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Construction of hydrogen molecule collisional-radiative model
水素分子衝突輻射モデルの構築

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A collisional-radiative model of molecular hydrogen, which includes electronic, vibrational and rotational states is constructed. Spontaneous transition probabilities for bound and continuum transitions are newly calculated. Cross sections are estimated from Franck-Condon and Hönl-London factors. Population density and emission spectra of the molecule are calculated.

1. Introduction

We have been developing collisional-radiative models and a neutral-transport code for hydrogen and helium species, which are used to investigate fusion plasmas.

As a revision of the molecular hydrogen collisional-radiative model, which includes electronic and vibrational states [1, 2], we are developing a model that includes rotational states in addition. This model will provide more precise effective reaction rate coefficients of the molecule. Emission line intensities of hydrogen molecules in plasmas are calculated as a function of n_{H2}, n_e, T_e, and T_v, T_{rot} in the ground electronic state. From observed spectra, these parameters can be determined.

2. Model

In the revised model which includes rotational states, assuming Hund’s (b) case, the levels are labeled by the principal quantum number of the united atom n, and Λ, N, and J. The number of 2131 levels for $n \leqq 4$, listed in Ref. [3], are included in the model.

Spontaneous transition probabilities $e^3\Sigma_u^+ \rightarrow a^3\Sigma_g^+$, $d^3\Pi_u \rightarrow a^3\Sigma_g^+$, $i^3\Pi_g \rightarrow c^3\Pi_u$, $j^3\Delta_g \rightarrow c^3\Pi_u$, $I^1\Pi_g \rightarrow C^1\Pi_u$, and $J^1\Delta_g \rightarrow C^1\Pi_u$ in Ref. [4] are included in the model. The values for other transitions are calculated according to Ref. [5]. Transition probabilities to continuum states, from $a^3\Sigma_g^+$, $h^3\Sigma_g^+$, $g^3\Sigma_g^+$, $i^3\Pi_g$, $r^3\Pi_g$ to $b^3\Sigma_u^+$, and from $B^1\Sigma_u^+$, $B'^1\Sigma_u^+$, $B''^1\Sigma_u^+$, $C^1\Pi_u$, $D^1\Pi_u$ to continuum of $X^1\Sigma_g^+$, are also calculated [8, 9].

The vibrationally resolved excitation cross section from the electronic ground state to $B^1\Sigma_u^+$, $B'\,^1\Sigma_u^+$, $B''\,^1\Sigma_u^+$, $C^1\Pi_u$, $D^1\Pi_u$, $D'\,^1\Pi_u$ in Ref. [6] are included in the model; for the excitation to other states, data in Ref. [7, 8] are included. There is not enough information to derive vibrationally and rotationally resolved cross sections. For an optically allowed transition, we assume that the rate coefficients are proportional to Franck-Condon and Hönl-London factors. For an optically forbidden transition, we use the Franck-Condon factor to obtain vibrationally resolved data and divide them evenly for rotational states. Excitation cross sections between excited states are estimated from united helium atom cross sections. Reaction rate coefficients which are essential to determine the vibrational and rotational population of the ground electronic state are included in the model.

3. Results and Discussion

We have calculated population of excited states and emission intensity. Figure 1 shows population distribution calculated with n_{H2}=1.0 cm^{-3}, n_e=2×10^{10} cm^{-3}, T_e=3.0 eV, and T_v=4200 K, T_{rot}=350 K. Electronic states of the levels are listed in Table I. Large values in Fig.1 are for metastable triplet c state. Figure 2(a) shows emission line intensity. Large emission intensity is seen in vacuum ultraviolet region. Figure 2(b) is enlarged one of Fig.2(a). Fülcher band around 600 nm is dominant in visible range. Continuum emission is seen in the wavelength from vacuum ultraviolet to around 400 nm.

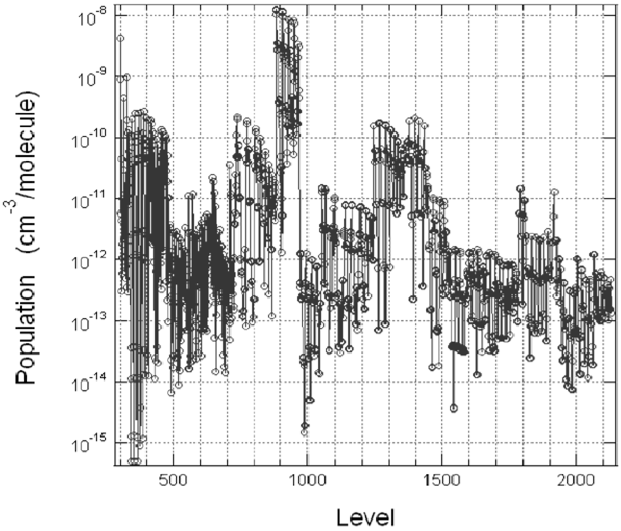

Fig.1. Calculated population with n_{H2}=1 cm^{-3}, n_e=2×10^{10} cm^{-3}, T_e=3.0 eV, and T_v=4200 K, T_{rot}=350 K. See Table I for levels.

Table I. Electronic states of levels in the model

X	1~301	S-	728~730
E	302~333	S+	731~733
B	334~423	a	734~881
C-	424~454	c-	882~965
C+	455~470	c+	969~1049
H	471~484	h	1050~1093
B’	485~512	e	1094~1243
D-	513~530	d-	1244~1372
D+	531~542	d+	1373~1438
G	543~577	g	1439~1523
I-	578~597	i-	1524~1598
I+	598~617	i+	1599~1661
J-	618~632	j-	1662~1724
J+	633~641	j+	1725~1784
O	642~661	f	1785~1810
B’’	662~676	k-	1811~1912
D’-	677~692	k+	1913~1930
D’+	693~708	r-	1931~1999
P	709~716	r+	2000~2062
R-	717~725	s-	2063~2098
R+	726~727	s+	2099~2131

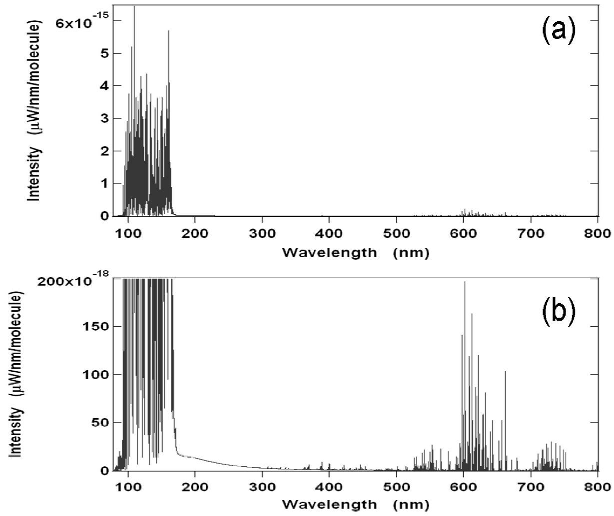

Fig.2. (a) Calculated emission lines. (b) Extended one of (a).

4. Conclusion

A molecular hydrogen collisional-radiative model which includes electronic, vibrational and rotational states has been constructed. We will apply this model to RF hydrogen plasmas at Shinshu University in order to test whether the model reproduces observed emission intensity. In the present model, Bolzmann distribution for vibrational and rotational population of the electronic ground state is assumed. If necessary, it will be improved.

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