

Abstract Submitted  
for the DAMOP07 Meeting of  
The American Physical Society

**Electron-impact ionization rates for  $\text{BF}_3$  fragments**<sup>1</sup> L. VUSKOVIC, M. RASKOVIC, S. POPOVIC, Old Dominion University, Norfolk VA — We calculated electron-impact ionization rates of  $\text{BF}_3$  and its fragments for electron energy distribution present in sheath mode of the repetitively pulsed d.c. diode system [1]. Data are being used for Ar/ $\text{BF}_3$  discharge modeling.  $\text{BF}_3$  and its fragments are reactive species that we are using to interact with niobium surface. The aim is to remove oxides and other impurities from the surface in the form of volatile compounds. This procedure of cleaning and smoothening improves the performance of the superconducting radiofrequency cavities used for particle accelerators. In our calculation electronic structures of  $\text{BF}_3$  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 [2]. Electron-impact ionization cross-sections were calculated employing the Binary-Encounter-Bethe approximation. Cross-section results were compared with available experimental data. Relative calculation errors were estimated, which was especially important for cross-sections obtained with CEP-31G basis set that is necessary to describe system containing niobium samples. [1] S. Radovanov, et al., J. Appl. Phys. 98, 113307 (2005). [2] Y-K. Kim, K.K. Irikura, AIP conferences proceedings, 543, 220 (2000).

<sup>1</sup>supported by DOE

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Date submitted: 16 Feb 2007

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