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Finding Key Diagnostic Lines for Divertor Molecular Dynamics based on Principal Component Analysis for Emission Spectral Dataset

Atomic and molecular reaction dynamics must be understood and controlled to realize efficient conversion of diverted heat load from fusion core plasmas to radiation. However, the current knowledge of the reaction dynamics is still insufficient. For example, experimentally observed radiated power in divertors is not explained by even the most advanced simulation codes. The challenge in understanding the atomic / molecular effects in the divertor is in their inherent complexity: many molecular species are involved and they interact with each other in a nonlinear manner. Exacerbating the complexities in the reaction paths, experimentally accessible quantities are very limited; analysis methods have been explored for only a few emission intensities of the atomic Balmer series and for limited molecular lines, such as Fulcher band. Although there are many emission lines from other excited states of hydrogenic and other impurity molecules, their analysis methods have not been established and thus they have been rarely measured.

In this work, in order to find unexplored features in molecular emission spectrum, a principal component analysis (PCA) is applied to high-definition spectra covering the entire visible range with 0.1 nm wavelength resolution, that are taken for 16 different experiment from the LHD divertor regions (totalling 150 frames). PCA approximates all the observed spectra by a sum of a few orthogonal bases. When the spectra are observed for variety of plasma conditions, emission lines that have different parameter-dependencies are categorized into different bases.

We found that most of the hydrogen molecular lines are categorized into a single basis, while a few distinct lines emerge in another basis. After the deeper examination, it is found that the lines extracted from PCA are H2 emission lines from the EF1Σg state and their distinct behavior is characterized by the long radiative lifetime of the state (˜102 ns). As the population influx and outflux of this state are dominated by electron-impact transitions, the ne dependence on the population is cancelled out. On the other hand, the intensity of typical emission lines is nearly proportional to the electron density as the spontaneous radiation determines the lifetime of their upper states (e.g., ˜100 ns for D1Πu state).

This finding leads to new diagnostic insights of the molecular reaction dynamics: the ratio of the two emission lines can be used to diagnose ne at the emission location, and the line intensity from the EF1Σg state can be used to infer the molecular density. A simplified collisional-radiative model is constructed from the electron-impact cross sections and spontaneous transition rates related to these states, which reveals a nearly linear ne-dependence of the line ratio and insensitivity on Te. We constructed a simple collisional-radiative model and estimate ne at the emission location (which is close to the divertor plate). This shows a strong correlation with but ˜3 times smaller than the value of ne measured independently on the last closed flux surface (LCFS). This correlation is consistent with previous studies.

In this work, the use of a pattern-recognition technique has been demonstrated to find underlying physics embedded in the complex spectra. This finding is not only useful for reaction studies in divertors, but also suggests the effectiveness of the approach. Application of a similar method to other parameter spaces, such as the high-density detached divertor in tokamaks and MPEX plasmas may reveal information more relevant to fusion power plant divertors.

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