

CHARACTERIZATION OF SINGLE-WALLED CARBON NANOTUBES CONTAINING DEFECTS FROM THEIR LOCAL VIBRATIONAL DENSITIES OF STATES

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The study of local vibrational properties of nanostructures is becoming of great interest since the development of resonant Raman enhanced spectroscopy, inelastic tunneling spectroscopy,... The latter technique has the advantage to authorize atomic resolution and could be used to detect the presence of a defect from the perturbation of the vibrational spectrum it induces. In this context, this work aims at exploring local vibrational structures of typical defects in carbon nanotubes.

We present a vibrational study of an isotopic substitution impurity in a (10,9) chiral nanotube, a Stone-Wales defect in a series of armchair tubes and, in addition, we have considered a intramolecular junction between (12,0) and (9,0) nanotubes. Our study emphasizes the differences of local vibrational densities of state (IVDOS) between perfect and imperfect nanotubes. We use a dynamical model where carbons interact up to their third nearest neighbours with force constants fitted to graphene [1]. IVDOS are computed with the recursion method. Our study is a first step towards a more complete approach for characterizing defects in carbon nanotube structures based on the recognition of local vibrational fingerprints of these defects.

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Reference

[1] R.A. Jishi and G. Dresselhaus, Phys. Rev. B **26** (1982), 4514-22