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Insight into carbon nanotube effect on polymer molecular orientation: an infrared dichroism study

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Materials and preparations.

The MWCNTs used here are commercial Baytubes C150 P from Bayer, MaterialScience AG, produced in a high-yield catalytic process based on chemical vapor deposition (CVD). The sPS, XAREC SP130, was kindly provided by Japan Idemitsu Kosan Co. Ltd. Its syndiotacticity, [rr], is larger than 97%.

The preparation of the sPS/MWCNT composite was described in the reference of G. Sun, G. Chen**,** Z. Liu and M. Chen, *Carbon*, 2010, **48**, 1434.

The sPS/MWCNT nanocomposite or pure sPS films with thickness around 100 μm were prepared by pressing the dried samples between two laminators with 15 MPa at 300 ℃ for 10min. Then, they were quickly immersed into ice/water mixture to obtain amorphous films.

Stretching procedure.

The film samples of the sPS or sPS/MWCNT nanocomposite were first fixed using a self-made stretching instrument by the two ends. Then, it was put into a thermostat. When the temperature reached 140 ^{o}C and became stable, the film was stretched to a certain length. After the stretching, it was cooled at room temperature.

Measurements.

The infrared dichroism measurements were carried out on a Perkin-Elmer System 2000 (Perkin-Elmer Corporation) Fourier transform infrared (FTIR) spectrophotometer with a Perkin-Elmer wire grid polarizer to record the polarized FTIR spectra. For all transmission FTIR spectra, the film planes of the samples were installed perpendicular to the incident beam direction. The FTIR spectra were recorded at 2 cm^{-1} nominal resolution with an accumulation of 126 scans. Polarization of the beam was conducted by rotating the polarizer.

Calculations.

The dichroic ratios (R) were measured by $R = A_{//} / A_{\perp}$, wherein $A_{//}$ and $A_{\perp}$ represent the absorbance of a band with incident light parallel and perpendicular to the stretching direction, respectively.

The draw ratios were calculated by draw ratio = L / L_0, wherein L and L_0 stand for the lenghs between the inner two fixed ends after and before stretching, respectively.

Table 1 Infrared band assignments of MWCNTs, sPS, and sPS/MWCNT nanocomposite.

Band / cm^{-1}	Assignment
3437	Hydrogen-bonded O–H stretching of MWCNTs
3082	$\nu_{20B}(B_1)$
3061	$\nu'_{20A}(A_1)$
3026	$\nu'_2\ (A_1)$
2922	-CH_2 asymmetric stretching
2848	-CH_2 symmetric stretching
1637	-C＝O stretching of MWCNT carboxylic acid groups
1601	$\nu_9(B_1)$
1583	$\nu_{9A}(A_1)$
1493	$\nu_{19A}(A_1)$
1453	$\nu_{19}(B_1)$
1029	$\nu_{18A}(A_1)$
903	$\nu_{17B}(B_2)$
755	$\nu_{10B}(B_2)$
699	$\nu_{11}(B_2)$
539	$\nu_{6A}(A_1)$