Poly(vinyl chloride)/Multi-Walled Carbon Nanotube Nanocomposites: Effect of the Tacticity Distribution on the Polymer/Nanofiller Interface

Horacio J. Salavagione, Gary Ellis, Gerardo Martinez

Instituto de Ciencia y Tecnología de Polímeros, CSIC, Juan de la Cierva 3, 28006, Madrid, Spain

Figure S1 shows the FTIR spectra of all of KBr dispersions of all the samples over the spectral range 4000 – 400 cm\(^{-1}\). All the nanocomposite samples show a displaced baseline due to absorption of the nanotubes. This is raw data with no baseline correction employed.

In the region between 800-600 cm\(^{-1}\) the bands associated with the different conformations of the C-Cl bonds are found. The assignment of this region has been extensively discussed in the literature (see references 30-32 in the manuscript). In order to clearly identify and locate these bands we have employed both derivative spectra and band deconvolution using PeakFit v4.12 software from Jandel Scientific. Figure S2 shows an example of a spectral deconvolution performed on sample P1, employing 9 Lorentzian peaks for the C-Cl modes, and the frequencies of the bands closely correspond with the
literature values described in the manuscript. Using the P1 deconvolution as an initial model we have attempted to follow the behavior of individual peaks with specific conformational assignments. However, we were able to generate multiple solutions. We consider that the high complexity of the system makes it impossible to reliably follow the differences without imposing strict restraints in for example band position, bandwidth, intensity range, etc. that are difficult to justify.

Figure S2. Deconvolution of the FTIR spectrum of P1 in the C-Cl bond region.

Figure S3 shows high magnification SEM images of each nanocomposite. The right image clearly shows the nanotubes out of the plane of section.
The next figure (S4) shows the variation of the storage modulus with the temperature for P2, P3 and its nanocomposites with 5 wt. % of eMWNTs. The curves are represented as $T - T_g$ in order to avoid any dependence on the glass transition temperature and make the comparison between pure polymers and nanocomposites clearer.
Figure S4. Comparison of the storage modulus of PCV produced at 70 °C (P2) and 0°C (P3) with its respective nanocomposites with 5 wt. % of eMWNTs.