A comprehensive xenon collisional-radiative model of atomic and ionic excited levels for Hall thruster

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Wang Yan-Fei[1] and Zhu Xi-Ming[2]
Harbin Institute of Technology, Harbin, Heilongjiang, 150001, China

Abstract: Collisional-Radiative (CR) model describes the kinetic mechanism of excited species in plasmas, it is the basis of optical emission spectroscopy (OES). In recent years, several xenon CR models for electric propulsion devices has been carried out, which allows us to diagnose plasma parameters in Hall thrusters using optical method. Kinetic mechanism of excited species in Hall thruster plasma also emerges as these works carry on. However, ionic excited levels, which are crucial to OES of some plasma parameters, e.g. electron density, are not incorporated in these models due to lack of cross sections. Information about xenon ionic lines are thus abandoned in OES, while kinetics of ionic species remain unknown. In this work, a comprehensive xenon CR model include atomic and ionic levels is presented. The model is verified by comparing modelled spectra with those measured in different regions of a Hall thruster. Using the model, kinetics of atomic and ionic levels in those different regions of Hall thruster are also studied. Development of a novel OES method using both atomic and ionic lines could be carried out by analyzing the relation between plasma parameters and spectrum character by using this model.

I.Introduction

Collisional-radiative (CR) model determines the distribution function of atoms and ions over their excited states. It describes the kinetic mechanisms of excited species, and is capable of predicting emission spectrum as a function of plasma parameters, e.g. electron temperature (T_e), electron density (n_e), etc., thus is the basis of optical emission spectroscopy (OES) method.

CR model for electric propulsion devices has been richly studied, especially for those devices which use xenon as propellant. In 2006, based on a set of measured emission cross sections, researchers from the TSNIIMASH of Russia and the Air Force Research Laboratory of the USA built a CR model for several atomic levels of Xe[1]. The model is capable of predicting several emission lines in the near-infrared region, and was used in determination of electron temperature in a Hall thruster. Three years later, using cross sections calculated by an R-Matrix method and by a distorted-wave method, they improved the model by replacing hypothetical cross sections of the metastable levels[2]. The improved model was tested on two types of Hall thrusters, and then used in studying the kinetics of metastable states in these devices. In 2010, researchers from the Northwestern Polytechnic University of China and the University of Tokyo proposed another Xe CR model. The model includes 173 atomic levels and is based on cross sections obtained by the atomic code of Los Alamos National Laboratory, which also uses distorted-wave method[3]. In early 2019, researchers from the India Institute of Technology and the Visvesvaraya National Institute of Technology presented a CR model incorporating 36 levels of Xe. And the model was used to determine plasma parameters from spectral of an ICP plasma[4].

By reviewing former researches, it is found that those models mainly focus on kinetic mechanisms of atomic species, and are capable of predicting emission intensity of lines from these atomic excited states, while ionic levels

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[1] Doctoral student, School of Energy Science and Engineering, arvin.yanfei.wang@outlook.com.
[2] Professor, School of Energy Science and Engineering, simon.ximing.zhu@outlook.com. (Corresponding author)

and related processes are not included. As a result, emission intensity of the lines in visible range that are mainly emitted by ionic states can't be predicted, and those lines are important when one analyze plume images captured by CCD cameras[5]. In addition, kinetic mechanisms of ionic levels remain unknown.

In this work, a comprehensive Xe CR model incorporates both atomic and ionic levels is presented, and is verified by comparing modelled spectra and spectra measured in a Hall thruster. The model is then used in studying the kinetic mechanism of excited atomic and ionic states in a Hall thruster.

II.Collisional-radiative model

For EP devices that use xenon as propellant, especially for Hall thruster and gridded ion thruster, it is found that emission lines emitted by 6p levels of atomic and ionic xenon excited particles are dominant in spectrum. On the one hand, a model which could well predict the behavior of 6p levels could be used in OES of EP devices, since these lines have the best signal to noise ratio (SNR) in spectrum measurement, using these lines in OES can reduce the errors caused by measurement. On the other hand, 6p levels of xenon are closely related to metastable states by radiative processes and electron collision processes, while metastable states may play a role in EP discharge. Thus it is important to include 6p and metastable states when one try to have a better understanding of the discharge by studying the kinetic mechanisms of excited species using CR model.

Under these concerns, the model presented in this paper considered atomic and ionic 6s, 6p and 5d levels of xenon. Table 1 lists the information about the atomic levels included in the model, while table lists the information about ionic levels. The model considers the lowest levels of each group, with the energy range given in the column named "Energy range".

Table 1 Atomic levels included in the CR model.

Group	Quantity	Energy range (eV)	Group	Quantity	Energy range (eV)
$5s^25p^6$	1	0	$5p^56d$	8	10.972 ~ 11.163
$5p^56s$	4	8.315 ~ 9.570	$5p^58s$	2	11.258 ~ 11.274
$5p^56p$	10	9.580 ~ 11.141	$5p^54f$	8	11.263 ~ 11.276
$5p^55d$	12	9.890 ~ 11.607	$5p^57d$	8	11.423 ~ 11.498
$5p^57s$	4	10.562 ~ 11.878	$5p^58p$	6	11.426 ~ 11.475
$5p^57p$	6	10.902 ~ 11.015	$5p^59s$	2	11.580 ~ 11.583

Table 2 Ionic levels included in the CR model

Group	Quantity	Energy range (eV)	Group	Quantity	Energy range (eV)
$5s^25p^5$	2	12.130 ~ 13.436	$5p^46s$	8	23.669 ~ 28.155
$5s5p^5$	1	23.367	$5p^46p$	21	25.991 ~ 30.627
$5p^46p$	28	23.958 ~ 29.248			

For collision processes, considering the characteristic of Hall thruster, the model takes electron collision process, ion-impact process as well as charge exchange process into account. Some other processes are not included because of their relatively low process rate. The electron-ion recombination process is weak due to high electron temperature in such plasma (T_e > 3eV). Collision between atoms, e.g. penning ionization and quenching process of excited atoms, are also not important, because of high ionization ratio and low pressures. As for radiation-related process, both spontaneous radiation process and self-absorption are considered. Processes considered in the model are listed below.

(a) Electron collision processes:

$$e+X \leftrightarrow e+X^* \ , \tag{1}$$

$$e+X^q \leftrightarrow e+X^{q+1} \ , \tag{2}$$

$$e+X^q \leftrightarrow e+X^{(q+1)*} \ . \tag{3}$$

(b) Ion-impact processes:

$$Xe^+ + X \leftrightarrow Xe^+ + X^* \ , \tag{4}$$

$$Xe^+ + X^q \leftrightarrow Xe^+ + X^{(q+1)*} \ . \tag{5}$$

(c) Photon-related processes:

$$X^* \rightarrow X+hv \ , \tag{6}$$

$$X+hv \rightarrow X^* . \tag{7}$$

(d) Charge exchange process,

(e) Diffusion process.

Considering all these processes, rate balance equation for atomic and ionic states can be written as:

$$\sum_{y\neq x} R_{y\to x}^{col} + \sum_{y>x} R_{y\to x}^{rad} + \sum_{y<x} R_{y\to x}^{abs} = \sum_{y\neq x} R_{x\to y}^{col} + \sum_{y<x} R_{x\to y}^{rad} + \sum_{y>x} R_{x\to y}^{abs} + R_x^{d/t}, \tag{15}$$

Here R is the rate of certain process that are distinguished by superscript. Superscript *col* denotes collision process; *rad* denotes radiation process; while *abs* denotes self-absorption process. $R^{d/t}$ is the loss rate caused by diffusion or transport process. The subscript y is a level different from the excited level x, including the atomic and ionic ground states; $y<x$ means level y is lower than level x in energy.

For level x, the rate of collisional population processes could be written as:

$$R_{y\to x}^{col} = n_e \cdot n_y \cdot Q_{y\to x}^{e} + n_i \cdot n_y \cdot Q_{y\to x}^{i} . \tag{16}$$

Here n_e and n_i represents density of electron and ion, respectively. And n_y is the density of level y. Q is the rate coefficient for collision process. Superscripts e and i over Q tells whether the transition is caused by electron-impact or ion-impact. And the rate coefficients could be calculated with collision cross sections by:

$$Q_{y\to x} = \int_{E_0}^{\infty} \sigma_{y\to x}(E) \cdot \sqrt{\frac{2E}{m}} \cdot g(E) \cdot dE . \tag{17}$$

Here $\sigma_{y\to x}$ is the cross section of collision-induced transition "$y\to x$". E is the energy of colliding system, m is system mass. $g(E)$ is the energy distribution function (EDF), e.g. for electron-impact system, it would be electron energy distribution function.

The rate of radiation and absorption processes could be expressed as:

$$R_{y\to x}^{rad} - R_{x\to y}^{abs} = \Gamma_{x\to y}(n_x) \cdot A_{y\to x} \cdot n_y . \tag{18}$$

Here A is the Einstein coefficient of spontaneous radiation, Γ is the escape factor due to the self-absorption effect, which could be calculated by:

$$\Gamma(\tau) = \frac{2-\exp(-c_1\cdot\tau)}{1+(c_2\cdot\tau)^k} , \tag{18}$$

where τ is the optical depth, c_1, c_2 and k are could be found in reference[6].

Loss frequencies due to diffusion and transport process are given by:

$$R_x^{d/t} = K_x \cdot n_x \text{ and } K_x^{-1} = (D_x \cdot \frac{\chi_{01}^{2}}{r^2})^{-1} + (\frac{v_0}{r})^{-1} , \tag{23}$$

where D is the diffusion coefficient, R is radius of plasma, v_0 is mean velocity of excited particles, and χ_{01} =2.405.

Collisional cross sections and Einstein coefficients are critical to a CR model. However, it is not so easy to attain these key data. For ionic electron impact processes, no literatures that report electron-induced excitation cross sections are found. Cross sections calculated in the first part of this series are used. As for atomic electron impact processes, Lin *et al* managed to measure cross sections for excitation into $5p^5 6p$, $5p^5 7p$ from both ground states and metastable states using optical method [CS 1-3]. Chiu *et al* reported a set of apparent cross sections for excitation into some xenon 6p sates, which are measured using optical method[9]. Srivastava *et al* calculated cross sections for excitation into $5p^5 6p$ states using relativistic distorted-wave method [CS 4]. Zatsarinny and Bartschat used *B*-spline *R*-Matrix approach to calculate excitation cross sections of xenon atoms, which produces accurate cross sections near the threshold [CS 5]. Cross sections for excitation into $5p^5 5d$ and other higher levels are calculated by them too, in addition to cross sections for excitation into $5p^5 6p$ and 7p, makes cross sections calculated by *R*-Matrix approach the most comprehensive ones. Thus the full set of *R*-Matrix cross sections are used in the model. Cross sections for de-excitation processes are obtained from the principle of detailed balance. Einstein coefficients calculated by *R*-Matrix approach are used for both atomic and ionic spontaneous radiation, to keep consistency of database.

III.Results

Spectra modelled by the CR model are compared with those measured in different regions of Hall thruster to examine the accuracy of the model. For the sake of conciseness and clarity in drawing, only the results of some strong lines are shown in figure 1. Emission lines of ionic lines are not observed in the near-anode region, thus only the comparison of atomic lines are shown. The reason why ionic lines are not observed in the near-anode region may be that ion density in this region is not high enough to emit observable amount of photons.

In general, the line intensities obtained from modelling and experiment are in agreement. It can also be seen that the emission intensities of ionic lines strengthens outward along the axial of the thruster. This reflects the variation of ion density along the axial direction of Hall thruster, and can be used to give a rough judgement of the location of ionization region in Hall thruster. Besides, atomic lines also have different pattern of variation. The lines with 916 nm and 904 nm strengthens as the ionic lines do, while those with 882 nm and 823 nm abates. Changes of these lines reflects the variation of plasma parameters, could be used in optical emission spectroscopy.

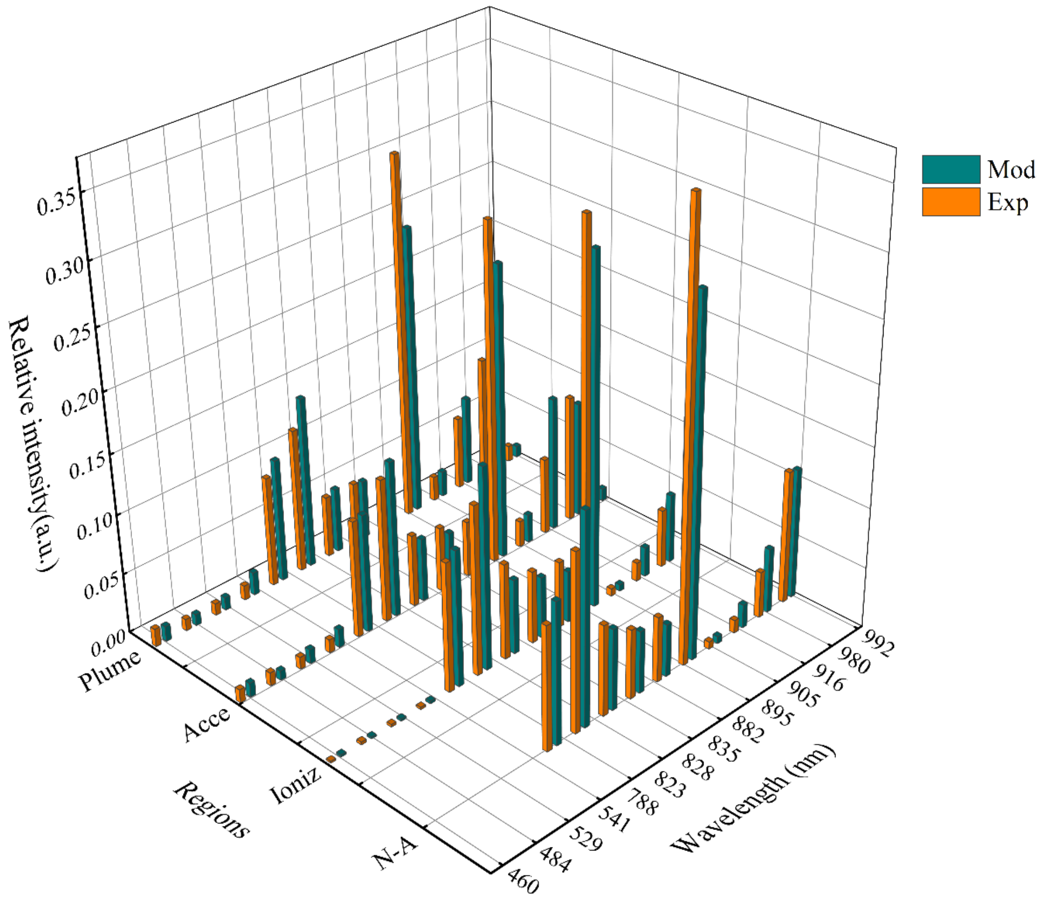

Figure 1 Comparison of observed and modeled line intensities in the near-anode region (N-A), ionization region (Ioniz), acceleration region (Acce), and plume region (Plume) of a Hall thruster. The results marked "Mod" are modelled results and those marked "Exp" are from experimental measurement.

Using the model, the kinetics of atomic and ionic 6p levels in different regions of Hall thruster are studied. It is found that for atomic 6p levels, radiation and ionization processes are the dominant de-populating processes; while for the ionic 6p levels, ionization process plays a limited role in de-population of these levels. The kinetics of populating process is more diverse. Figure 2 and gives the rate proportion for dominant populating processes of several atomic and ionic 6p levels, respectively. These levels are the upper levels of spectral lines shown in figure 1.

For atomic levels shown in figure 2, the production processes are divided into three groups: group (a) includes excitation from the ground-state by electron impact and radiative decay from the high-lying levels, group (b) includes the electron-impact excitation or de-excitation processes from the metastable and excited levels, and group (c) indicates self-absorption process. The processes in group (a) are mainly sensitive to the density of high energy electrons, due to the high threshold of electron-impact processes. Processes in group (b) are sensitive to low energy electrons, since threshold of these processes are relatively lower. And group (c) is highly related to metastable density.

As is shown in figure 2, process in group (b) or group (c) barely plays a role in populating the upper level of line 828 nm. In fact, the electron-impact cross section for excitation process that from atomic ground state to the upper level of 828 nm line is bigger than to other levels, e.g. the upper level of 823 nm or 881 nm, note that the emission intensity of 881 nm line is about 4 times stronger than 828 nm. The reason that the 882 nm line is the strongest atomic line without the biggest excitation cross section from ground state is due to the contribution of processes in group (b) and group (c). As is shown in figure 2, the contribution from group (b) is the most important production channel, which contribute at least 1/3 of production rate. While the contribution of self-absorption process cannot be ignored in the thruster channel.

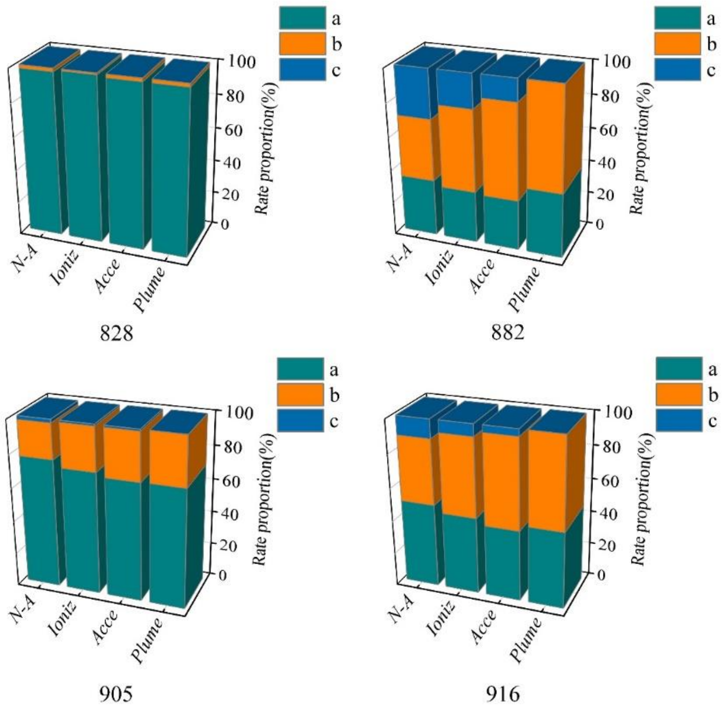

Figure 2 Ratios of production rates of atomic 6p levels from three groups of processes: (a) ground-state excitation by electron impact and radiative decay from high-lying levels, (b) excitation or de-excitation by electrons from metastable or excited levels, and (c) self-absorption process. The ratios of (c) are omitted when very small.

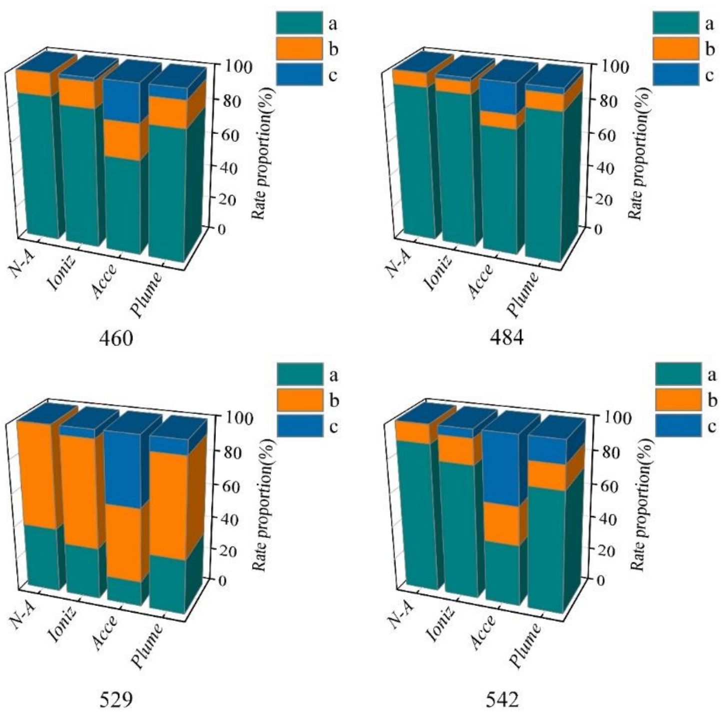

Figure 3 Ratios of production rates of ionic 6p levels from three groups of processes: (a) ground-state excitation by electrons and radiative decay from high-lying levels, (b) excitation or de-excitation by electrons from metastable or excited levels, and (c) electron-impact ionization-excitation process. The ratios of (c) are omitted when very small.

It is also found that the contribution of self-absorption process abates as the atom density decrease along the thruster channel.

For ionic levels shown in figure 3, the production processes are also divided into three groups: group (a) includes excitation from the ground-state by electron impact and radiative decay from the high-lying levels, group (b) includes the electron-impact excitation or de-excitation processes from the metastable and excited levels, while group (c) is electron-impact ionization-excitation process. The first two groups have similar characteristic, while group (c) depends on the very high energy tail of EEDF.

It is found that the contribution of processes in group (c) is highly related to location. For all the ionic levels, the greatest contribution of processes in group (c) is made in the acceleration region. It is because the electron temperature has a maximum around this region, which means electrons with enough energy to trigger ionization-excitation process have the largest amount in this region. Although electron temperature in the plume region is not very high, the electron energy distribution function is maxwellian distribution, which provides bigger probability in high energy region. In addition, production mechanism of the upper level for 529 nm line is quite different from the other three lines. The contribution from group (b) is the most important production channel for this level, while for the upper level of 460 nm, 484 nm and 542 nm, contribution of group (a) are the most important.

Information about kinetic mechanisms of atomic and ionic levels is useful when one studies how to select emission lines for diagnostic purpose. Rate proportion of ion-impact processes can be directly obtained by subtracting the values of groups (a)-(c) in these figures from 100.

IV.Conclusion

In this work, we propose a collisional-radiative model includes both atomic and ionic energy levels of xenon. The model considers kinetic important processes in electric propulsion plasma, and is verified by comparing the modelled spectra and the spectra measured in different regions of a Hall thruster. The modelled and measured results are in general agreement. Based on this model, kinetics of atomic and ionic 6p levels are discussed.

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