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Supplementary Information

Coaxial Structure of Multiwall Carbon Nanotubes on

Vertically Aligned Si Nanorods and Its Intrinsic

Characteristics

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1.1 Electron energy loss spectroscopy (EELS)

Electron energy loss spectroscopy (EELS) of the Si NR/(SiO₂)/MWCNT core/multishell nanocomposites in the vicinity of the K edge are useful indicators of the density of states of unoccupied electron levels. The spectra of Figure S1 show the evolution of the π^* and σ^* features recorded point by point from across the Si NR/(SiO₂)/MWCNT core/multishell layers. The spectroscopy exhibit the peak at 281 eV and a broadened peak ranging from 298 to 306 eV, near the K-edge, are assigned to a transition to antibonding π^* orbitals and to a transition to antibonding σ^* orbitals, respectively.

1.2 X-ray photoelectron spectroscopy (XPS)

XPS represents an effective technique for surface analysis, so the compositions and chemical states of the as-synthesized Si NR/(SiO₂)/MWCNT core/multishell were characterized by XPS. The absence of peaks related to the metal catalysts used for the CNT synthesis in the XPS spectra indicated that the SiO₂ act as an efficient catalyst in this study. Figure S4 shows fine scanned XPS results of the C1s region with each sample. As seen from its general XPS spectra, the relative intensity ratio of sp² and carbon peak shift can be observed with varying reaction gas. Quantitative analysis for high resolution C1s XPS spectra through curve fitting are carried out to determine the relative percentage of sp², sp³, and etc. At the binding energy about 284.4 - 284.2 eV originated in both sp²-hybridized graphite like carbon atoms (C=C). A peak at 286 - 285.9 eV can be assigned to sp³-hybridized carbon atoms as in diamond like carbon (C-C). Other peak with higher binding energies about 287.4 - 287.3 eV correspond to carbon atoms attached to different oxygen containing moieties. With respect to the peak positions of sp² and sp³ carbon hybridization in C1s spectra of Si NR/MWCNT(7nm) core/shell nanocomposite and Si NR/SiO₂(2nm)/MWCNT(15nm) core/multishell nanocomposite, the peak positions of Si NR/MWCNT(18nm) core/shell nanocomposite and Si NR/SiO₂(10nm)/MWCNT(15nm) core/multishell nanocomposite are shifted to 284.2 eV and 285.9 eV, respectively. According to Wan et al., high residual stress would induce shift in binding energy position of sp² and sp³ hybridized carbon atoms. In MWCNTs, the sidewall curvature poses strain energy to the bonding and they can cause a shift of the binding energy to lower energy level.

XPS survey spectra of Si NR, Si NR/MWCNT(7nm), Si NR/MWCNT(18nm), Si NR/SiO₂(2nm)/MWCNT(15nm), and Si NR/SiO₂(10nm)/MWCNT(15nm) are plotted in Figure S5.

Supporting Figures



Figure S1. EELS spectra recorded point by point across a Si NR/MWCNT core/shell nanocomposite. The annular dark field image (left panel) shows where each spectra set was taken. The right panel shows the C K edges.



Figure S2. (a) element mappings of an Si NR/SiO₂ (2nm)/MWCNT(15nm) nanocomposites, (b) Si, (c) C, (d) O, respectively.



Figure S3 At the [110] zone axis, the fast Fourier-transformed electron diffraction pattern confirms the single crystalline Si with the [100] direction along the axis. The MWCNT shell consisted of crystalline graphitic layers in 0.34 nm along the NW axis, corresponds to the (002) basal plane of graphitic layers.



Figure S4. Fine-scanned XPS C1s peaks of the (a) Si NR/MWCNT(7nm) core/shell, (b) Si NR/MWCNT(18nm) core/shell, (c) Si NR/SiO₂(2nm)/MWCNT(15nm) core/multishell, and (d) Si NR/SiO₂(10nm)/MWCNT(15nm) core/multishell nanocomposites.





Figure S6. XRD data for Si NR/MWCNT core/shell. Graphite like peaks, (002) and (100), are shown.