Application of the Zeeman patterns to local measurements of diatomic molecular spectra

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Introduction

Spatially resolved measurements of the translational, vibrational, and rotational temperatures of diatomic molecules are significant to understand molecular relevant plasma surface interactions. In the vicinity of the surface, desorbed molecules are excited through the surface recombination and electron-impact processes. These ro-vibrationally excited molecules contribute to several plasma reactions. H_2 molecules, for instance, play an essential role in determining the rate coefficients of molecular assisted recombination (MAR) or volume production of negative ions. In addition, the physical and chemical sputtering of plasma facing components generate molecules such as CH and C_2, BH, and BeH. The creation and annihilation balance of these radicals as well as their transport is of importance to estimate the amount of the redeposition and to reduce the contamination of the bulk plasma.

For local measurements by means of optical emission spectroscopy, a technique based on measurements of the Zeeman patterns appeared in the emission line shapes has been developed for atomic (D [1, 2], H [3–5], and He [5, 6]), ionic (O^{4+} [3]), and molecular (H_2 [7]) spectra. In this paper, we further extend this technique to general light diatomic molecules. A scheme for computation of the line shapes under magnetic and electric fields is summarized. The possibility of application is discussed for H_2 $d^3\Pi_u - a^3\Sigma_g^+$, CH $A^2\Delta - X^2\Pi$, C_2 $d^3\Pi_g - a^3\Pi_u$, BH $b^3\Sigma^- - a^3\Pi$, and BeH $A^2\Pi - X^2\Sigma^+$ band spectra which may be observable in fusion edge plasmas.

Methods

The effect of external magnetic and electric fields on diatomic molecules has been extensively studied in the field of astrophysics (*e.g.*, [8, 9]). The most straightforward approach to calculation of the angular momenta is to take Hund's case (a) [10] basis wavefunction for analytically expressing the Hamiltonian matrix elements. The details of the calculation are summarized in elsewhere (*e.g.,* [8, 9]). For light molecules, however, the coupling of the angular momenta becomes close to Hund's case (b), and the adoption of the case (b) basis may help us to understand

the physical meaning directly. We therefore dare to use the case (b) description. In the presence of external magnetic and electric fields, the total Hamiltonian H_{tot} can be written as

$$H_{\text{tot}} = H_{\text{ele}} + H_{\text{vib}} + H_{\text{rot}} + H_{\text{cd}} + H_{\text{so}} + H_{\text{sr}} + H_{\text{ld}} + H_{\text{B}} + H_{\text{E}}, \qquad (1)$$

where the terms in the right-hand side denote the ro-vibronic energies, centrifugal distortion, spin-orbit interaction, spin-rotation interaction, Λ-type doubling, Zeeman effect, and Stark effect. In the most cases expected for fusion applications, these terms are sufficient to be considered. In our calculation code, we can treat the Zeeman and Stark effects simultaneously, and obtain the emission spectra in any direction of observation. In this paper, however, both the effects are treated separately because the latter affects only the heteronuclear molecules.

Results and Discussions

Figure 1 illustrates the magnetic field effect on the H_2 $d^3\Pi_u - a^3\Sigma_g^+$, known as the Fulcher-α, band ($v' = v'' = 0$) $Q1$ and $Q2$ transitions. Figure 1 (a) shows the Zeeman split of the spectra as a function of the magnetic field strength, and (b) and (c) shows the spectra with magnetic field strengths of 0.0, 1.7, and 3.5 T, and the π and σ polarization components at 3.5 T, respectively. In the calculation, the molecular constants were taken from a database [11]. The $d^3\Pi_u$ state rotational population was assumed to be the Boltzmann distribution with a rotational temperature of 500 K, and the translational temperature was assumed to be the same as the rotational one which corresponds to the Doppler broadening of 0.0068 nm. In Figures 1 (b) and (c), an instrumental function

Figure 1: Magnetic field effect on the H_2 $d^3\Pi_u - a^3\Sigma_g^+$ band Q-branch spectra:(a) the Zeeman split of the spectra as a function of the magnetic field strength, (b) the spectra with magnetic field strengths of 0.0, 1.7, and 3.5 T, and (c) the π and σ polarization components in the case of 3.5 T.

of $\Delta\lambda_{\text{FWHM}} = 0.02$ nm was assumed. We calculated these spectra in the Voigt configuration. Compared to the other molecular spectra shown below, the rotational spectra have larger wavelength separation. Furthermore, the effects of the spin-orbit and spin-rotation interactions are negligible both for the upper and lower electronic states, which results in the relatively simple pattern of the Zeeman split well described by the Paschen-Back regime. By measuring only
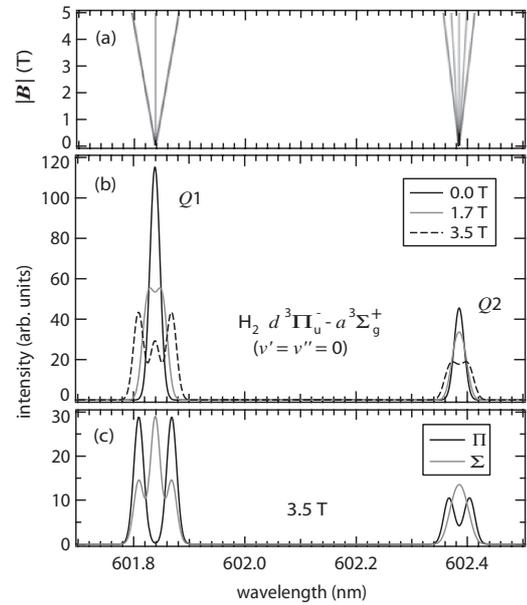
the π components, the split of the spectra becomes more salient. This can be confirmed in Figure 1 (b). In our previous paper, we reported the measurements of the π and σ polarization components in the TRIAM-1M tokamak [7].
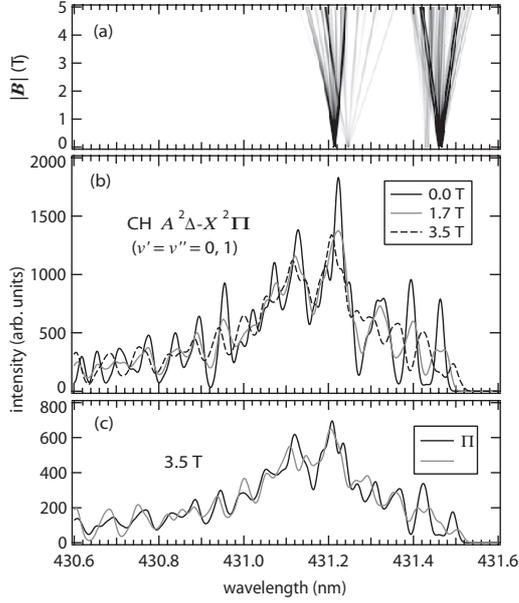

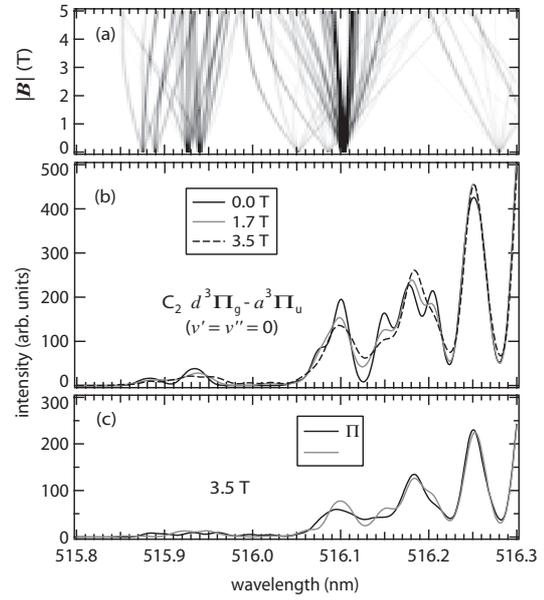Figure 2: Magnetic field effect on the CH $A^2\Delta - X^2\Pi$ band Q-branch spectra.

Figure 3: Magnetic field effect on the C_2 $d^3\Pi_g - a^3\Pi_u$ band P-branch spectra.

Figure 2 shows the magnetic field effect on the CH $A^2\Delta - X^2\Pi$ band ($v' = v'' = 0, 1$) Q-branch spectra, while Figure 3 shows the effect on the C_2 $d^3\Pi_g - a^3\Pi_u$ band ($v' = v'' = 0$) P-branch spectra, the so-called Swan band. The molecular constants and FC factors for the CH were taken from [12], while the molecular constants for the C_2 were taken from [13]. The vibrational temperature of the CH $A^2\Delta$ state was assumed to be 5000 K, and the rotational temperatures of the CH $A^2\Delta$ and C_2 $d^3\Pi_g$ states were assumed to be the equal superposition of 3000 and 500 K. The translational temperature was assumed to equal to the latter, which corresponds to the Doppler broadening of 0.0019 nm for the CH and 0.0016 nm for the C_2. The spectra are continuous because of the smaller separation between rotational energy levels than H_2 molecules. The magnetic field effect is described by the anomalous Zeeman or intermediate regime due to the larger spin-orbit interactions. For the C_2 spectra, the split is observable only in the band head, while for the CH that is rather conspicuous up to larger N as shown in Figure 2. This feature can be explained by the relative magnitudes of $\Delta\lambda_{FWHM}$, $\Delta\lambda_{so}$, and $\Delta\lambda_{ld}$, where the latter two are the wavelength shifts by the spin-orbit interaction and Λ-type doubling, respectively. For the C_2, $\Delta\lambda_{so}$ and $\Delta\lambda_{ld}$ are much smaller than $\Delta\lambda_{FWHM}$, and thus the split is mainly determined by $\Delta\lambda_{FWHM}$. By contrast, these three quantities are of the same order up to larger N for the CH. This results in the continuous change in the envelope of the spectra.

We also calculated the spectra of the BH $b^3\Sigma^- - a^3\Pi$ band ($v' = v'' = 0$) and BeH $A^2\Pi - X^2\Sigma^+$ band ($v' = v'' = 0$, 1) taking the molecular constants of the BH from [14] and BeH from [15]. The FC factors for the BeH were taken from [16]. In the calculation, the ro-vibrational temperatures of the BeH and BH upper states were assumed to be the same as those of the CH and C_2, respectively. We found that the magnetic field effect is not large on both the spectra. The change in the shape of the envelope is measurable only in the band head like the C_2 spectra.
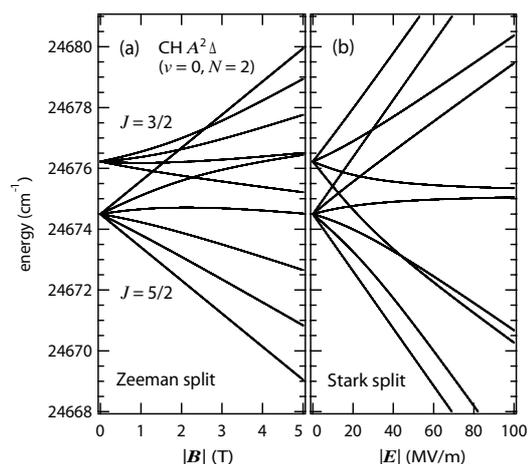

Figure 4: (a) Magnetic and (b) electric field effects on the CH $A^2\Delta$ state.

Finally, we compare the magnetic and electric field effects on the CH $A^2\Delta$ state, which are plotted in Figure 4 (a) and (b), respectively. The permanent electric dipolar moment was taken from [17]. We can see that the latter effect is negligible in the fusion application.

Acknowledgement

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