Raman Scattering as a Probe of the Electronic Structure of Single-Wall Carbon Nanotubes Under High Pressure

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Abstract. Single-wall carbon nanotubes (SWNTs) under *in-situ* pressures of 0-0.5 GPa have been studied using Raman scattering in a diamond anvil cell (DAC). The pressure-induced changes in electronic structure of SWNT were related to changes observed in resonant Raman spectra. In particular, the radial breathing Raman modes show a strong pressure dependence. At ambient conditions the band at 191 cm^{-1}, corresponding to SWNTs with a diameter of 1.29 nm was a dominant spectral feature, whereas at pressures above 0.3 GPa, the band at 211 cm^{-1}, corresponding to nanotubes with a smaller diameter (1.16 nm), became dominant. The switching of resonance enhancement in selective diameter SWNTs is interpreted as a pressure-induced narrowing of the corresponding electronic gap. Upon decompression these effects are reversed. Our estimation of the band gap narrowing with pressure is in agreement with the direct measurement from optical absorption experiments on SWNT surfactant liquid suspension pressurized in a DAC.

INTRODUCTION

Raman scattering has been used as a common diagnostics of the electronic properties in SWNTs (single-wall carbon nanotubes), primarily due to the photo-selective resonance response for the radial breathing modes (RBM) [1]. The SWNTs exist in ropes, where each nanotube possesses an individual 1D electronic density of states (DOS). It is dominated by a set of van Hove singularities situated symmetrically relatively to the Fermi level (Figure 2) [2]. Optical transitions are allowed between the symmetrical maxima, and the energy separation ("pseudo"-gap) is almost inversely proportional to the tube diameter. Hence, laser Raman spectroscopy provides a diameter size selective resonance excitation when the laser photon energy matches one of the allowed optical transitions for a specific diameter SWNT. The most common way to achieve selective Raman excitation of different diameter carbon nanotubes in the rope is through tuning of the laser wavelength to match the resonance optical gap. However, another way to achieve selectivity is either through pressure or temperature tuning of the electronic structure in SWNTs. In our previous work, elevated temperature was used to narrow the SWNT pseudo-gap and providing a selective excitation of Raman scattering in narrow

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