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Photoemission Spectroscopy of Single-Wall Carbon Nanotube

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Introduction

A SWNT becomes a metal or semiconductor depending on its chirality, and has characteristic peak structures due to one-dimensional van Hove singularities (1D VHS) in the density of states because of the periodic boundary condition along the circumference. In this study, we investigated the electronic states of SWNTs by photoemission spectroscopy.

Experimental

The photoemission experiments were performed using synchrotron radiation at the beam line BL-11D of the Photon Factory, High Energy Accelerator Research Organization (KEK). The instrumental resolutions were 50 meV.

Results and Discussion

Figure 1 shows the photoemission spectra of SWNT and graphite measured at $h\nu$=65 eV. The intense structure around the 8 eV peak and the structure around the 3 eV peak are due to the σ and π bands, respectively. The broad trapezoid structure around 19 eV is the C 2s band. The shapes and positions of these structures are similar to the results of Suzuki *et al*. [1]. The valence band spectrum of the SWNT is similar as a whole to that of graphite. The difference in spectral features between the SWNT and graphite appeared in the energy region near the Fermi level (E_F).

The photoemission spectra near E_F are shown in Fig. 2. For the SWNT samples, three peak structures denoted by S_1, S_2 and M_1 can be clearly seen around the binding energies of 0.45, 0.75 and 1.0 eV, respectively. On the other hand, the spectrum of graphite shows no structure in this energy region. We estimated the mean diameter of the SWNT-A sample to be 1.37 nm from the A_{1g} breathing mode frequencies in the Raman spectra. The structure and electronic properties of SWNTs can be defined by a pair of integers, the so-called chiral index expressed in (n_1, n_2) [2]. For SWNTs with diameters near 1.37 nm, for example, a metallic SWNT with a chiral index (10, 10) has a diameter of 1.375 nm and a semiconducting SWNT with (16, 2) has a diameter of 1.357 nm. The densities of states for the SWNTs with these chiral indices calculated by Maruyama [3] are also shown in Fig. 2. As can be seen from the figures, the S_1 and S_2 peaks and the M_1 peak can correspond to the structures of semiconducting and metallic SWNTs, respectively. For the SWNT-B sample, the peak structures appeared at higher binding energies than the respective corresponding structures of the SWNT-A sample. The mean diameter of the SWNT-B sample was estimated to be 1.25 nm. The fact that the difference in peak position comes from the difference in diameter is consistent with the result of the band structure calculation [2]. From the above comparison, the three observed peak structures are due to the spikes caused by the 1D VHS in the occupied density of states.

[1] S. Suzuki *et al*., Phys. Rev. B 63, 245418 (2001).

[2] R. Saito, G. Dresselhaus and M. S. Dresselhaus, *Physical Properties of Carbon Nanotubes* (Imperial College Press, London, 1998).

[3] S. Maruyama, private communication.

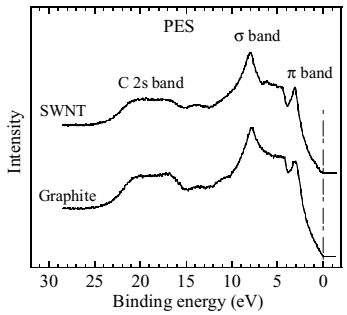

Figure 1: Photoemission spectra of SWNT and graphite.

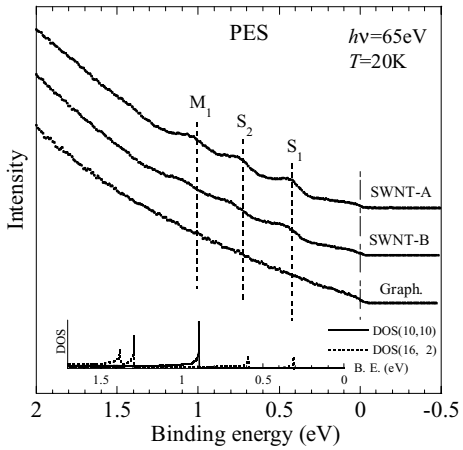

Figure 2: Photoemission spectra of SWNT samples and graphite.

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