Supplementary Information

Chirally Selective Growth and Extraction of Single-Wall Carbon Nanotubes via Fullerene Nano-Peapods

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Stone-Wales transformation

Stone-Wales transformation gives a hypothetical mechanism for structural interconversion of sp^2-bonded carbon nanosystems. Two carbon atoms are manually rotated for 90^o with respect to the midpoint of the bond. The structure after Stone-Wales transformation is geometry optimized by a semi-empirical simulation (PM3) implemented in Gaussian 03 package.[1] The corresponding energy evolution during Stone-Wales transformation is also recorded.

Characterization details

UV-vis-NIR spectroscopy (V-570, JASCO) was applied to measure the optical absorption. Raman spectra were taken in a back-scattering geometry using a single monochromator with a microscope (HR-800, Horiba Jobin Yvon) equipped with a charge coupled device detector and an edge filter. The samples were excited by lasers at 488nm, 514nm, and 633 nm. PL was measured by a Shinadzu NIR-PL system equipped with a liquid nitrogen cooled InGaAs detector. The emission spectra of the pristine and extracted tubes were taken in 1% DOC aqueous solution with exposure time of 5 sec. HRTEM measurements were performed by using a JEOL JEM 2100F microscope. HRTEM images were acquired at an electron acceleration voltage of 80 KV. The referred sample was dispersed in 1,2-dichloromethane by a weak bath sonication technique for 5 min and then drop onto the a thin carbon film coated copper grid.

Experimental details

The DWCNTs were heated at 600 °C for 10 min under air to re-open the ends and create defects in outer tubes. The open capped DWCNTs (ca. 2.4 mg) were dispersed in 2.5 mL 1% sodium deoxylcholate (DOC, TCI-EP) aqueous solution. The inner tubes were then extracted from the

DWCNTs by the ultrasonication method using Nanoruptor NR-350 (Cosmo Bio Co. Ltd) for 20 h at 20 °C. The inner tubes were further separated and isolated from the outer tubes and residual DWCNTs by the density gradient ultracentrifugation (DGU) method. The density gradients were created from aqueous solutions of iodixanol, purchased as OptiPrep (60% w/v iodixanol, Sigma-Aldrich), directly into centrifuge tubes. Three discrete layers with decreasing iodixanol concentrations (30%, 1.5 mL; 20%, 1.5 mL; 15%, 1.0 mL) were layered from bottom to top into a centrifuge tube. The sample (1.0 mL) was layered on top of the iodixanol layers. All the layers contain 1% DOC surfactants. Centrifugation was carried out using a swing bucket S52ST rotor (Hitachi Koki) at 52,000 r.p.m. for 12 h at 22 °C. The sample was fractioned after centrifugation and was subjected to further characterized. The DGU separation of inner tubes from C_{60} and C_{70} coalescence is shown in Fig. S2. A thin light purple layer and a thin light red layer were detected on the top of the solution after 12 h centrifugation, respectively. The different sections of the samples were pipetted and measured by optical absorption. The optical absorption (Fig. 2c and Fig. S2) and Raman spectra (Fig. 2d and Fig. S1) of the sample indicates that the top thin layers are the extracted inner tubes.

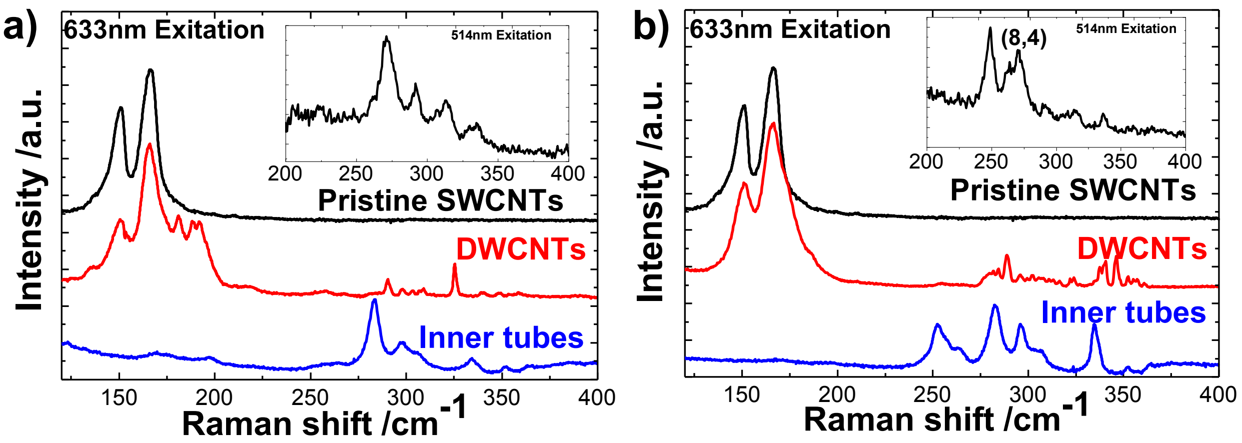

Fig. S1. Raman spectra of inner tubes extraction of DWCNTs derived from a) C_{60}@CNTs; b) C_{70}@CNTs (633 nm). (Insets show the corresponding inner tubes at wavelength of 514nm).

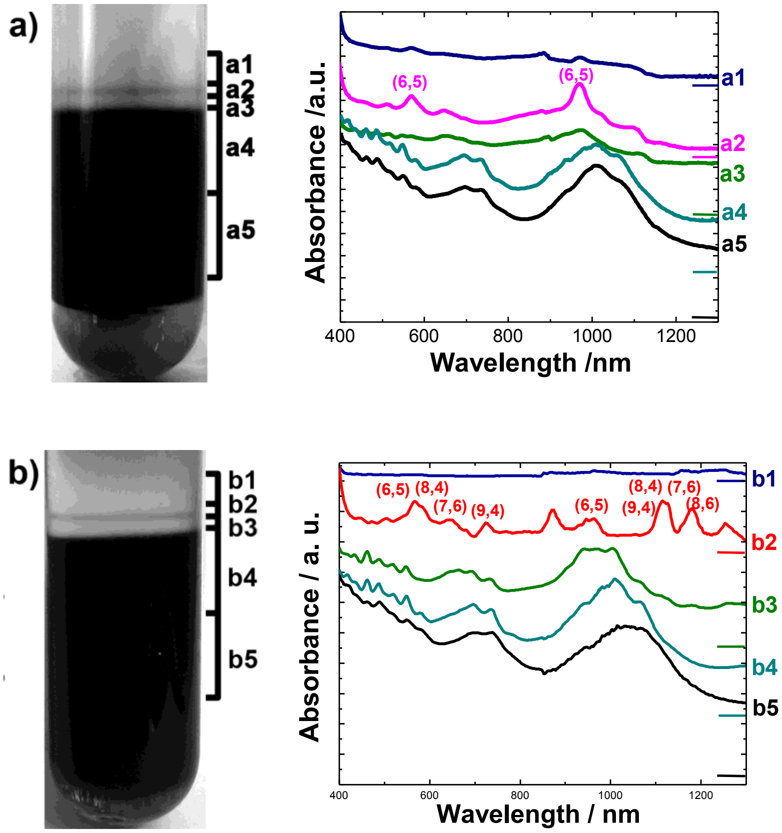

Fig. S2. DGU separation and optical absorption spectra of inner tubes extraction of DWCNTs produced from a) C_{60}@CNTs; b) C_{70}@CNTs.

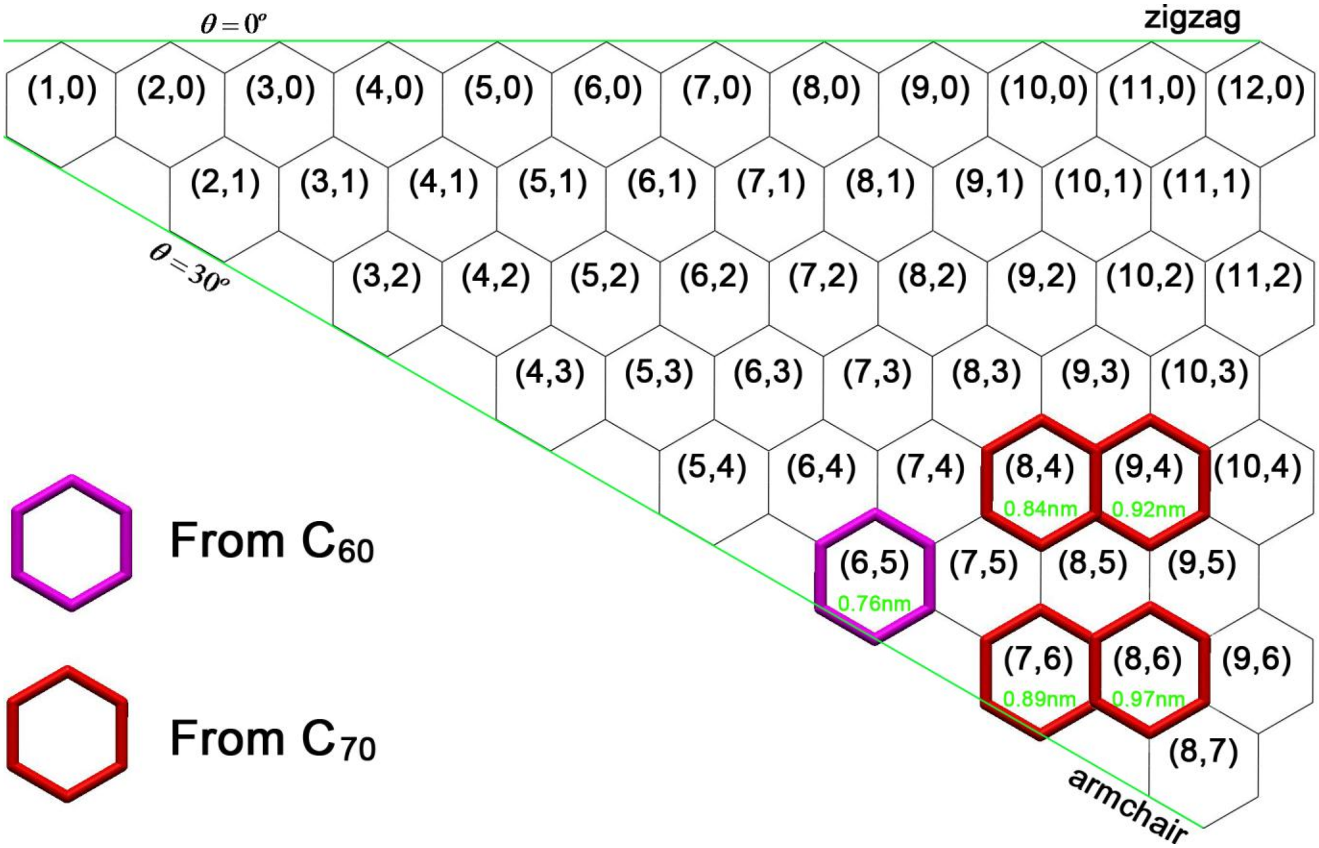

Fig. S3. chirality map of the extracted inner tubes from C60 and C70 coalescence.

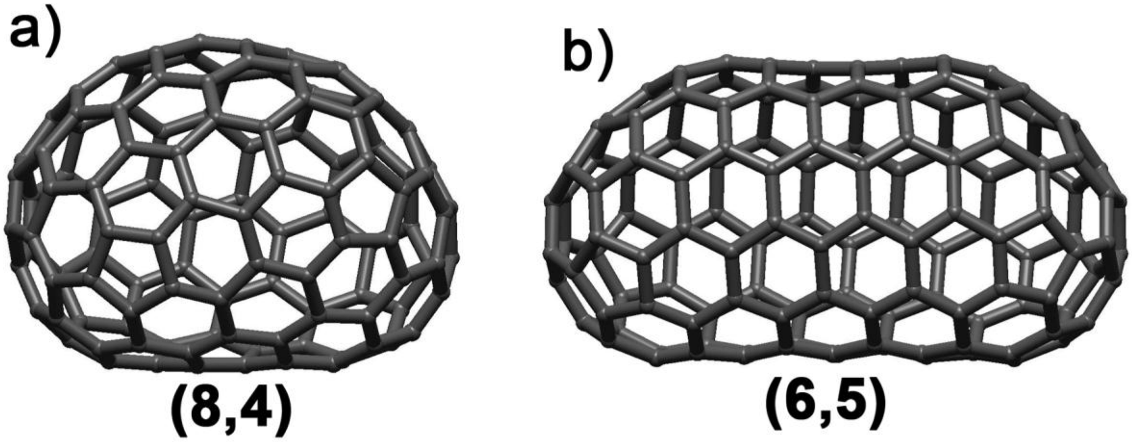

Fig. S4. Structural models of a) C_{120} tube with chirality of (8,4), b) C_{140} tube with chirality of (6,5).

Table S1. Relative Photoluminescence Intensities of the Extracted Inner Tubes from C_{60} and C_{70} Coalesence

(n,m)	diameter (nm)	θ (degree)	Diff PL peak intensity (C_{60})[a]	Diff PL peak intensity (C_{70})[a]
(6,5)	0.76	27.0	100	40
(8,3)	0.78	15.3	22	0
(7,5)	0.83	24.5	20	33
(8,4)	0.84	19.1	24	56
(7,6)	0.89	27.5	0	92
(9,4)	0.92	17.5	0	100
(8,6)	0.97	25.3	0	69

[a] Differential PL intensity: the amplitude of the partial derivative of the PL map, as suggested by Arnold *et al.*[2]

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2. Arnold, M. S.; Green, A. A.; Hulvat, J. F.; Stupp, S. I.; Hersam, M. C., Sorting carbon nanotubes by electronic structure using density differentiation. *Nature Nanotechnology* 2006, 1, 60-65.