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Photoemission Spectra of Carbon Nanotube and C_{60} Fullerene-Peapod

Hiroyoshi ISHII*[1], Hidetsugu SHIOZAWA[1], Hideo KIHARA[1], Naoya SASAKI[1], Satoshi NAKAMURA[1], Tetsuo YOSHIDA[1], Yasuhiro TAKAYAMA[1], Tsuneaki MIYAHARA[1], Masashi NAKATAKE[2], Takeshi KODAMA[1], Shinzo SUZUKI[1], Yohji ACHIBA[1] and Hiromichi KATAURA[3]
[1]Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan
[2]HiSOR, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan
[3]National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8562, Japan

Introduction

A single-wall carbon nanotube (SWNT) encapsulating C_{60} fullerenes, which is called a C_{60} peapod (C_{60} PPD), has attracted much attention because of its exotic nano-scale structure; many theoretical and experimental studies of the C_{60} PPDs have been performed. According to the results of the local density approximation calculation performed by Okada *et al*. [1] and Otani *et al*. [2], the orbital mixing between the nearly-free-electron states of SWNTs and the π orbitals of C_{60} fullerenes leads to the intersection of the lowest unoccupied molecular orbital (LUMO) band of the C_{60} fullerene with the Fermi level (E_F); it is expected that the LUMO band of the C_{60} fullerene appears near E_F in the photoemission spectrum. In this study, we have measured the photoemission spectra of SWNT and C_{60} PPD samples.

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 resolution was 50 meV. SWNT samples were prepared by the laser vaporization method [3]. The mean diameters of SWNTs in the samples are 1.40 nm.

Results and Discussion

Figure 1 shows the photoemission spectra of the SWNT and C_{60} PPD samples measured at $h\nu$ = 65 eV. The photoemission spectrum of the C_{60} PPD is, as a whole, similar to that of the SWNT [3].

The spectrum of the C_{60} fullerenes inside the SWNT was obtained by subtracting the empty SWNT spectrum from the C_{60} PPD spectrum and is shown in the figure. The overall spectral features are very similar to those of the C_{60} solid spectrum [4]. The peaks in the binding energy region between 5 eV and E_F correspond mostly to the π band structures of an isolated C_{60} fullerene. The structures at the binding energies above 10 eV correspond mostly to the σ band. The several peaks in the binding energy region between 5 eV and 10 eV are mixture of the π and σ bands. The peak at the binding energy of 2.3 eV is derived from the highest occupied molecular orbital (HOMO) having h_u symmetry with 5-fold degeneracy. The peak at 3.6 eV is derived from the next HOMO (NHOMO) having g_g and h_g symmetry with 9-fold degeneracy.

As shown in the figure, the NHOMO and HOMO peak positions are nearly equal to the respective corresponding peak positions in the C_{60} solid spectrum [4]. According to the theoretical calculation by Okada *et al*. [1] and Otani *et al*. [2], the t_{1u} level of the C_{60} fullerene intersects with E_F when the SWNT diameter is larger than 1.3 nm. For the present C_{60} PPD sample with the SWNT mean diameter of 1.4 nm, however, there is no structure in binding energies ranging from the onset of the HOMO peak to E_F. This result is consistent with the experimental results of the potassium doping effect and the electron-energy-loss spectroscopy [5]. It is concluded that the t_{1u} level of the C_{60} fullerenes inside the SWNT stays above E_F even when the SWNT mean diameter is larger than 1.4 nm.

References

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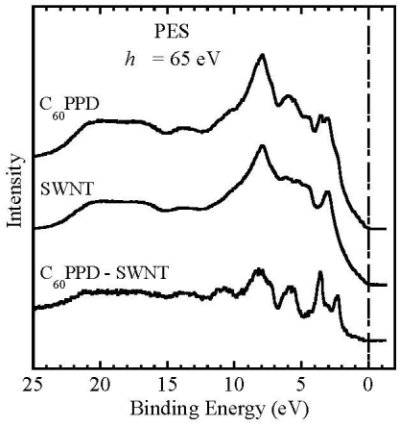

Figure 1: Photoemission spectra of the C_{60} peapod and SWNT samples, and C_{60} fullerenes in SWNTs.

* ishii@comp.metro-u.ac.jp