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Polymer dynamics and morphology in LDPE nanocomposites studied by NMR spectroscopy and relaxometry

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Low density polyethylene (LDPE) is commonly used for food packaging [1]. The addition of nano-clays often improves the mechanical, thermal and gas-barrier properties of the polymer matrix, making the composite a potentially superior industrial product.

In this work, solid state NMR spectroscopy and ^1H NMR relaxometry techniques were applied to a neat LDPE and a LDPE/montmorillonite nanocomposite sample [2] in order to investigate the effect of the filler on polymer morphology and dynamics, molecular level properties which are related to the mentioned macroscopic properties.

The studied LDPE sample showed a glass transition at -45°C and a melting point at 114°C . The analysis of ^1H low field NMR Free Induction Decays in the temperature range between 26 and 100°C allowed three components with different mobility to be identified: crystalline, amorphous, and rigid amorphous fractions. ^{13}C direct excitation NMR spectra were also recorded at room temperature to further characterize these fractions. In addition, in order to get insight into the phase heterogeneity we measured the ^1H longitudinal relaxation times in the laboratory frame (T_1) at 300 MHz and in the rotating frame ($T_{1\rho}$) using ^{13}C detection through Cross Polarization Magic Angle Spinning (CP MAS) at room temperature and performed spin diffusion experiments. Moreover, the chain segmental and collective dynamics was characterised by measuring ^1H T_1 at Larmor frequencies ranging from 10 kHz to 30 MHz, exploiting a Fast Field-Cycling NMR relaxometer in the $26\text{-}120^\circ\text{C}$ temperature interval. The results obtained for the neat polymer and the nanocomposite were compared and discussed.

References

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