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Phonon anomalies in the resonance Raman spectra of graphite and single-wall carbon nanotubes GEORGII G. SAMSONIDZE, HYUNGBIN SON, Department of Electrical Engineering and Computer Science, MIT, Cambridge, MA, SHIN GRACE CHOU, Department of Chemistry, MIT, Cambridge, MA, GENE DRESSELHAUS, Francis Bitter Magnet Laboratory, MIT, Cambridge, MA, MILDRED S. DRESSELHAUS, Department of Electrical Engineering and Computer Science and Department of Physics, MIT, Cambridge, MA, RIICHIRO SAITO, JIE JIANG, Department of Physics, Tohoku University and CREST JST, Japan, EDUARDO B. BARROS, ANTONIO G. SOUZA FILHO, Departamento de Fisica, Universidade Federal do Ceara, Fortaleza, CE, Brazil — Phonon dispersion relations for a graphene sheet and single-wall carbon nanotubes (SWNTs) are calculated within the extended tight-binding model that has recently been shown to accurately predict the optical transition energies in small-diameter SWNTs. Anomalies in the dispersion relations are found at certain high- symmetry points of the reciprocal lattice and these anomalies are attributed to the strong electron-phonon coupling. These anomalies are very sensitive to changes to electron and lattice temperatures, electron doping, mechanical stress, SWNT diameter, and SWNT metallicity. Resonance Raman measurements of doping and strain induced shifts of the phonon frequencies in SWNTs are in qualitative agreement with the present calculations. The MIT authors acknowledge support under NSF Grant DMR 04-05538.

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