LOW-FREQUENCY RAMAN SPECTROSCOPY OF CARBON NANOTUBES

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Since mechanical, elastic, and thermal properties are strongly influenced by phonons, Raman spectra provide much information about the structure, quality and utility of single-walled carbon nanotubes (SWCNTs). Unprecedented NIST-prepared samples combined with theoretical calculations and unique instrumentation permit a thorough study of the low-energy phonon modes of SWCNTs. Observed in the four to seven THz region of the spectrum, the radial breathing modes (RBMs) have A symmetry and are inversely proportional to the diameter of the SWCNT. The lowest lying E2g mode, has yet to be observed and is the focus of this study. Phonon energies using both the local density approximation (LDA) and the generalized-gradient approximation (GGA) to density functional theory (DFT) have been calculated as a function of nanotube radius and chirality. Novel SWCNT samples have been developed to enable experimental tests of the theory. Furthermore, multiple laser lines for resonant enhancement and a triple-grating monochromator for ultimate rejection capabilities make possible our studies of these vibrations predicted in the tens of wavenumbers or less than 0.5 THz. A detailed examination of the complex low-frequency Raman spectra of SWCNTs will be presented.