Electron collision processes for BH and BH^+ molecules

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In magnetically confined fusion devices, BH spectral emission is a good diagnostic of boron deposition onto plasma-facing materials. BH (or boron deuteride, BD) molecular bands have been confirmed in discharges after fresh boronization. Kawate et al.[1] performed impurity powder dropping experiments[2] with boron powders in the Large Helical Device toward real-time wall conditioning. Their spatially-resolved spectroscopic measurements of BH molecular bands suggest deposition and desorption of boron on the divertor plates.

Especially aiming at fusion plasmas, electron collisional cross sections for hydride molecules related to plasma-wall interactions are crucial and have been discussed intensively. Despite the importance in fusion plasma applications and the long discussions of the spectroscopic characteristics, systematic investigations of cross sections and rate coefficients of e^-–$BH^{(+)}$ collision had not been in the literature.

In this study, we numerically investigate electronic excitation and ionization cross sections for the e^-–BH and e^-–BH^+ collision processes and the rate coefficients. In addition, we derive S/XB and compare it to the preceding study, aiming for an application to plasma diagnostics and modeling near plasma-facing materials in fusion devices. The calculations were performed by the R-matrix and Binary Encounter Bethe methods by using the UKRmol+ software suite[4]. To examine the uncertainty due to the calculation conditions, we compared the results by different basis sets and internuclear distances of the target model. We found that the uncertainties are typically within 10%. Rate coefficients were derived and fitted to an Arrhenius function. The derived S/XB values for e^-–BH collisions agreed with the value presented by Lieder et al.[5].

References

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