HRTEM, DFT modeling and Raman Spectroscopy of Extreme Nanowires within Single Walled Carbon Nanotubes

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Extreme nanowires formed by filling the central pore of single walled carbon nanotubes (SWCNTs) have extreme diameters and thus extreme properties. In some instances the extreme confinement causes entirely new crystalline forms not observed in bulk and these structures are investigated by high performance electron microscopy (i.e. hardware corrected HRTEM and exit wave reconstruction (EWR)). Until recently, there has been only limited research into the physical properties of these extreme nanowires. While there has been a significant effort in terms of revealing the physical properties of, for example, KI and HgTe extreme nanowires in SWCNTs by density functional theory (DFT) [1,2] there are few experimental studies besides imaging. A significant impetus towards new studies in these materials has been given by the observation that under beam irradiation or induced strain, some materials undergo significant 'phase change' behaviour [3,4,5] We report here investigatio ns into two new systems, SWCNT embedded SnSe [5] which undergoes band gap expansion, as well as shear induced phase change behaviour in SWCNTs with diameters >1.4 nm and also experimental studies into two-atom thick SWCNT-embedded HgTe extreme nanowires. Raman spectra have been measured for ensembles of bundled filled tubes for excitation photon energies in the ranges 3.39 to 2.61 eV and 1.82 to 1.26 eV for Raman shifts down to 25 cm^{-1} and sample temperatures in the range 4-300K. All of the evidence support the hypothesis that the observed Raman features are not attributable to single walled carbon nanotubes, but instead to the HgTe nanowires. The observed additional features are due to four distinct phonons, with energies 47, 51, 94 and 115 cm^{-1} respectively, plus their overtones and combinations [6].

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