

## Segmental Mean Square Displacement: Field-Cycling $^1\text{H}$ Relaxometry vs Neutron Scattering

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### Abstract

© 2016 American Chemical Society. Proton ( $^1\text{H}$ ) field-cycling (FC) NMR relaxometry is applied to monitor the crossover in the segmental subdiffusion from the Rouse to the constrained Rouse regime in an entangled linear polymer melt. The method probes the dispersion of the spin-lattice relaxation rate  $R_1(\omega)$ . Via Fourier transformation the segmental mean square displacement  $\langle r^2(t) \rangle$  is calculated from the intermolecular relaxation contribution  $R_{1\text{inter}}(\omega)$  to the total  $^1\text{H}$  spin-lattice relaxation dispersion  $R_1(\omega)$ . As an example we chose poly(ethylene propylene) ( $M = 200\text{k}$ ), and  $R_{1\text{inter}}(\omega)$  is singled out by performing an isotope dilution experiment. The  $\langle r^2(t) \rangle$  data obtained by FC NMR is directly compared to such of neutron scattering (NS) available from the literature. Because of different experimental time windows the NS data is converted to a reference temperature assuming frequency-temperature superposition. Absolute agreement is revealed between FC NMR and NS. The data on  $\langle r^2(t) \rangle$  confirm the predictions of the tube-reptation model; i.e., the crossover from Rouse regime to constraint Rouse regime is identified, and the tube diameter is estimated to  $d \approx (4.6 \pm 0.2)$  nm. Thus,  $^1\text{H}$  FC NMR has established itself as an alternative route to access subdiffusion.

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