Straightening Single-Walled Carbon Nanotubes by Adsorbed Rigid Poly(3-hexylthiophene) Chains via π – π Interaction

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Introduction

Carbon nanotubes (CNTs) have a wide range of applications in many fields. However, because of their high aspect ratio, bending and twisting usually occur for CNTs, which result in decreased performance of electronic devices. Straightened and aligned CNTs will be beneficial to the properties and performance of the CNT-containing materials and devices. In the present work, we demonstrate that adsorbed rigid P3HT chains can straighten single-walled carbon nanotubes (SWCNTs) under suitable conditions.

Experiment and result

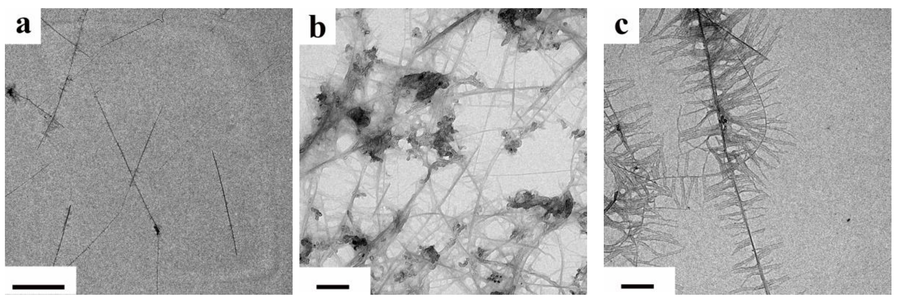


Figure 1. TEM images of SWCNTs/LM-P3HT supramolecular structures after crystallization from mixed solvent of anisole/heptane (1/1 v/v) at T_c = 45 ℃ for 24 h. (a) C_{SWCNT} = 1.0×10^{-3} mg/mL, W_{SWCNT}/W_{P3HT} = 1/50. Scale bar = 500 nm. (b) C_{SWCNT} = 0.2 mg/mL, W_{SWCNT}/W_{P3HT} = 1/50. Scale bar = 200 nm. (c) C_{SWCNT} = 1.0×10^{-3} mg/mL, W_{SWCNT}/W_{P3HT} = 1/250. Scale bar = 200 nm.

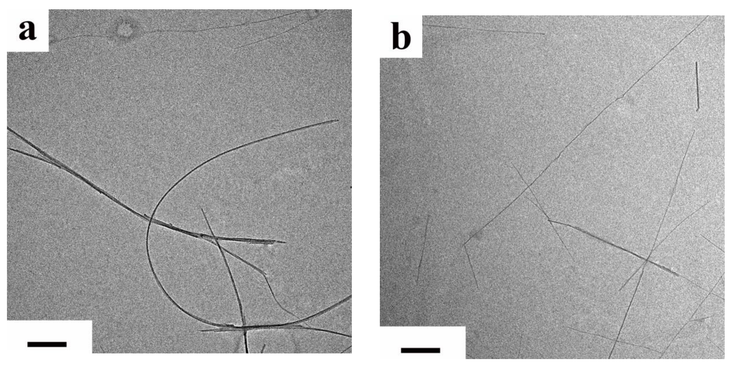


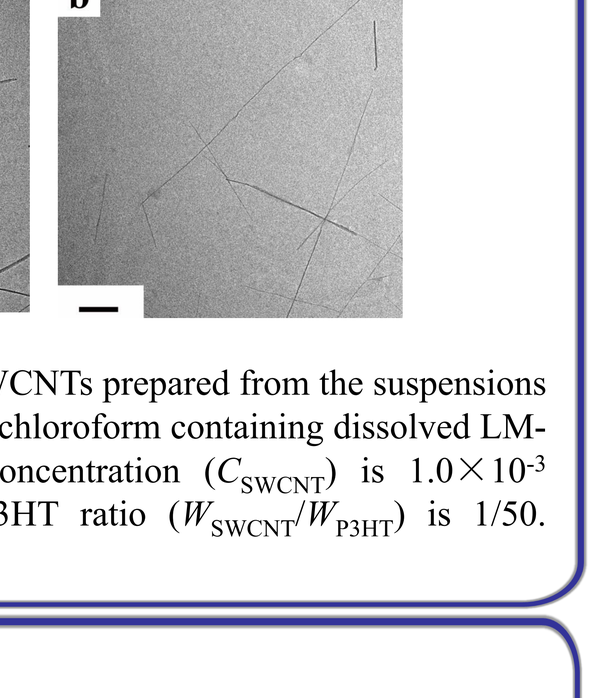
Figure 2. TEM images of SWCNTs prepared from the suspensions in neat chloroform (a) and in chloroform containing dissolved LM-P3HT (b). The SWCNT concentration (C_{SWCNT}) is 1.0×10^{-3} mg/mL and the SWCNT/P3HT ratio (W_{SWCNT}/W_{P3HT}) is 1/50. Scale bar = 200 nm.

Conclusions

1. Straightening of the bent SWCNTs was achieved by mixing with a conjugated polymer, P3HT. UV-Vis and PL spectra revealed that there was strong π-π interaction between P3HT chains and SWCNTs.

2. The straightening effect originated from the rigid P3HT chains adsorbed on the surface of SWCNTs, instead of the epitaxial P3HT crystals.

3. The straightening force exerted by P3HT chains is relatively weak and may be counteracted by entanglement and bridge among SWCNTs, which usually occurred at a high SWCNT concentration and a low SWCNT/P3HT ratio.



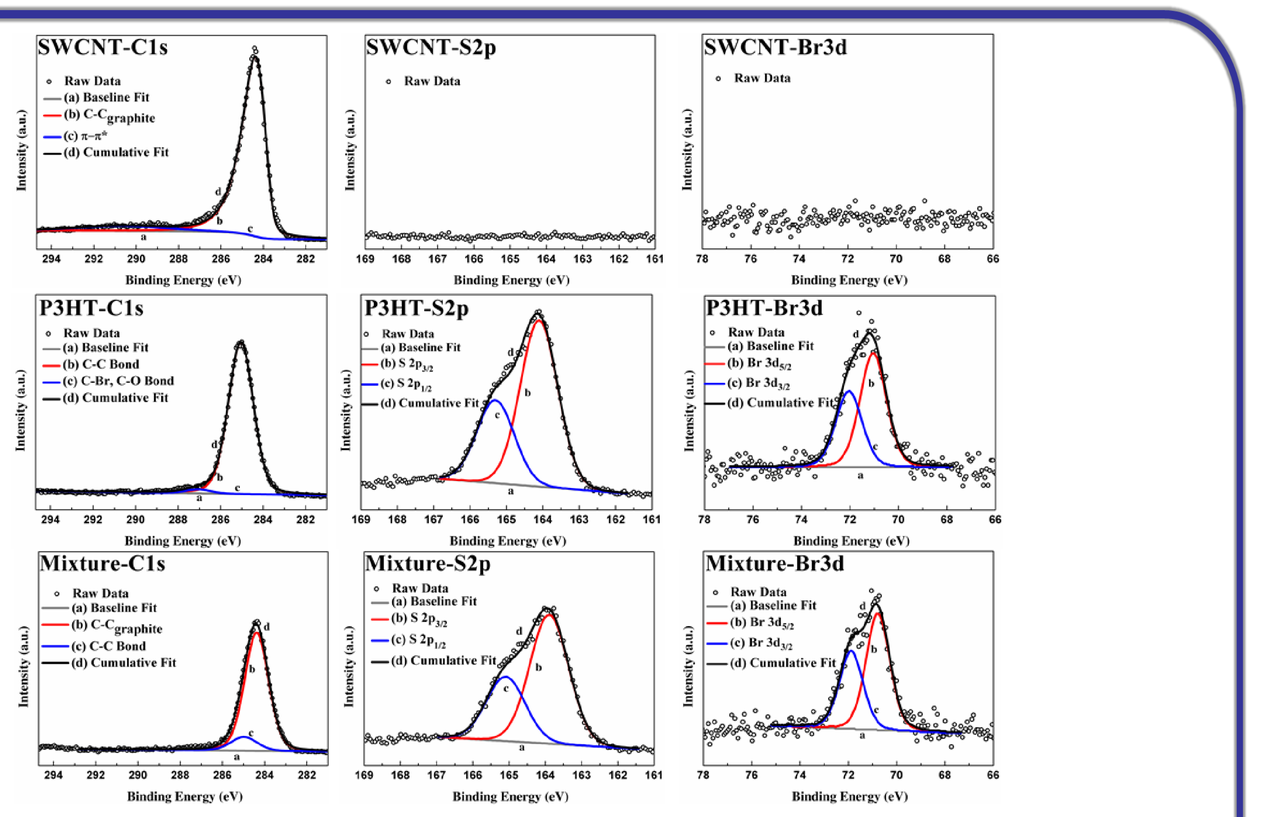


Figure 3. High resolution XPS scans for the carbon (C 1s), sulfur (S 2p), and bromine (Br 3d) signals obtained for the SWCNTs, P3HT and the composite. The S 2p peak was resolved via the Gauss-Lorentz fit-functions into a set of S 2p3/2 (164.1 eV) and S 2p1/2 (165.3 eV), accounting for the sulfur in the thiophene ring. The Br 3d peak was resolved into a set of Br 3d5/2 (70.8 eV) and Br 3d3/2 (71.9 eV), accounting for the covalently bonded C-Br end group.

Table 1. Assignments of Binding Energy (BE) and Weight Percentages of Atoms for the High-Resolution XPS Spectra of SWCNTs, P3HT and the Composite

Peak	BE/eV	at %			Entity
		SWCNT	P3HT	Mixture	
C 1s	284.4	91.4	-	85.7	C-C$_{graphite}$
	285.0	-	90.4	11.3	C-C, C-H
	287.0	-	1.2	-	C-Br, C-O
	290.6	8.6	-	-	π-π*
S 2p	163.9	-	7.9	2.6	S-C
Br 3d	70.9	-	0.5	0.4	Br-C

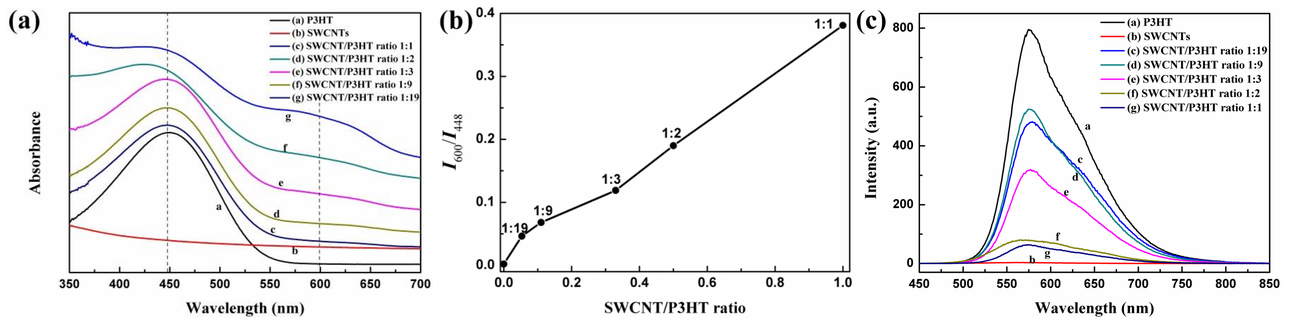


Figure 4. (a) UV-Vis spectra of the neat LM-P3HT, SWCNTs and SCWNTs/LM-P3HT mixtures with different SWCNT/P3HT ratios in chloroform. The concentration of P3HT is fixed at 0.02 mg/mL. The curves are shifted vertically for visual clarity. (b) Plot of the intensity ratio of the absorption at 600 nm over that at 448 nm (I_{600}/I_{448}) versus the SWCNT/P3HT ratio. (c) Photoluminescence spectra of the above samples used in UV.

Acknowledgement

This work was supported by National Natural Science Foundation of China (21574116) and Zhejiang Provincial Natural Science Foundation of China (LY15B040002).

References

[1] Liu, J. H.; Moo-Young, J.; McInnis, M.; Pasquinelli, M. A.; Zhai, L. *Macromolecules* **2014**, *47*, 705-712.

[2] Bernardi, M.; Giulianini, M.; Grossman, J. C. *ACS Nano* **2010**, *4*, 6599-6606.