phys. stat. sol. (b) **215**, 393 (1999)

Subject classification: 78.30.Na; 62.50.+p; S5

Pressure Behaviour of Single Wall Carbon Nanotube Bundles and Fullerenes: A Raman Study

A.K. Sood (a, b), Pallavi V. Teresdesai (a), D.V.S. Muthu (a), Rahul Sen (b), A. Govindaraj (b), and C.N.R. Rao (b)

(a) Department of Physics, Indian Institute of Science, Bangalore–560 012, India

(b) Jawaharlal Nehru Center for Advanced Scientific Research, Jakkur Campus, Jakkur P.O., Bangalore–560 064, India

(Received May 7, 1999)

We shall discuss our recent high pressure Raman studies on single wall carbon nanotube (SWNT) bundles and compare them with pressure-induced amorphous and polymeric phases of crystalline C_{60} and C_{70}. Our high pressure Raman studies on SWNT bundles carried out upto 25.9 GPa show that the intensities of both the radial modes ($\omega \approx 170$ cm^{-1}) as well as tangential modes (around 1590 cm^{-1}) decrease significantly with pressure, so much that the radial modes cannot be observed beyond 2.6 GPa. Most interestingly, the frequency of the dominant tangential mode increases upto 11 GPa, then decreases till 16 GPa and again increases. Raman spectra were resolved into four modes upto 10 GPa beyond which only one or two modes could be fitted to the recorded spectra. The pressure-softening of the mode between 11 and 16 GPa as well as other features of the Raman spectra are reversible in the decreasing pressure cycle. These results, though not understood at present, can be associated with the distortion of the circular cross-section of the tubes in the bundle, eventually leading to a possible transition of the SWNT bundle to graphite like carbon at 11 GPa which is completed at 16 GPa. This transition is reversible on decompression.

1. Introduction

In recent years, there has been intense activity, both experimental and theoretical, in exploring fascinating physical properties of newer forms of carbon, namely fullerenes and single wall carbon nanotubes (SWNT) [1]. These properties include high structural stability and novel electronic transport. It is hoped that SWNT will have potential applications in nanometer-sized electronics and in development of high strength polymeric composite materials. Initially fullerenes C_{60} and C_{70} had occupied a center-stage, but in recent years most of the attention is focussed on carbon nanotubes. After the first observation [2] of multiwall nanotubes in 1991, a major breakthrough occurred in 1996 when bundles of aligned SWNT with narrow-size distribution could be produced in large quantities by laser pulse vaporization [3], followed by electric arc method [4]. The SWNT in a bundle are arranged in nearly a two dimensional triangular lattice, with intertube spacing of $\approx$3.4 Å, typical of van der Waals interaction between the tubes. Recent scanning tunneling spectroscopy experiments [5] have verified the theoretical predictions that the electronic properties of SWNT are given by one-dimensional density of states. These isolated tubes can be semiconducting or metallic, depending on their diameter and the chiral angle defined by the orientation of the hexagons with respect to the nanotube axis. The chiral vector which connects two crystallographically equivalent sites on a 2D graphene sheet is $n\mathbf{a}_1 + m\mathbf{a}_2$, where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the unit