

Structural studies of N-doped multi-wall carbon nanotubes by high-energy X-ray diffraction

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The structure of the nitrogen doped multi-wall carbon nanotubes (~6 at. %) have been studied using the high-energy X-ray diffraction and molecular dynamics (MD) techniques. The diffraction measurements were carried up to a maximum value of the scattering vector $K_{max}=24 \text{ \AA}^{-1}$. The obtained diffraction data were then converted to a real space representation in the form of the pair correlation function. Structural models containing four walled carbon nanotube 300 Å in diameter and 25 Å in length (~35 000 atoms) were computer generated and then relaxed using the Tersoff potential [1] with parameters reported by Matsunaga et al. [2] for carbon-carbon, carbon-nitrogen, nitrogen-nitrogen interactions and the Lennard-Jones potential for inter-layer interactions. According to the previous studies there are three types of nitrogen arrangement in the N-doped carbon nanotubes: in a sp^3 bonding configuration, which represents N atoms in out-of-plane positions, in a sp^2 graphite-like configuration, which represents substitutions of carbon by N atoms, and the pyridine-like N defect (substitutional nitrogen creating a carbon vacancy) [3,4,5]. These three types of nitrogen positions were taken into account. The MD simulations were performed at 2 K. In order to account for the thermal oscillations and static disorder the Debye-Waller factor and the Stone-Wales defects were introduced respectively. For such relaxed models the intensity and pair correlation functions were computed. Correctness of the models was verified by comparison of the simulations with the experimental data both in real and reciprocal space. Effects of three types of nitrogen arrangements (sp^3 bonding configuration, sp^2 graphite-like configuration, and pyridine-like configuration) and the Stone-Wales defects on the resulting structure were investigated.

- [1] J. Tersoff, Phys. Rev. B 39 (1989) 5566.
- [2] K. Matsunaga, C. Fisher, H. Matsubara, Jpn. J. Appl. Phys. 39 (2000) L48.
- [3] M. Zhao, Y. Xia, J.P. Lewis, R. Zhang, J. Appl. Phys., 94 (2003) 2398.
- [4] S.H. Lim, H.I. Elim, X.Y. Gao, A.T.S. Wee, W. Ji, J.Y. Lee, J. Lin, Phys. Rev. B, 73 (2006) 045402.
- [5] H.Ch. Choi, J. Park, B. Kim, J. Phys. Chem. B, 109 (2005) 4333.