Nitrogen doping of carbon nanotubes

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We investigate nitrogen doping in single and multi-walled carbon nanotubes (SWNTs and MWNTs) using a combination of EEL spectroscopy and density functional calculations. Nitrogen doping in SWNTs is limited to concentrations of up to 1%, whereas MWNTs show localized doping of up to 30%. Spatial EELS mapping of individual SWNTs shows nitrogen in the nanotube walls, with two distinct N1s peaks at 398.6eV and 402eV [1]. MWNTs show a distinct morphology with 'bamboo-like' interior compartments arranged uniformly along the nanotube length. In addition to the peaks at 398.6 and 402eV, two further N(1s) peaks are discerned, at 400.5 and 406eV. We further investigate variations in the N(1s) and C(1s) edges at different locations within the nanotubes. The high nitrogen concentrations within the tube occur primarily on the inner nanotube surface and within the bamboo wall structures. This region shows a less pronounced $\pi^*$ C(1s) peak. This nitrogen rich region rapidly becomes amorphous under the irradiating electron beam.

We perform density functional calculations of various configurations of nitrogen in graphitic carbon and nanotube structures, notably exploring the influence of the metallic or semiconducting character of the nanotube on the nitrogen behavior. Substitutional nitrogen binds strongly to isolated vacancies leading to a local acceptor state, while isolated substitutional nitrogen remains in-plane giving rise to a strong donor peak just below the conduction band. We explore the potential for coupling between nitrogen defects in semiconducting tubes, and discuss the possibility of heterogeneous nitrogen distribution via islands of CNₓ within the tube wall. [2]

References

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