## Multiscale phenomena in molecular matter



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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 <sup>1</sup>H 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 macrocroscopic properties.

The studied LDPE sample showed a glass transition at -45°C and a melting point at  $114^{\circ}$ C. The analysis of  $^{1}$ H low field NMR Free Induction Decays in the temperature range between 26 and  $100^{\circ}$ 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  $^{1}$ H 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  $^{1}$ H  $T_1$  at Larmor frequencies ranging from 10 kHz to 30 MHz, exploiting a Fast Field-Cycling NMR relaxometer in the 26-120°C temperature interval. The results obtained for the neat polymer and the nanocomposite were compared and discussed.

## References

[1] Ray, S.; Quek, S. Y.; Easteal, A.; Chen, X. D. Int. J. Food Eng. 2006, 2(4), art. 5.

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