VUV spectroscopic diagnostics of the vibrational temperature to the ground state of hydrogen/deuterium molecules

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The vacuum ultraviolet (VUV) spectroscopic method has been evaluated for measuring of the vibrational temperatures T_{vib} of H_2 and D_2 to the electronic ground state in a plasma on a linear plasma device, TPD-SheetIV. This is inferred from the comparison of simulated Lyman, Werner spectra for H_2 and D_2 taking into account radiation trapping effects with measured VUV spectra in the range from 90 to 150 nm. T_{vib} of H_2 and D_2 is around 4000-5000K in the plasma.

1. Introduction

The vibrationally excited molecules of hydrogen and deuterium molecules (H_2 or D_2) to the electronic ground state play a significant role for the ionization and dissociation processes in space plasma, plasma processing, and the boundary layer of fusion plasma. In order to understand these processes, measurements of vibrational temperatures of H_2 or D_2 to the electronic ground state, T_{vib}, have been given by many authors using the spectroscopic diagnostic method.

The Fulcuer-band spectroscopy for H_2 or D_2 has been employed for the indirect determination of the gas temperature of technical plasma by visible spectroscopy [4]. Using the Fulcher-band spectroscopy for molecules, the relative ground state population can be determined sensitively for vibrational levels up to v = 4, while the main contributor to the negative and molecular ions production is the population in v > 4. If a tail, bi-Maxwellian region exists in the vibrational distribution in the ground electronic state, the production cannot be predicted from the Fulcher-band spectroscopy on the basis of T_{vib}. Therefore, it has to be supplemented by a CR model for the levels 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 [5,6]. 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 or D_2 with excellent sensitively [6,7]. Thus, the VUV spectroscopic method is an effective approach to measure the vibrational temperatures of H_2 or D_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 plasma.

However, these diagnostics are rather complicated, especially with regard to a diagnostics. Also, a complete description of VUV spectrum has proved elusive because of the radiation trapping [8]. Various VUV spectroscopic studies have shown clear signal of opacity (line absorption) effects, that is, radiation trapping for dense plasma conditions [9,10]. In case of the high neutral and density plasma, it is necessary to take account of the radiation trapping to theoretical and experimental investigation of VUV spectroscopy.

In this paper, VUV spectroscopic method for determination of the ground-state vibrational temperature of H_2 or D_2, T_{vib}, is presented which make use of naturally emitted radiation in plasma on a linear plasma device, TPD-SheetIV [11]. T_{vib} was deduced by applying the corona equilibrium by using the electron impact excitation rate and the spontaneous emission coefficient between the upper electronic states $B^1\Sigma_u^+$, $C^1\Pi_u$ with vibrational level and the ground state $X^1\Sigma_g^+$, taking into account the radiation trapping. The role of the vibrationally excited hydrogen or deuterium molecules, H_2 or D_2, in the plasma is discussed.

2. Experimental apparatus and Method

The experiment was performed in the linear plasma device TPD-SheetIV [11-13]. The hydrogen or deuterium sheet plasma was produced by a modified Test Plasma produced by Directed Current (TPD)-type dc discharge. The anode slit was 2 mm thick and 40 mm wide. Ten rectangular magnetic coils formed a uniform magnetic field of 0.7 kG in the experimental region. The sheet plasma was terminated by an electrically floating and water-cooled target plate (tungsten) axially positioned at z = 70 cm from the discharge anode

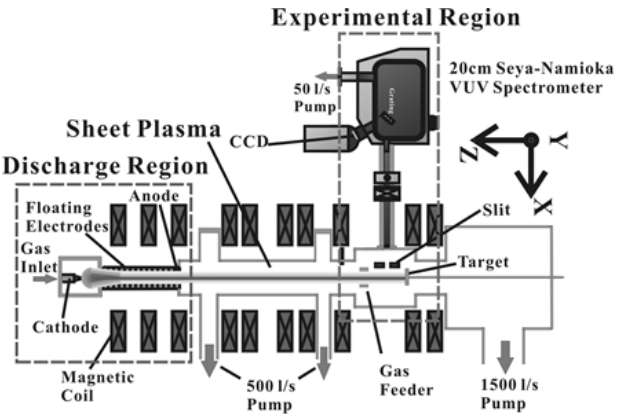

Fig.1 Schematic diagram of the linear plasma device, TPD-SheetIV, and measuring system

electrode. The hydrogen plasma was generated at a hydrogen gas flow of 70 sccm with a discharge current of 30-70 A.

The magnetized sheet plasma and measuring system is shown in Fig. 1. The secondary gas was locally fed by gas feeder. This gas feeder was placed in the experimental region located 60 cm in front of the anode and 2.0 cm below the sheet plasma. The secondary hydrogen or deuterium gas was fed perpendicularly into the sheet plasma in the low-pressure experimental region (< 0.1 Pa). The neutral pressure P in the experimental region was controlled by feeding the secondary hydrogen gas at pressures from 0.05 to 3 Pa. The change in P in the experimental region had no effect on the plasma production in the discharge region, because of the poor conductance. The pressure difference between the discharge and the experimental regions extends to 3 orders of magnitude.

The n_e and T_e of the sheet plasma were measured using Langmuir probes. A plane Langmuir probe was located 3 cm from the target plate. The vibrationally excited hydrogen molecules H_2*($X^1\Sigma_g^+$, $v''>5$) result from the de-excitation of electronically excited hydrogen molecules H_2($B^1\Sigma_u^+(v')$, $C^1\Pi_u(v')$, and $D^1\Pi_u(v')$) by electron impact[5]. Through a viewing port installed in the sidewall of the experimental region, the plasma is observed using the VUV spectrometer (20cm Seya-Namioka VUV Spectrometer, nominal resolution of 0.1nm) 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. Modelling the VUV spectroscopy

The vibrational excited deuterium/hydrogen molecules $D_2/H_2(v'')$ result from the electron impact excitation rate 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 $X^1\Sigma_g^+(v)$ [14,15]. Assuming a thermal (Boltzmann) population of ground state vibrationally excited levels and given the Franc-Condon matrix for electron-impact excitation from the ground state to the upper state [16], the electron impact excitation rate of $X^1\Sigma_g^+(v) \rightarrow B^1\Sigma_u^+(v')$, $C^1\Pi_u(v')$, and $D^1\Pi_u(v')$ states given by

$$c_{Xv}^{Bv',Cv',Dv'} = <\sigma_{Xv}^{Bv',Cv',Dv'}\upsilon_e> = \frac{q_{Xv}^{Bv',Cv',Dv'}\exp(\frac{\Delta G_{B,C,D}(v')}{Te})}{\sum_{v'} q_{xv}^{Bv',Cv',Dv'}\exp(\frac{\Delta G_{B,C,D}(v')}{Te})} < total\,\sigma_{Xv}^{Bv',Cv',Dv'}\upsilon_e > \quad (1),$$

where the $q_{Xv}^{Bv',Cv',Dv'}$ is Franck-Condon Factors, $\exp \Delta G_{B,C,D}(v')$ is exponential factor using the energy difference between the vibrational state of interest and $v = 0$, $\sigma_{Xv}^{Bv',Cv',Dv'}$ is the cross section of the electron impact excitation rate of $X^1\Sigma_g^+(v) \rightarrow B^1\Sigma_u^+(v')$, $C^1\Pi_u(v')$, and $D^1\Pi_u(v')$ states, respectively.

The rate coefficients $< total\,\sigma_{Xv}^{Bv',Cv',Dv'}\upsilon_e >$ are calculated using cross sections over a Maxwellian energy distribution faction of the electrons.

The corona model used to calculate the population distribution of the vibrational levels resulting from a Boltzmann population distribution in the ground state characterized by a temperature of hydrogen molecule. The calculated relative intensities of VUV spectrum of the transitions from $B^1\Sigma_u^+(v') \rightarrow X^1\Sigma_g^+(v'')$ (The Lyman Band), $C^1\Pi_u(v') \rightarrow X^1\Sigma_g^+(v'')$ (The Werner Band), and $D^1\Pi_u(v') \rightarrow X^1\Sigma_g^+(v'')$ are given by

$$I_{Xv''}^{Bv',Cv'} = \frac{A_{Xv''}^{Bv',Cv',Dv'}}{\sum_{v'} A_{Xv''}^{Bv',Cv',Dv'}} \frac{hc}{\lambda_{Xv''}^{Bv',Cv',Dv'}} n_e \sum_v [c_{Xv}^{Bv',Cv',Dv'} n_{Xv} \exp[-\frac{G_x(v)}{k_B T_{vib}}]] \quad (2),$$

where, $A_{Xv''}^{Bv',Cv',Dv'}$ is spontaneous emission coefficient, $\lambda_{Xv''}^{Bv',Cv',Dv'}$ is the wavelength of the measured line, $G_x(v)$ is the vibrational energy in the $X^1\Sigma_g^+$ state, $c_{Xv}^{Bv',Cv',Dv'}$ is The electron impact excitation rate of

$X^1\Sigma_g^+(v) \rightarrow B^1\Sigma_u^+(v')$, $C^1\Pi_u(v')$, and $D^1\Pi_u(v')$ states, respectively [15].

In high natural density such as the divertor plasma or processing plasma, it is necessary to take into account of the radiation trapping to theoretical and experimental investigation of the VUV spectroscopy [7,17]. In case of the consideration of the radiation trapping, the brightness of line will be in the ratio of their spontaneous emission coefficients.

The emitted radiation intensity decay with the common rate $g_0 A$ (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

$$g_0 \cong \frac{1.92 - 1.3/\left[1+(\kappa_0 R)^{6/5}\right]}{(\kappa_0 R + 0.62)\left[\pi \ln(1.37+\kappa_0 R)\right]^{1/2}} \quad (3),$$

where κ_0 is absorption coefficient at the line center [8]. The characteristics of the escape factor as function of the optical depth. Figure 2 shows an example of the calculated VUV spectra of of (a) H_2 (T_e = 4 eV) and (b) D_2 (T_e = 5,5 eV) molecules with effect of radiation trapping at T_{vib} = 3300K, T_n = 500 K and P = 0.3 Pa. The solid line represents the calculated with radiation trapping and the dotted line give that without radiation trapping, respectively. The intensity of the wave length 80-110 nm, which overlaps with the Werner band system and $C^1\Pi_u$ state, decay about 40-80% for the radiation trapping effect. The theoretical intensity of VUV spectra is decreases in the spectral range 80-105 nm, provided that radiation trapping effects are taken in account.

4. Experimental Results

In the VUV wavelength region, there are three band system for H_2 and D_2 ($B^1\Sigma_u^+$, $C^1\Pi_u$, and $D^1\Pi_u$) and emission lines (Lyman α, β, γ) for H and D atoms. An example of the measured VUV spectra of (a) H_2 (T_e = 4 eV, P = 0.3 Pa) and (b) D_2 (T_e = 10.6 eV, P = 0.06 Pa) molecules in the range from 90 nm to 150 nm compared with a calculated spectrum is shown in Fig. 3. The dotted line represents the experimental results, the solid line give the calculated results, respectively. While the calculated spectra resemble the measured spectra very well both in the line positions and in the line intensities, there are also lines that have not been identified yet. The calculated values and the experimental results show good agreement. These results show no major difference in the quality of the fits with respect to hydrogen or deuterium. The presented method for determination of the ground state vibrational temperature of H_2 and D_2, using VUV emission spectroscopy, is well suited for both molecular hydrogen and deuterium.

T_{vib} can be found which results in a fit to the measured relative intensities of VUV spectrum in the range from 80 nm to 150 nm comparisons with the calculated spectra at the discharge current I_d of 50 A in H_2 and D_2 plasma. The small amount of secondary H_2/D_2 gas puffing into a H_2/D_2 plasma, T_e rapidly decreases below 2 eV and n_e has a maximum value at P = 0.5~ 0.6 Pa. Above P ~ 0.5 Pa, n_e falls and Te gradually decreases with increasing P. T_{vib} of both H_2 and D_2 gradually decreases from 4000-5000 to 1000K with increasing the P. The effect of increasing P is a decrease in T_{vib} due to increasing dissociation which leads to a loss of vibrationally excited molecules. The loss of T_{vib} for D_2 is smaller than that for H_2 because of greater mass.

5. Conclusions

In this work a method has been presented for the determination of the ground state vibrational temperature of H_2 and D_2 molecule T_{vib} using VUV emission spectroscopy in plasma. T_{vib} was deduced by applying the corona equilibrium by using 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 $X^1\Sigma_g^+$. The experimental results and the theoretical values show good agreement. The intensity of the wavelength range 80-110nm decay about 40-80% for the radiation trapping effects. With increasing the gas pressure P, T_{vib} gradually decreases from 4000-5000K to 1000 K in the plasma.

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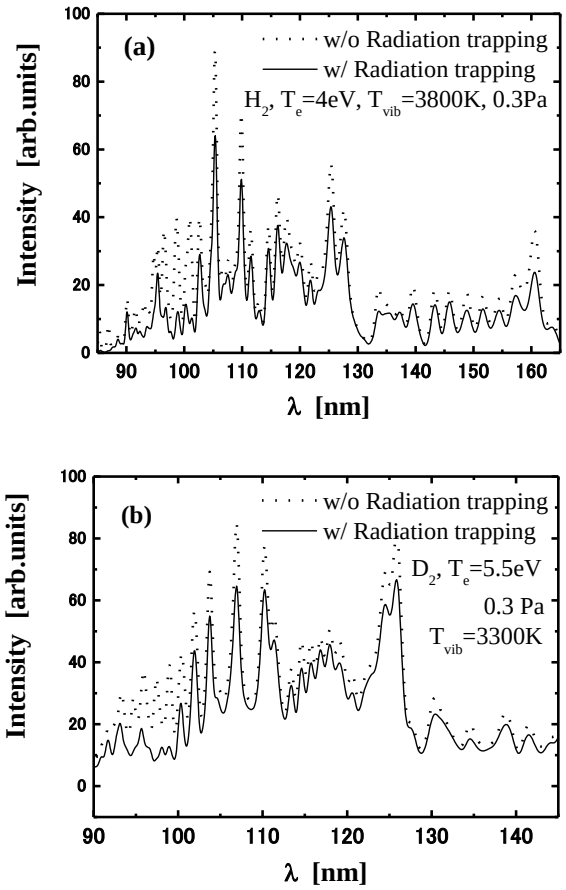

Fig.2 Example of the calculated VUV spectra of (a) H_2 (T_e = 4 eV) and (b) D_2 (T_e = 5,5 eV) molecules with effect of radiation trapping at T_{vib} = 3300K, T_n = 500 K and P = 0.3 Pa. The solid line represents the calculated with radiation trapping and the dotted line give that without radiation trapping, respectively.

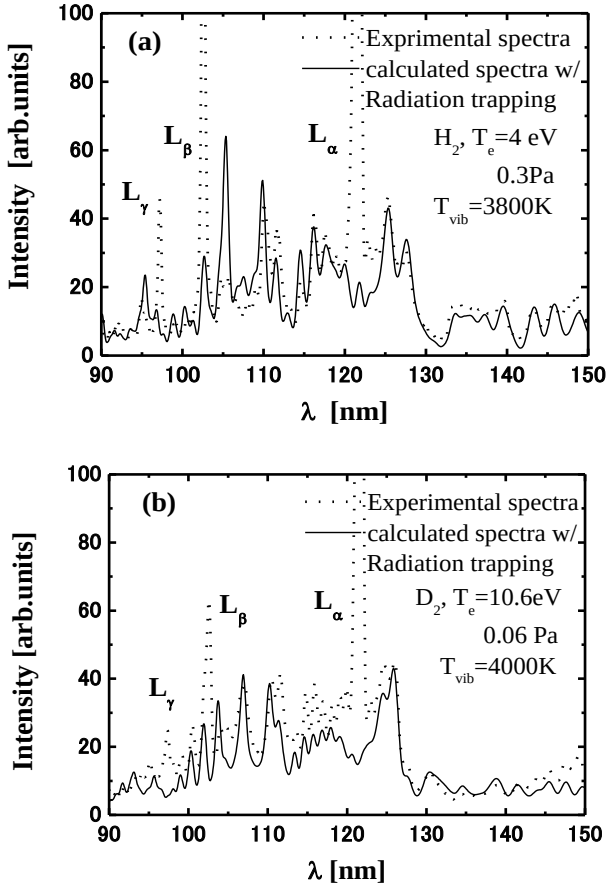

Fig.3 Example of the measured VUV spectra of (a) H_2 (T_e = 4 eV, P = 0.3 Pa) and (b) D_2 (T_e = 10.6 eV, P = 0.06 Pa) molecules in the range from 90 nm to 150 nm compared with a calculated spectrum. The dotted line represents the experimental results, the solid line give the calculated results with radiation trapping, respectively.