Intertubular interaction in bundled single-walled carbon nanotubes studied by Raman scattering at high pressure and temperature

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Raman spectra of bundled single-walled carbon nanotubes (SWCNTs) were measured at high temperature up to 400° C and pressure up to 4.5 GPa. The SWCNTs were synthesized by the arc discharge method in helium atmosphere at a pressure of 0.86 bar, using a metallic Ni/Y catalyst The average diameter of the tubules was 1.5 nm as anticipated for the preparation method applied, as well as by TEM and Raman characterization. The main impurities were graphite particles, while the content of metal impurities was ~1.3 %.

Raman spectra at high pressure and high temperature were recorded *in-situ* using spectrograph Acton SpectraPro-2500i equipped with a Peltier-cooled CCD Pixis2K, high pressure diamond anvil cell of Mao-Bell type and a high temperature cell. The 514.5 nm Ar^+ laser line was focused on the sample by means of a 50× objective in a spot of ~10 μm diameter, while the beam intensity on the sample was ~5 mW.

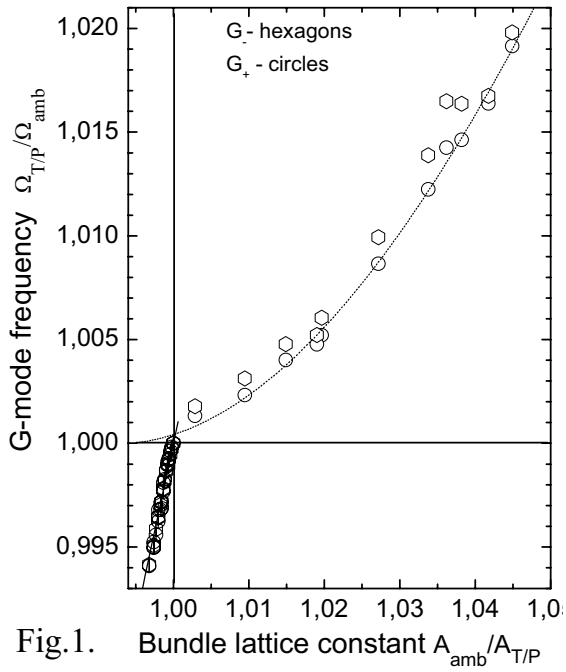

Fig.1.

Raman spectra show reversible pressure- and temperature-induced shift for the G_- and G_+ bands. The temperature shift is negative and practically the same for the G_- (-0.0230± 0.0007) cm^{-1}/K and G_+ (-0.0229±0.0002) cm^{-1}/K bands, whereas the pressure shift is positive with pressure coefficients for the G_- and G_+ (7.23±0.33) cm^{-1}/GPa and (7.02±0.15) cm^{-1}/GPa, respectively. The Raman data do not show changes in the tube diameter upon heating and compression of bundles. The dependence of the G_- and G_+ band shift on the relative variation of the triangular lattice constant was calculated on the basis of the linear compression and dilatation constants, obtained by XRD-measurements [1,2] (Fig.1). These data show that the dilatation constant is not compatible with the compressibility constant, whereas the inter-tubular interaction is mainly of the van-der-Waals type.

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[1] S. Sharma et al., *PRB* **63**, 205417 (2001).
[2] Y. Maniwa et al., *PRB* **64**, 241402R (2002).