Abstract Submitted
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Electron-impact ionization rates for BF_3 and its fragments[1] M. RASKOVIC, S. POPOVIC, L. VUSKOVIC, Old Dominion University — We have calculated the electron-impact ionization rates of BF_3 and its fragments for electron energy distribution present in sheath mode of the repetitively pulsed d.c. diode system. Data are required for BF_3 discharge modeling. BF_3 and its fragments are reactive species used to interact with niobium surface in order to remove oxides and other impurities from the surface in the form of volatile compounds. This cleaning and smoothening treatment of bulk niobium improves the performance of the superconducting radiofrequency cavities used for particle accelerators. In our calculation electronic structures of BF_3 and its fragments were described with several empirical basis sets. After geometry optimization using density functional method B3LYP, MO parameters were calculated with UHF, CCSD(T) and OVGF methods. Electron-impact ionization cross-sections were calculated employing the Binary-Encounter-Bethe approximation and results were compared with available experimental data. Relative calculation errors were estimated, which were especially important for the cross-sections obtained with CEP-31G basis set, necessary to describe system containing niobium samples. These cross-sections are used to calculate rates for electron energy distributions of BF_3 plasmas.

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