain radiation power and its ability to be less contaminated by plasma with low fuel retention. In this sense, it is very important to obtain accurate collisional data of EII on Be. The estimation of coefficient rates is based on analytical concepts developed in previous works and datasets [7]. These studies on hot electrons were related to specific experiments, and the results obtained were restricted to specific types of energy distribution used to characterize these electrons. It should be noticed that rates of collisional ionization, resonant excitation, and radiative recombination present a relative sensitivity with characteristic energy and functional shape of the electron distribution, which may have significant consequences on collisional radiative two-temperature models. These models usually include distributions of hot electrons with much greater energies than the usual transition gaps, where the sensitivity of hot electron effects for both Gaussian and Maxwellian distributions is observed separately [8].

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In this study, an analytical and numerical investigation on the ionization rates of plasma made from a population of electrons including a non-Maxwellian distribution of a given initial velocity, was conducted. The effects of the simultaneous presence of electrons with low and high energies on the calculation of ionization rate coefficients and their energy distribution functions are discussed. This approach aimed to present the influence of hot electrons and investigate the impact of the electron energy distribution functions on the measurement of the ionization rates for Be^{+2} using a non-Maxwellian energy distribution for various hot electron fraction values. The non-Maxwellian distribution used gave satisfactory results for larger fractions of hot electrons. This study focused on larger fractions of hot electrons because using a non-Maxwellian distribution gives unacceptable results on weak fractions. Compared to previous works on neutral helium ionization rates calculated using a non-Maxwellian distribution and the power-law distribution functions of electrons [9], this study exhibits a great improvement in the curves obtained, particularly for the Maxwellian and power-law distribution functions.

II. THEORETICAL ASPECT

A. *Ionization Cross-sections*

In laboratory or astrophysical plasma studies, it is very crucial to understand the ionization balance based on the estimation of ionization rates for different ions involved in such plasmas. Many analytical and statistical formulas are dedicated to the estimation of ionization rates and the related cross-sections. In this way, the Lotz formula has been frequently used in plasma-related fields as one of the most suitable empirical formulas to calculate the cross-sections of the ionization rates [10], based on experimental measurements of ionized elements with low Z [11, 12]. Similarly in [13], the parametric formula initially introduced in [14, 15] was used. Recently, dedicated codes were built to calculate the corresponding atomic structure and data related to interaction processes (recombination, ionization, excitation, etc.). Therefore, the Flexible Atomic Code (FAC) was mainly made to accommodate radiative transformation, direct collisional excitation, and ionization [16]. This robust package was presented in [17] to combine different atomic processes into a common theoretical system and provide a uniform, flexible, and easy-to-use user interface to access all computational tasks. FAC was used to calculate the EII cross-section, based on the Distorted Wave (DW) relativistic approximation and the interpolation-factorization methods [16, 17]. The cross-section of the transition:

$$2s^2 \rightarrow 1s2s^2$$

for Be was generated using this code on a varying energy range from 0 to 1000eV, as shown in Figure 1. The FAC code included the DW method and generated cross-section data with a satisfactory level. Figure 2 shows the cross-sectional data of the ionization processes, obtained according to the DW method, taking into account the potential felt by the incident electron when approaching the nucleus of the target ion [18]. Thus, it was possible to generate the cross-sections needed over a large interval of incident electron energies, starting from the ionization threshold [17].

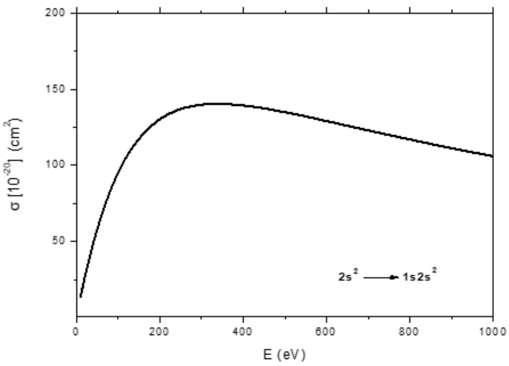

Fig. 1. Cross-section of Be obtained by FAC.

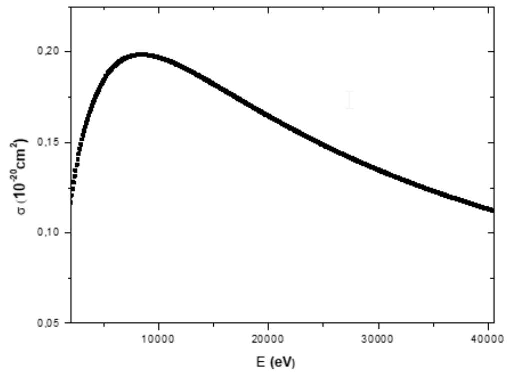

Fig. 2. Cross-section of Be^{+2} obtained by FAC.

B. *The Effects of Hot Electrons on the Calculation of Ionization Rates*

Free electrons in a plasma are characterized by a given energy distribution. The quantity of interest is the ionization rate coefficient per electron impact, obtained by averaging the product of the electron velocity by the corresponding ionization cross-section. In the case of direct ionization, the coefficient of ionization rates is given by [19, 20]:

$$\tau[cm^3.s^{-1}] = \int v\sigma(E)F(E)dE \quad (1)$$

where v and E are the velocity and energy of the incident electron respectively, $\sigma(E)$ represents the impact ionization cross-sections calculated by FAC, $F(E)$ is the electron energy distribution function, and E is the energy of the impacting electron. A non-Maxwellian distribution function of the energy $F(E)$ was used to calculate the ionization rates by the mean of cross-sections. The produced plasma under low pressure often exhibit a non-Maxwellian behavior of electron distributions. Such a distribution can be represented by a function of two temperatures corresponding to both hot and cold electron populations. The following non-Maxwellian distribution was chosen to study the effects of hot electrons on the ionization rates of Be [20]:

$$F_{NM}(E) = (1 - f_{hot})F_M(T_{bulk}) + f_{hot}F_X(T_{hot}) \quad (2)$$

where f_{hot} is the normalized hot electron fraction, F_M is the Maxwell energy distribution function, and T_{bulk} and T_{hot} are the bulk and hot electron temperatures respectively.

By substituting (2) in (1) and including the effective ionization cross sections generated by the FAC code for Be atoms, it was possible to obtain the ionization rates for different values of hot electron fractions f_{hot}, as shown in Figure 3 by plotting the obtained curves representing the variation of the ionization rate coefficients of Be using the non-Maxwellian distribution. This was carried out for different values of hot electron fractions f_{hot} as a function of the electron temperature T, taken between 1.0 and 10^3eV, including the results obtained by applying a Maxwell distribution for f_{hot}=1. The temperature T_{bulk} was taken equal to an average value of k_bT_{bulk}=0.85eV [19]. The fractions of cold electrons are less than those of hot electrons. The rate coefficients at very low temperatures are very sensitive to the cross-section behavior near the threshold and significant discrepancies may be observed between various theoretical calculations and/or empirical scaling. The plane wave of Born approximation is not valid at low energies and gives typically lower cross-sections than the DW computation method near the threshold by a factor of 2 [10].

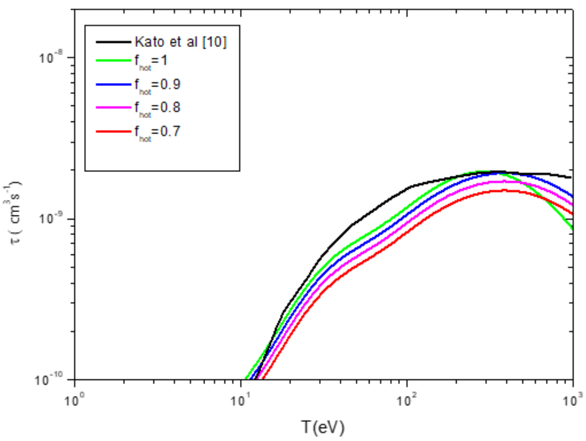

Fig. 3. Ionization rates of Be obtained for a non-Maxwellian distribution with different values of hot electrons fraction f_{hot}=0.7, 0.8, 0.9, and 1.0.

Figure 3 shows that the curves obtained for the various fractions (70%, 80%, 90%) are generally quite close to the plotted for the referential fraction value f_{hot}=1 representing the Maxwellian distribution. As a matter of fact, in the case of low temperatures, the ionization rates are very sensitive to the cross-section behavior [21]. There are noticeable differences between theoretical and experimental methods. Examining the published results in [10] for comparison, the plotted curves of ionization rates in Figure 3 are shifted down from the Maxwellian distribution for f_{hot}=1 as the hot electron fraction decreases. This shows a remarkable sensitivity of the ionization rates related to hot electron fractions.

C. Distribution Functions

The electron energy distribution is highly important in plasma physics, nuclear fusion reactions, and astrophysics [22]. Consequently, collisional-radiative atomic models assessing the effect of a non-Maxwellian distribution and hot electrons are extremely important to apprehend the obtained data in atomic physics, such as in spectroscopic analysis to establish the existence and characteristics of the behavior mechanisms of electrons in studied plasmas [23, 24]. Dedicated experiments and research on hot electrons provided valuable contributions to build suitable energy distribution functions, as given by the following expressions [20]:

Maxwellian:

$$F_M(\varepsilon, T_e) = 2\sqrt{\frac{\varepsilon}{\pi T_e^3}}\, exp\left[{}^{-\varepsilon}/_{T_e}\right] \quad (3)$$

Gaussian:

$$F_G(\varepsilon,\ T_e) = \frac{1}{T_e\sqrt{\pi}}\left(\frac{2}{1+erf\left({}^{+\varepsilon_0}/_{T_e}\right)}\right) exp\left[-\left(\frac{(\varepsilon-\varepsilon_0)}{T_e}\right)^2\right] \quad (4)$$

Power- law:

$$F_p(\varepsilon, T_e) = \left(\frac{\gamma-1}{T_e{}^{1-\gamma}}\right)\varepsilon^{-\gamma}; \varepsilon \geq T_e \quad (5)$$

where T_e, ε, ε_0 are the energies of electrons corresponding to each distribution, and γ is the decay constant.

The energy distribution helps to examine how the used model affects the estimation of the ionization rates for given cross-sections. For plasma described by a single-temperature Maxwellian distribution, it is possible to calculate de-excitation and recombination rates with accurate precision, explicitly from the coefficients of collisional excitation and ionization rates. In the case of plasmas with atoms described by non-Maxwellian distributions, the cross-sections related to calculated rates must be integrated through the entire distribution of electron energies. A simple analytical formula could express the associated rate coefficients when using the appropriate approximation of the cross-sections as an energy-dependent function. This study aims to extend the calculations for plasmas described by a non-Maxwellian distribution. Plasmas containing a small proportion of hot electrons may be observed in the universe or in the laboratory, and induced plasmas often exhibit non-Maxwellian distributions with hot and cold electrons. Therefore, using cross-sections generated by the FAC, the ionization rates were calculated using different energy distribution functions $F(\varepsilon)$. Ionization rates were obtained for various values of hot electron fractions f_{hot} by separately substituting $F_x(\varepsilon, T_e)$ from (2) with Maxwellian (3), Gaussian (4), and Power-law (5).

III. RESULTS AND DISCUSSION

Figures 4 and 5 show the ionization rates for Be^{+2} for different values of hot electron fractions using Maxwellian, Gaussian, and Power-law models in (2). In the case of the Maxwellian model shown in Figure 4, the values of the coefficient rates increased very rapidly at low temperatures. Figure 5 shows the comparison between different distribution functions for a specific value. A good agreement can be observed between the ionization rate curves for hot electron fractions ranging from 1 to 10% over the whole energy range. Furthermore, the value of the decay constant γ does not significantly affect the calculation estimation for a given value of the fraction of hot electrons [9]. The relative susceptibility of the ionization rates to the form of the electron energy distribution functions when γ=2 and the hot electron fraction assume high values have significant consequences for collisional radiative models at two temperatures. When the temperature of electrons increases, the hot electron distribution takes a thermal form with a long tail compared to the Maxwellian distribution at thermal equilibrium electron distribution functions over the whole energy range for various values of given hot electron fractions f_{hot}.

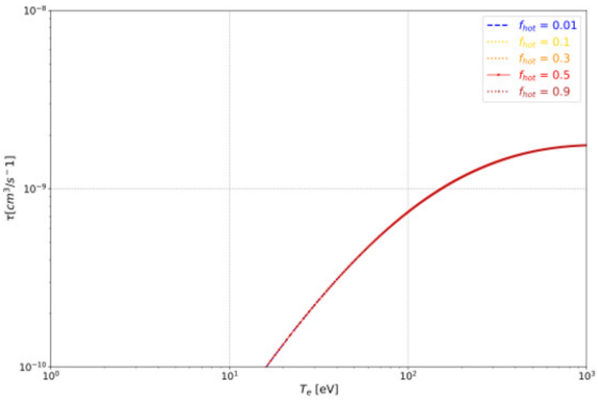

Fig. 4. Ionization rates of Be^{+2}: Coefficient rates obtained for the Maxwellian distribution function with various fractions of hot electrons f_{hot}.

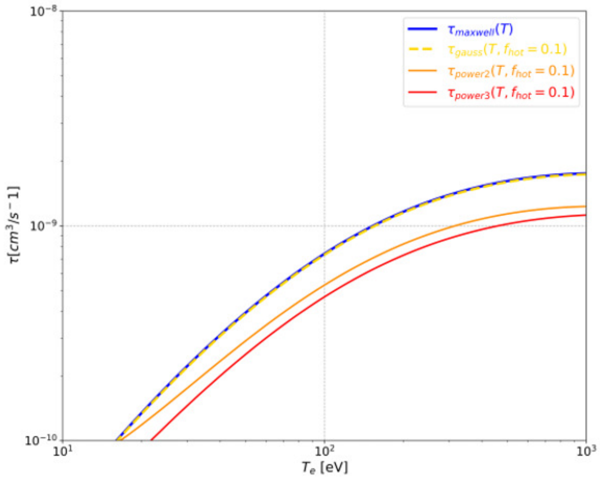

Fig. 5. Ionization rates of Be^{+2}: Coefficient rates obtained for Maxwellian, Gaussian, and Power-law distribution functions with f_{hot}=0.1.

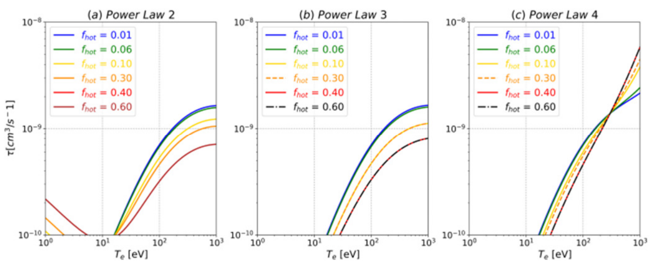

Fig. 6. Ionization rates of Be^{+2}: Coefficient rates obtained for different power distribution functions with various decay constants: (a) γ=2, (b) γ=3, (c) γ=4 and different hot electron fractions.

Figure 6 shows the ionization rates of Be^{+2} obtained for different power-law distributions defined by a given decay constant γ. Figures 6(a) and (b) show the generated results for both power 2 and 3 models at low temperatures and indicate the presence of susceptibility to the fractions of hot electrons as the value of the constant of decay γ increases. Figure 6(c) shows significant variations within the 10-100eV range, where a considerable improvement in curve shape is registered for the power 4 model (γ=4).

IV. CONCLUSION

This study used the FAC code and a non-Maxwellian distribution function to calculate the ionization rates and the corresponding cross-sections of Be and Be^{+2}. Most collisional rates were more sensitive to the hot electron fractions than to the exact functional form of the electron energy distributions. Greater hot temperatures naturally contain larger numbers of superthermal electrons and thus allow larger fractions of hot electrons, which may cause profound impacts. Ionization rates are very sensitive to the behavior of cross-sections. It should be also noticed that considerable differences between theoretical and empirical methods may be registered. The use of a non-Maxwellian energy distribution demonstrated that the estimated rates are sensitive to the forms of electron energy distributions used [25, 26]. In the case of beryllium, it was shown that the curves of ionization rates are responsive to the hot electron fractions of 70 and 80%. The curve of the ionization rate approaches that of [10] for the fraction of 100% of hot electrons. The results obtained from the ionization rates for Be^{+2} and different energy distribution functions showed an acceptable agreement between the curves of various figures, except for the Maxwellian distribution function. Furthermore, significant deviations were observed for low temperatures in the 20-200eV energy range. Finally, exceptional sensitivity of the ionization rates for Be^{+2} was shown for various fractions of hot electrons.

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