Experimental report

04/09/2022

Proposal: 9-11-1947 **Council:** 10/2019

Title: Exploration and validation of random phase approximation (RPA) effects on the observed dynamical scattering from polymer mixtures.

Research area: Soft condensed matter

This proposal is a new proposal

Main proposer: Margarita KRUTEVA

Experimental team:

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Samples: (C2H4)n
(C2D4)n

Instrument	Requested days	Allocated days	From	To
IN15	6	6	14/08/2020	20/08/2020

Abstract:

The structure of polymer blends is commonly described in terms of the RPA approximation, that considers incompressibility and interactions in terms of the Chi-parameter. The dynamics of such blends also needs dynamic RPA corrections that for dynamically asymmetric systems could turn out to be very significant. Using a blend of short un-entangled polyethylene in a highly entangled matrix this proposal will demonstrate the huge distortions of the short chain dynamic structure factor by the RPA caused intermixing with the dynamics of the long chain. The proposal serves to validate a code that will allow very generally to correct for dynamic RPA effects with the perspective to become a standard correction program.

Exploration and validation of random phase approximation (RPA) effects on the observed dynamical scattering from polymer mixtures.

To test the predictions of the RPA model treatment, we conducted an experiment at the refurbished spin-echo spectrometer IN15 at the ILL, Grenoble, on short polyethylene (PE) chains in a melt of long PE-chains at different concentrations. The sample consisted of h-PE chains with about 200 monomers (Mn = 2.9 kg/mol) and a deuterated matrix polymer (d-PE) with about 2700 monomers per chain (Mn = 45 kg/mol). The volume frac- tions φ of the short chains were 0.02, 0.06, 0.12, and 0.24. Data were collected for 3 scattering angle settings corresponding to momentum transfers Q = 0.05, 0.08, 0.12 $Å^{-1}$ and covering a time range between t = 0.05 and 477 ns using neutron wavelengths of10 and 13.5 Å. The temperature was T = 509 K as in all previous NSE experiments on PE. Background scattering as measured from a sample of pure long d-PE chains has been subtracted.

The results of the experiment were published in Journal of Chemical Physics [1].

[1] Monkenbusch, M.; Kruteva, M.; Zamponi, M.; Willner, L.; Hoffman, I.; Farago, B.; Richter, D. J. Chem. Phys. 2020, 152 (5), 054901.