

Structure and dynamics of supramolecular poly(alkyl ether)-based polymers: insights from neutron scattering and complementary methods

Wednesday, 26 April 2023 16:30 (30 minutes)

In this talk, a number of key results converged from neutron scattering, rheology and dielectric relaxation spectroscopy (DRS) on the association and chain structure of supramolecular polymers from the bulk to the diluted state in the melt will be highlighted. These consist of well-defined hydrogenated (H) polymers with a polyethylene oxide (PEO) and polypropylene oxide (PPO) backbone (molar mass is 2000 g·mol⁻¹), carrying at the ends either two different hydrogen bonding (H-bonding) functional groups types (H-bond pair diaminotriazine (DAT) and thymine-1-acetic acid (THY) or homoassociative 2-ureido-4[1H]-pyrimidinone (UPY)) differing in both association pattern and strength. Small angle neutron scattering (SANS) results in the bulk reveal that while PEO and PPO functionalized with THY/DAT self-assemble as linear chains, PEO and PPO functionalized with UPY form spherical UPY clusters responsible for the physical crosslinks of the formed transient network [1,2]. Also in the bulk, a molecular view on the association lifetimes for the supramolecular PEO and PPO functionalized with the pair THY/DAT is provided by neutron spin echo spectroscopy (NSE) in combination of rheology and DRS [1]. For a better insight at a molecular level on the association dynamics of UPY based supramolecular polymers, PEO functionalized with UPY functional groups is diluted in deuterated (D) covalent short linear non-functionalized PEO chains in the melt (the non-functionalized (D) PEO chains molar mass is 500 g·mol⁻¹). It is observed that upon dilution the supramolecular PEO functionalized with UPY changes from spherical ring-like to linear conformation, which is confirmed as well by NSE and rheology analysis [3]. Ultimately, it is concluded that at sufficient dilution the structure and dynamics of supramolecular PEO polymers become independent on the H-bonding type and association strength.

[1] A. R. Brás, A. Arizaga, D. Sokolova, U. Agirre, M.T. Viciosa, A. Radulescu, S. Prévost, M. Kruteva, W. Pyckhout-Hintzen, A. M. Schmidt, *Macromolecules*, 2022, 55, 10014.

[2] A. Brás, A. Arizaga, U. Agirre, M. Dorau, J. Houston, A. Radulescu, M. Kruteva, W. Pyckhout-Hintzen, A. M. Schmidt, *Polymers* 2021, 13, 2235.

[3] A. R. Brás, R. Pasquino, T. Koukoulas, G. Tsolou, O. Holderer, A. Radulescu, J. Allgaier, V. G. Mavrantzas, W. Pyckhout-Hintzen, A. Wischniewski, D. Vlassopoulos, D. Richter *Soft Matter*, 2011, 7, 11169.

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Session Classification: Large scale structures