2nd Asia-Pacific Conference on Plasma Physics, 12-17,11.2018, Kanazawa, Japan

Atomic and ionic processes in low-temperature Ar, Kr, and Xe plasmas: cross section data and collisional-radiative model

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I. Introduction.

Collisional-radiative (C-R) model is a powerful tool for describing the interactions between electrons, neutrals, ions, and radiation throughout a plasma. However, conducting C-R model requires knowledge of cross section data of fundamental atomic and ionic processes, which may be not available in literatures [1]. In this work, we report the recent progress in calculating cross section data of rare-gas atoms and ions by the Dirac *B*-spline *R*-matrix approach [2] and in measuring their excitation rate coefficients by the method of combined diagnostics in afterglow plasmas (CDAP) [3]. The kinetics of excited atoms and ions in several kinds of non-equilibrium plasmas is then investigated by C-R modelling using these data.

II. Cross section

Benchmark calculations of oscillator strengths and electron-impact excitation cross sections of rare-gas atoms have been carried out using the Dirac *B*-spline *R*-matrix (DBSR) method in literatures [2]. However, research on ionic cross sections are rarely reported, which are also important for plasma applications. In this work, we report a comprehensive investigation on the structural parameters of rare gas ions e.g. Xe^+ important for the electric propulsion. The Dirac–Coulomb Hamiltonian is performed to describe the target and the collision systems. As shown in table 1, the calculated oscillator strengths for typical transitions of Xe^+ (in the velocity form) are in good agreement with the available experiment measurements from the NIST. Based on this structure description, The electron impact excitation cross sections of Xe^+(6s), Xe^+(6p), and Xe^+(5d) levels are obtained, which are used in combination with the atomic cross sections in literatures for the following collisional-radiative model.

Table 1. Comparison of oscillator strengths

Upper level	Lower level	Theory	NIST
$5p^4(^3P_2)6p^2[1]^\circ_{3/2}$	$5p^4(^3P_2)6s^2[2]_{3/2}$	0.238	0.26
$5p^4(^3P_2)6p^2[3]^\circ_{7/2}$	$5p^4(^3P_2)6s^2[2]_{5/2}$	0.517	0.52
$5p^4(^3P_2)6p^2[2]^\circ_{5/2}$	$5p^4(^3P_2)6s^2[2]_{5/2}$	0.404	0.37
$5p^4(^3P_1)6p^2[0]^\circ_{1/2}$	$5p^4(^3P_1)6s^2[1]_{3/2}$	0.191	0.16
$5p^4(^1D_2)6p^2[3]^\circ_{5/2}$	$5p^4(^1D_2)6s^2[2]_{3/2}$	0.130	0.16
$5p^4(^3P_2)6p^2[2]^\circ_{5/2}$	$5p^4(^3P_2)5d^2[2]_{3/2}$	0.020	0.032

III. Rate coefficient

Cross section and rate coefficient data for electron-impact processes play an important role in the low-temperature plasma modelling; however, there is a lack of data for processes between excited levels. Recently, a method for determining electron excitation rate coefficients between Ar and Kr excited states in afterglow plasmas is successfully implemented and further developed to obtain large sets of collisional data [3]. This method combines diagnostics for electron temperature, electron density, and excited species densities and the kinetic modelling of excited species, from which the electron excitation rate coefficients between excited levels can be determined. Here we compare the experimental data from CDAP with the theoretical results given by the *R*-matrix method.

IV. Collisional-radiative model and kinetic processes

By using the above oscillator strength, cross section, and rate coefficient data, a kind of collisional-radiative model for the important *n*s, *n*p, and (*n*-1)d levels for the atoms and ions of Ar(*n*=4), Kr(*n*=5), and Xe(*n*=6) are built [4-5]. For example, figure 1 shows the prediction of the relative line intensities emitted by Xe(6p) and Xe^+(6p) levels in the ionization region of the discharge channel of a Hall thruster, which are not reported in the literatures before. It shows that the modelling results are in good agreement with those measured by using the optical line-ratio method. This kind of model becomes a useful tool to reveal the fundamental kinetic processes of the species in the region with strong electromagnetic field, as well as to support the widely-used optical emission spectroscopy (OES) method. A discussion about the above topics will be given in detail in this work.

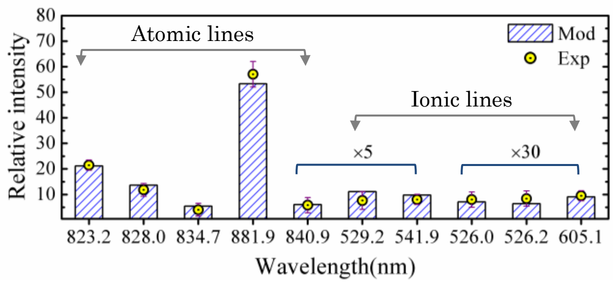

Figure 1. Comparison of line intensities from a Hall thruster.

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