§29. Construction of a Molecular Hydrogen Collisional-radiative Model for Ionizing and Recombining Plasmas

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We are developing a collisional-radiative model of H_2 in which the electronic, vibrational, and rotational states are resolved. In this study, we constructed D_2 code for future LHD experiments. In this model, assuming Hund's (b) case, the levels are labeled by n, v and Λ, N, J. 7817 levels for $n \leq 6$ are included. Level energies are taken from Ref.[1]. Transition probabilities from $B^1\Sigma_u^+$, $B'^1\Sigma_u^+$, $C^1\Pi_u$, $D^1\Pi_u$, to $X^1\Sigma_g^+$ are taken from Ref.[2]. Other transition probabilities are newly calculated according to Ref.[3]. Electron excitation cross section from $X^1\Sigma_g^+$ to $B^1\Sigma_u^+$, $B'^1\Sigma_u^+$, $B''^1\Sigma_u^+$, $C^1\Pi_u$, $D^1\Pi_u$, $D'^1\Pi_u$ are taken from Ref.[4]. For other excitations from $X^1\Sigma_g^+$, data in Ref.[5] are mainly used. Electron impact excitation cross sections between the electronic states are estimated from those for united atom helium.

In order to test the newly developed model, we applied it to D_2 RF plasmas (13.56 MHz) at Shinshu University. Emission spectra in 380 nm - 800 nm were measured with an echelle spectrometer. The electron temperature T_e and the density n_e were determined from mixed helium atom emission intensities [6], and the vibrational temperature T_{vib} and the rotational temperature T_{rot} in the electronic ground state were determined from the $d^3\Pi_u$ - $a^3\Sigma_g^+$ emission line intensities. Using these values, D_2 emission line spectra are calculated.

Calculated spectra of the continuum $a^3\Sigma_g^+$ - $b^3\Sigma_u^+$ and $d^3\Pi_u$ - $a^3\Sigma_g^+$ band well reproduce the experimental ones. For other bands, in order to improve absolute intensity, we corrected the electron impact excitation rate coefficients from the electronic ground state in Ref.[5]. Figure 1 shows the experimentally corrected rate coefficients for $X^1\Sigma_g^+$ - $E^1\Sigma_g^+$ as an example. These data are fitted using a formula in Ref.[5]. As shown in Fig.2, spectra of the $E^1\Sigma_g^+$ - $B^1\Sigma_u$ and $e^3\Sigma_u^+$ - $a^3\Sigma_g^+$ bands are especially well reproduced. This suggests that the model with the corrected rate coefficients can be used for the spectroscopic diagnostic of the above input parameters by analyzing the spectra of these transitions.

As for H_2 code, we have calculated the time dependent vibrational and rotational population in the electronic ground state of the molecules which are released from a wall. In this model, various processes which determine the vibrational and rotational population of the electronic ground state $X^1\Sigma_g^+$, e.g., the electron impact dissociative attachment, the electron impact and the molecule impact excitations in $X^1\Sigma_g^+$, are considered. Effective reaction rate coefficients for various molecular processes in plasmas are also calculated considering the time dependent population.

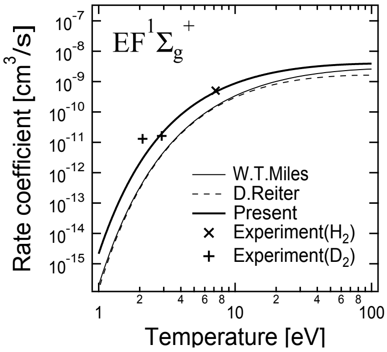

Fig. 1: $X^1\Sigma_g^+ \rightarrow E^1\Sigma_g^+$ electron impact excitation rate coefficients determined from the experimental emission intensity.

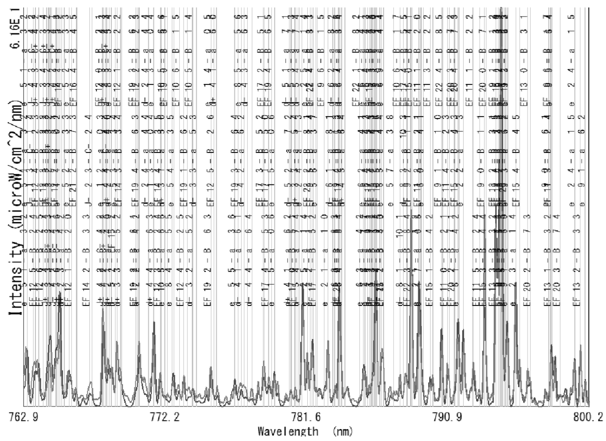

Fig. 2: Spectrum of D_2 (762.9 nm -800.2 nm). Experiment (gray) and calculation (black).

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