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Characteristics of vibrational temperature of hydrogen molecules in detached plasma

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ABSTRACT

The ground-state vibrational temperature of hydrogen molecules, T_{vib}, is observed in detached plasma using a VUV spectrometer on a linear plasma device, TPD-SheetIV. T_{vib} was deduced by applying the corona equilibrium model by using the electron impact excitation rate and the spontaneous emission coefficient, taking into account the cascade contribution of $E,F^1\Sigma_g^+$ and the radiation trapping. T_{vib} can be found which results in a fit to the observed relative intensities of VUV spectrum in the range from 90 to 150 nm. With increasing gas pressure P, T_{vib} gradually decreases from 5000 to 3000 K and remains nearly constant at around 1000 K in detached plasma at discharge current of 50 A.

1. Introduction

The vibrationally excited hydrogen molecules, $H_2(v)$, in their electronic ground state play a significant role in fusion plasma because of the increase in ionization and dissociation rate coefficients. In the divertor region of tokamak experiments, $H_2(v)$ lead to enhance the reduction of ion particle flux as the plasma volume recombination associated with $H_2(v)$, that is, molecular activated recombination (MAR) [1–3] Also, the most volume formation of negative ions (H^-) is the dissociative electron attachment to $H_2(v'')$. In order to understand these processes, measurements of the ground-state vibrational temperature of hydrogen molecules, T_{vib}, have been given by many authors. In particular, the Fulcher-band spectroscopy was used for T_{vib} determination not only in technical but also in tokamak plasma [4–6].

Using the Fulcher-band spectroscopy for $H_2(v)$, the relative ground state population can be determined sensitively for vibrational levels up to $v = 4$ for hydrogen [4]. Since transitions between higher vibrational levels were not observed because of predissociation, T_{vib} cannot be predicted from the Fulcher-band spectroscopy accurately. The main contributor to the negative and molecular ions production on the basis of T_{vib} is the population in $v > 4$.

On the other hands, vacuum ultraviolet (VUV) emission spectroscopy in the spectral range 80–180 nm are investigated for basic research in laboratory experiments [7–9] VUV emission intense line spectrum is observed at the Lyman ($B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$) and Werner ($C^1\Pi_u \rightarrow X^1\Sigma_g^+$) bands of H_2 or D_2. Also, several active laser methods in VUV lights have been applied successfully for the detection of vibrationally excited H_2 with excellent sensitivity [8,10]. Thus, the VUV spectroscopic method is an effective approach to measure the vibrational temperatures of H_2 to the electronic ground state, T_{vib}, in the low temperature and high density plasma when the molecular and negative ions are produced in the detached plasma.

However, these diagnostics are rather complicated, especially with regard to a diagnostics to the divertor region. Also, a complete description of VUV spectrum has proved elusive because of radiation trapping, that is, opacity effects [11]. Various VUV spectroscopic studies have shown clear signal of opacity effects for dense divertor plasma conditions in various tokamaks [12,13] In case of the high neutral density such as detached divertor plasma, it is necessary to take into account of radiation trapping to theoretical and experimental investigation of VUV spectroscopy.

In this paper, we obtain the ground-state vibrational temperature of hydrogen molecule T_{vib} using a VUV spectrometer on a linear plasma device, TPD-SheetIV. T_{vib} was deduced by applying the corona equilibrium model by using the electron impact excitation rate and the spontaneous emission coefficient between the upper electronic states $B^1\Sigma_u^+$, $C^1\Pi_u$, and $D^1\Pi_u$ with vibrational level and the ground state $X^1\Sigma_g^+$, taking into account the cascade contribution of $E,F^1\Sigma_g^+$ and the radiation trapping. T_{vib} can be found which results in a fit to the observed relative intensities of VUV spectrum in the range from 90 to 150 nm. The role of the vibrationally excited hydrogen molecules, $H_2(v)$, in detached plasma is discussed.

2. Experimental apparatus and method

The experiment was performed in the linear plasma device TPD-SheetIV. [9,14,15] Ten rectangular magnetic coils formed a

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uniform magnetic field up to 0.1 T in the experimental region. The hydrogen plasma was generated at a hydrogen gas flow of 75 sccm, with a discharge current of 30–100 A. The neutral gas pressure P in the experimental region was controlled between 0.01 and 2.0 Pa with a secondary gas feed. The sheet plasma flowed from the plasma source along the magnetic field to a floating endplate located about 1.0 m downstream.

Electron density and electron temperature were measured using a planar Langmuir probe in front of the endplate. The rate coefficients are calculated using cross sections over a Maxwellian energy distribution function of the electrons. Through a viewing port installed in the sidewall of the experimental region, the emission intensity from the plasma is observed using the VUV spectrometer (20 cm Seya-Namioka VUV Spectrometer, nominal resolution of 0.1 nm) with a differential pumping system by a 150 l/s turbo-pump and a charge-coupled device (CCD) camera. The VUV spectra from electronically excited hydrogen molecules were detected 3 cm from the target plate.

3. Modeling the VUV spectroscopy

The vibrational excited hydrogen molecules $H_2(v'')$ result from the electron impact excitation rate and the spontaneous emission coefficient between the upper electronic states ($B^1\Sigma_u^+(v')$, $C^1\Pi_u(v')$, and $D^1\Pi_u(v')$) with vibrational level and the ground state $X^1\Sigma_g^+(v'')$ [16,17]. Assuming a thermal (Boltzmann) population of ground state vibrational levels and given the Frank–Condon matrix for electron-impact excitation from the ground state to the upper state [18], the electron impact excitation rate $c_{Xv}^{Bv',Cv',Dv'} = \langle \sigma_{Xv}^{Bv',Cv',Dv'} v_e \rangle$ of $X^1\Sigma_g^+(v) \to B^1\Sigma_u^+(v'), C^1\Pi_u(v')$, and $D^1\Pi_u(v')$ states given by

$$c_{Xv}^{Bv',Cv',Dv'} = \langle \sigma_{Xv}^{Bv',Cv',Dv'} v_e \rangle = \frac{q_{Xv}^{Bv',Cv',Dv'} \exp\left(\frac{\Delta G_{B,C,D}(v)}{T_e}\right)}{\sum_{v'} q_{Xv}^{Bv',Cv',Dv'} \exp\left(\frac{\Delta G_{B,C,D}(v)}{T_e}\right)} \langle total\ \sigma_{Xv}^{Bv',Cv'',Dv'} v_e \rangle, \quad (1)$$

where the $q_{Xv}^{Bv',Cvn,Dv'}$ is Frank–Condon factors, $\Delta G_{B,C,D}(v)$ is the energy difference between the vibrational state of interest and $v = 0$, v_e is the thermal velocity of electron in plasma, $total\sigma_{Xv}^{Bv',Cv',Dv'}$ stands for the total cross-section for electronic transition from the initial and final state of the electron impact excitation of $X^1\Sigma_g^+(v) \to B^1\Sigma_u^+(v'), C^1\Pi_u(v')$, and $D^1\Pi_u(v')$ states.

The corona equilibrium model used to calculate the population distribution of the vibrational levels resulting from a Boltzmann population distribution in the ground state. The calculated relative intensities of VUV spectrum $I_{Xv''}^{Bv',Cv',Dv'}$ for the transitions from $B^1\Sigma_u^+(v') \to X^1\Sigma_g^+(v'')$ (the Lyman-band), $C^1\Pi_u(v') \to X^1\Sigma_g^+(v'')$ (the Werner-band), and $D^1\Pi_u(v') \to X^1\Sigma_g^+(v'')$ are given by

$$I_{Xv''}^{Bv',Cv',Dv'} = \frac{A_{Xv''}^{Bv',Cv',Dv'}}{\sum_{v'} A_{Xv''}^{Bv',Cv',Dv'}} \frac{hc}{\lambda_{Xv''}^{Bv',Cv',Dv'}} n_e \times \sum_v \left\{ C_{Xv}^{Bv',Cv',Dv'} n_{Xv} \exp\left[-\frac{G_X(v)}{kT_{\text{vib}}^X} \right] \right\}, \quad (2)$$

where $A_{Xv''}^{Bv',Cv',Dv'}$ is spontaneous emission coefficient [18] $\lambda_{Xv}^{Bv',Cv',Dv'}$ is the wavelength of the measured line, $G_X(v)$ is the vibrational energy in the $X^1\Sigma_g^+$ state, n_{Xv} is the neutral density, $c_{Xv}^{Bv',Cv'Dv'}$ is the electron impact excitation rate from the $X^1\Sigma_g^+(v)$ state to the $B^1\Sigma_u^+(v')$, $C^1\Pi_u(v')$, and $D^1\Pi_u(v')$ states, respectively [17]. Fig. 1 shows calculated individual spectrum of H_2 from the $B^1\Sigma_u^+$ (the Lyman-band), $C^1\Pi_u$ (the Werner-band), and $D^1\Pi_u$ states at the electron density $n_e = 10^{18}$ m^{-3} and $T_e = 10$ eV. These calculated spectra are the resolution of 0.1 nm and neglect a rotational structure of molecules. The

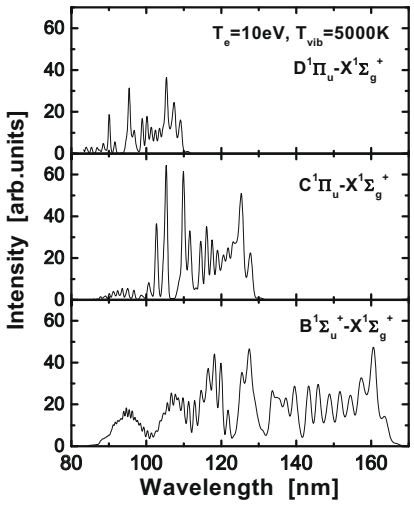

Fig. 1. Calculated individual spectrum of H_2 from $B^1\Sigma_u^+$ (the Lyman-band), $C^1\Pi_u$ (the Werner-band), and $D^1\Pi_u$ states at electron density $n_e = 10^{18}$ m^{-3} and $T_e = 10$ eV.

spectral region shifts to the short-wavelength with increasing the excitation level from $B^1\Sigma_u^+$ to $D^1\Pi_u$ states. Also, $D^1\Pi_u$-state span the wavelength range 50–110 nm and overlap with the Lyman and Werner-bands.

It is necessary to consider cascade contributions to $B^1\Sigma_u^+$, that is, $E,F^1\Sigma_g^+ \to B^1\Sigma_u^+$. The electron impact excitation rate of $X^1\Sigma_g^+(v) \to E,F^1\Sigma_g^+(v')$ state given by the same calculated technique for $c_{Xv}^{Bv',Cv',Dv'}$. Fig. 2 shows the calculated Lyman spectra with the cascade contributions with changing the electron temperature T_e from 3 to 40 eV. These spectra are normalized by that of the electron density $n_e = 10^{18}$ m^{-3} and $T_{\text{vib}} = 5000$ K. The line intensity of the cascade region (130–160 nm) increases with increasing T_e. This cascade spectrum overlaps with the Lyman-band. It is estimated from this calculation that the effect of the cascade contribution on $E,F^1\Sigma_g^+ \to B^1\Sigma_u^+$ transition produce about 30% of intensity of the cascading band system at $T_e = 40$ eV.

In high neutral density such as detached divertor plasma, it is necessary to take into account of radiation trapping to experimental investigation of the VUV spectroscopy [9,18]. In case of the consideration of radiation trapping, the brightness of line will be in the ratio of their spontaneous emission coefficients. The emitted radiation intensity decays with the common rate g_0A (escape factor $g_0 < 1$). In the case of a Gaussian profile for an infinite cylinder with radius R, an approximate expression for g_0 is given as

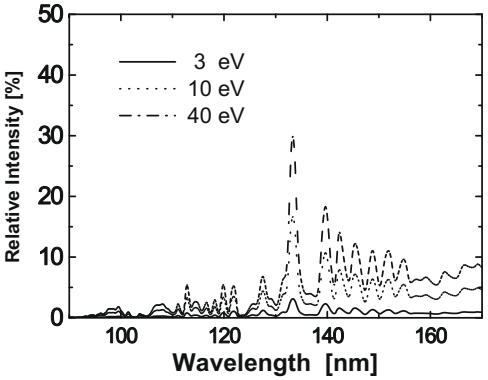

Fig. 2. Calculated Lyman spectra with cascade contributions with changing electron temperature T_e from 3 to 40 eV. These spectra are normalized by that of electron density $n_e = 10^{18}$ m^{-3} and $T_{\text{vib}} = 5000$ K.

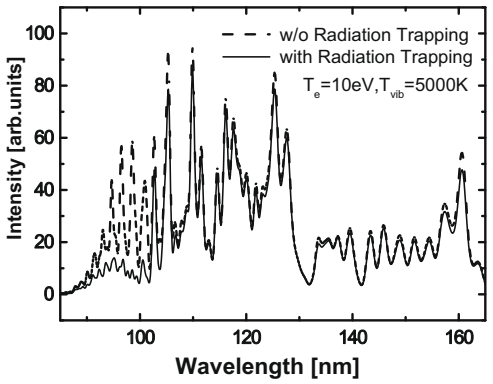

Fig. 3. Example of the calculated VUV spectra of hydrogen molecules with effect of radiation trapping at T_n = 500 K and P = 0.1 Pa.

$$g_0 \cong \frac{1.92 - 1.3/[1 + (\kappa_0 R)^{6/5}]}{(\kappa_0 R + 0.62)[\pi \log_e(1.357 + \kappa_0 R)]^{1/2}}, \quad (3)$$

where κ_0 is absorption coefficient at the line center [19]. The characteristics of g_0 is as function of the optical depth $\kappa_0 R$. Fig. 3 shows an example of the calculated VUV spectra of the hydrogen molecules with the effect of radiation trapping at T_n = 500 K and P = 0.1 Pa. The solid line represents the calculated intensity with radiation trapping and the dotted line gives that without radiation trapping, respectively. The intensity of the wavelength range 80–110 nm decays about 80% for radiation trapping effects. The intensity of calculated spectra resemble the experimental spectra very well taken into account the radiation trapping effects in the range of 80–110 nm.

4. Experimental results

In the VUV wavelength for the spectral range 80–180 nm, there are two strongest band system for H_2 (the Lyman-band $B^1\Sigma_u^+ \rightarrow X^1\Sigma_g^+$, and the Werner-band $C^1\Pi_u \rightarrow X^1\Sigma_g^+$) and emission lines (Lyman α, β, γ) for atomic hydrogen. An example of the measured VUV spectrum compared with a calculated spectrum except the Lyman α, β, γ for atomic hydrogen is shown in Fig. 4 at T_e = 13.9 eV, $n_e = 9.3 \times 10^{17}$ m^{-3} and P = 0.07 Pa. The solid line represents the experimental result, the dotted line and the dashed-dotted line give the calculated results with radiation trapping (T_{vib} = 6000 K) and without one (T_{vib} = 4500 K), respectively. T_{vib}

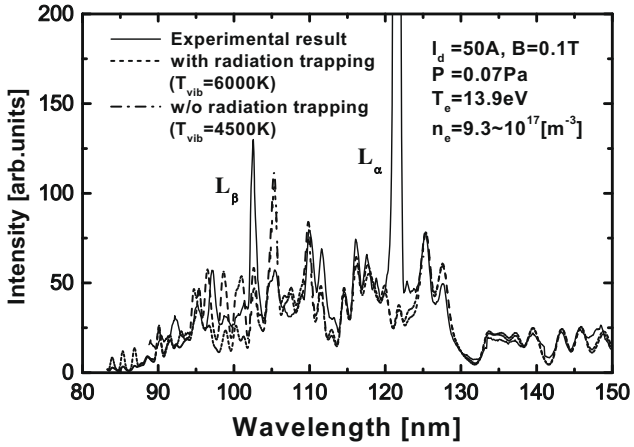

Fig. 4. VUV spectra of the intensity compared to the predicted result (except the Lyman α, β, γ for atomic hydrogen) by calculation of model with that of the experimental result at T_e = 13.9 eV, $n_e = 9.3 \times 10^{17}$ m^{-3} and P = 0.07 Pa.

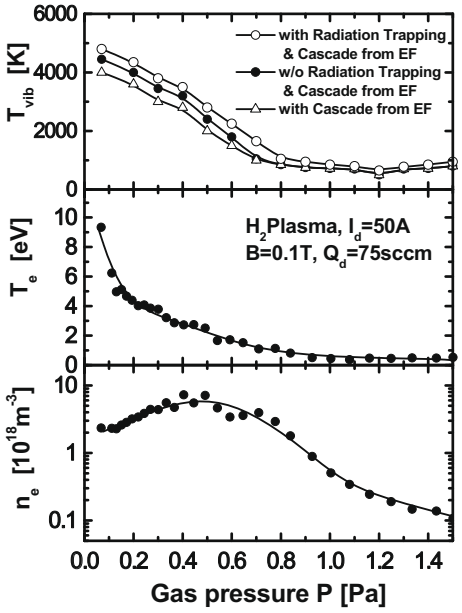

Fig. 5. Calculated vibrational temperature of hydrogen molecule T_{vib}, electron temperature, T_e, electron density, n_e, are plotted against gas pressure P at discharge current I_d of 50 A in hydrogen plasma.

can be estimated which results in a fit to the observed relative intensities of VUV spectrum in the range from 90 to 150 nm. These calculated spectra resemble the measured spectra very well. However, the predicted T_{vib} without radiation trapping is about 0.75 times as small as that of T_{vib} with radiation trapping. It is necessary to take into account of the radiation trapping in experimental investigation of the VUV spectroscopy.

Fig. 5 shows the calculated vibrational temperature of hydrogen molecule T_{vib}, electron temperature, T_e, electron density, n_e, are plotted against gas pressure P at the discharge current I_d of 50 A in the hydrogen plasma. T_{vib} can be found which results in a fit to the observed relative intensities of VUV spectrum in the range from 80 nm to 150 nm comparisons with the calculated spectra taking into account cascade contribution of $E, F^1\Sigma_g^+$ and radiation trapping. Using a small amount of secondary hydrogen gas puffing into a hydrogen plasma, n_e has a maximum value of 8.0×10^{18} m^{-3} at $P \sim 0.5$ Pa and T_e decreases rapidly from 9.5 to 2 eV at $P \sim 0.5$ Pa. Above $P \sim 0.5$ Pa, T_e gradually decreases below 1 eV and n_e falls with increasing P. T_{vib} gradually decreases from 5000 to 3000 K with increasing P and remains nearly constant at around 1000 K above $P \sim 0.8$ Pa.

5. Conclusions

We obtain the ground-state vibrational temperature of hydrogen molecule T_{vib} can be found which results in a fit the calculated VUV spectrum to the observed relative intensities of VUV spectrum. T_{vib} was deduced by applying the corona equilibrium model by using the electron impact excitation rate and the spontaneous emission coefficient between the upper electronic states $B^1\Sigma_u^+$, $C^1\Pi_u$, and $D^1\Pi_u$ with vibrational level and the ground state $X^1\Sigma_g^+$. The experimental results and the theoretical values show good agreement, taking into account cascade contribution of $E, F^1\Sigma_g^+$ and radiation trapping. The line intensity of the cascade region (130–160 nm) increases with increasing T_e. The intensity of calculated spectra resemble the experimental spectra very well taken into account radiation trapping effects in the range of 80–105 nm which overlap with the Werner-band system and $D^1\Pi_u$ state. With increasing gas pressure P, T_{vib} gradually decreases from

5000 to 3000 K and remains nearly constant at around 1000 K in detached plasma.

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