Electronic Supplementary Material for *PCCP*

Determining Exact Molar Absorbance Coefficients of Single-Wall Carbon Nanotubes

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Electronic Supplementary Information (ESI):

Degree of impurities of the CNTs used in this study

The thermogravimetric analysis (TGA) data for HiPco, CoMoCAT and as-produced SWNTs synthesized by pulsed laser vaporization (LV-SWNTs) in air at a ramp rate of 10 ºC/min are used for evaluating the degree of impurities in samples. TGA was conducted using a Shimadzu TA-60WS and samples were placed in a quartz pan. The change in TGA residue at 800 ºC shows the degree of impurities, especially metal catalyst impurities (typically, -HiPco: ~ 20 % w/w, CoMoCAT: ~ 20 % w/w, LV-SWNTs: ~ 10 % w/w).

Quality of the CNTs used in this study determined by Raman studies.

Raman studies were carried out on as-prepared HiPco samples and HiPco samples sonicated after ultracentrifugation at 197,000 *g* to determine the quality of the samples used. The surfactants were removed from dispersed HiPco samples using dialysis membranes (visking tube; MW ~ 12,000). A thin film of such samples was then prepared on a membrane filter (Omnipore membrane, JGWP, Millipore). Raman spectra were measured on a single-grating spectrometer (Jobon Yvon HR-800) equipped with an Ar^+ ion laser at 488 nm and a He-Ne laser at 632.8 nm for excitation.

Figures S1 and S2 show the Raman spectra of the (a) as-prepared HiPco and (b) sonicated HiPco samples excited at 488 nm and 632.8 nm, respectively. The peak distribution of the radial breathing mode (RBM) with the known reciprocal relation between the diameters and RBM frequency did not change before and after the sonication process, indicating that the diameter distribution of SWNTs also did not change. A vibrational line centered at 1300 cm^{-1} (D-band) characterizes defects in bonding and sidewall vacancy, such as changes in the carbon-carbon bonding and the presence of amorphous carbon. The intensity of the D-band normalized by the intensity of the G-band at around 1590 cm^{-1} slightly increased after the sonication process as shown in Figs. S1 and S2, indicating that nanotube shortening and defect induction occurred during the sonication process[1].

Expression of the absorption probability of randomly oriented CNTs

To evaluate the probability that an individual CNT has a proper angle to incident light, we need to determine the total probability that one side of a CNT is set at a zero point and the other side is set anywhere on the surface of a sphere of radius L, which is the length of a CNT. Such a model is illustrated in Fig. S3, where the angle notations are defined and incident light comes from the direction parallel to the y-axis. The probability that an SWNT has a tilt $\theta \sim \theta + d\theta$ and $\varphi \sim \varphi + d\varphi$ is given by

$$\frac{L^2 \sin\theta d\theta d\varphi}{4\pi L^2} \qquad (1)$$

and the corresponding absorption area is defined by

$$\pi d_{NT} L \sin\theta , \qquad (2)$$

where d_{NT} is the diameter of CNTs. CNTs show a polarization dependence of $\sin^2\varphi$.[2, 3] Using the above relations, we can estimate absorption probability as follows[4,5]:

$$\iint \frac{L^2 \sin\theta d\theta d\varphi}{4\pi L^2} \cdot \pi d_{NT} L \sin\theta \cdot \sin^2\varphi$$

$$= \frac{d_{NT} L}{4} \int_0^{2\pi} \sin^2\varphi d\varphi \int_0^{\pi} \sin^2\theta d\theta$$

$$= \frac{\pi^2 d_{NT} L}{8} \qquad (3)$$

References

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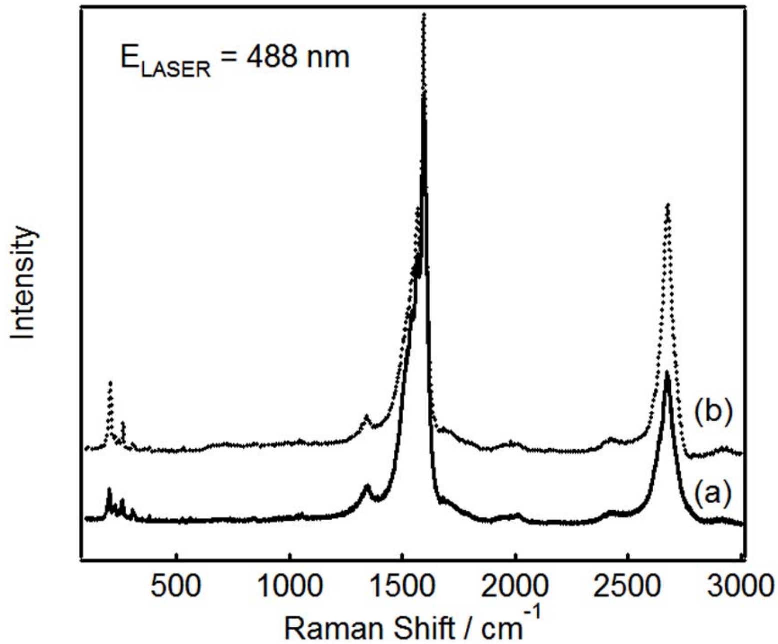

Fig. S1 Raman spectra of (a) as-prepared HiPco (solid line) and (b) sonicated HiPco (dotted line). The excitation is at 488 nm.

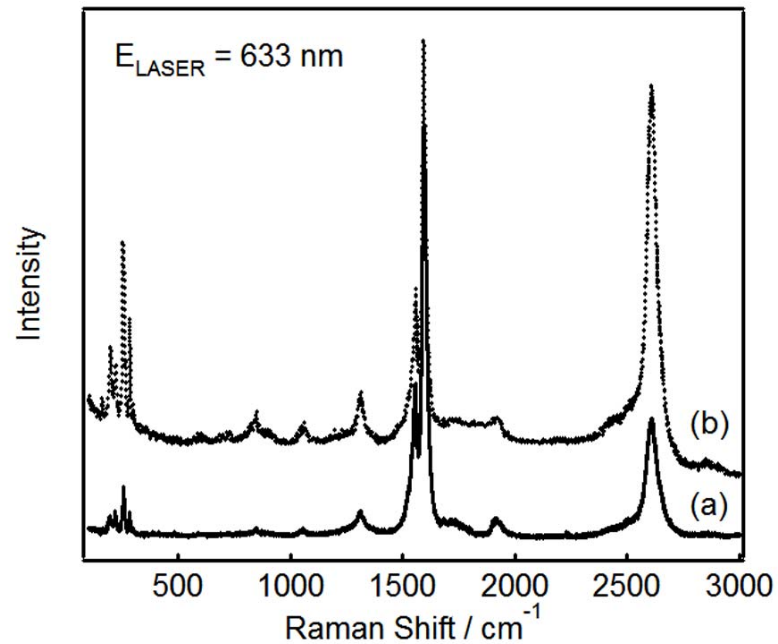

Fig. S2 Raman spectra of (a) as-prepared HiPco (solid line) and (b) sonicated HiPco (dotted line). The excitation is at 633 nm.

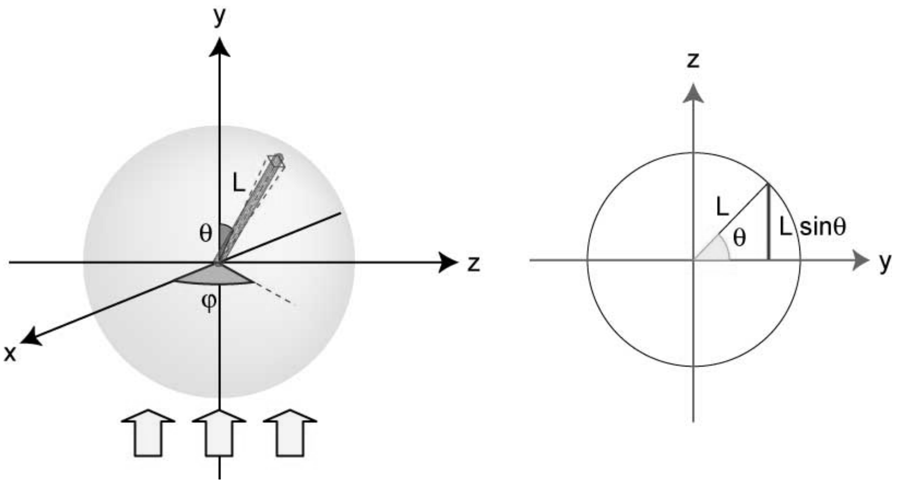

Fig. S3 Illustration of the model of CNTs adopts various angles to incident light.