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Boron Substitution in Disordered Graphene-like Carbon JOE SCHAEPERKOETTER, ANDREW GILLESPIE, CARLOS WEXLER, PETER PFEIFER, University of Missouri, MATERIALS RESEARCH INSTITUTE- MISSOURI S&T COLLABORATION, PAUL RULIS COLLABORATION — X-ray photoelectron spectroscopy was used to determine both the elemental composition of boron doped carbons as well as gain insight into the arrangement of atoms in the material. The hypothesized arrangement of atoms is a direct substitution of boron for carbon into a graphene like sheet, maintaining the hexagonal honeycomb lattice of sp^2 sigma bonds. Such a boron atom would have an electronic configuration of $1s^2(sp^2)^3$. With a graphitic carbon atom, the p_z orbitals are maintained and participate in mobile pi bonds with neighboring carbon atoms, as understood in the aromatic model. Boron, however, would require a charge donation to fill its p_z orbital. Thus, three possible models are proposed for the out of plane electron density: (1) the orbital remains unoccupied and the boron is a free radical, (2) charge is donated from a neighboring atom and the boron atom is ionic, (3) the delocalization of charge in the aromatic system results in a partial charge transfer with an effective charge somewhere between neutral and anionic. Our results suggest that boron is not in an anionic state, and, by doing a quantitative and simultaneous analysis from multiple elemental spectra, we conclude that no more than 2 wt% of boron is being substitutionally doped into the system.

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