Nano-segregation and dynamics of ter-butanol/toluene binary liquids confined in mesoporous materials

Ramona MHANNA[1,2], Abdel Razzak ABDEL HAMID[1], Sujeet DUTTA[1], Ronan LEFORT[1], Denis MORINEAU[1], Bernhard FRICK[2], Christiane ALBA-SIMIONESCO[3], Laurence NOIREZ[3]

[1]Institute of Physics of Rennes, CNRS-University of Rennes 1, Rennes France
[2]Institut Laue-Langevin, Grenoble France
[3]Laboratoire Léon Brillouin, Saclay France

Different mesoscopic structures have been observed in binary mixtures of alcohol, often related to their incomplete mixing at the molecular level in apolar solvent or in aqueous solution. Recent neutron diffraction studies have revealed that the fully miscible ter-butanol/toluene binary mixtures form supra-molecular assemblies under confinement in the straight and mono-disperse rigid channels of mesoporous MCM-41 and SBA-15 silica molecular sieves. Indeed, systematic H/D contrast matching experiments suggest the possible formation of a surface-induced nano-segregation of the two components (core-shell structure) (Fig.1). Quasielastic neutron scattering experiments (BS and TOF) have been performed to assess the molecular dynamics of these nano-segregated mixtures, aiming to disentangle the main structural relaxation related to the 'macroscopic' glass transition from putative distinct modes arising from the different nano-segregated regions. Indeed, BS fixed window scans performed on IN16 and IN10 reveals the composition dependence of the glass transition of the confined mixture around 150 K, while at high temperature the slow dynamics of the TBA component is probed (Fig.2).

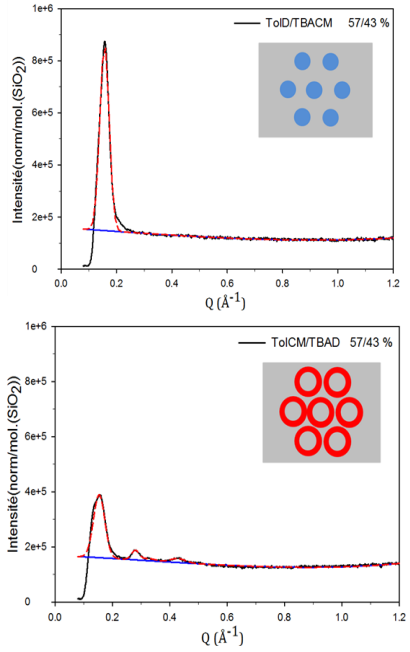

Fig.1. Neutron diffraction of TBA/TOL mixtures confined in MCM-41 with the same chemical but different isotopic compositions. The modulation of the MCM-41 Braggs peaks intensity reflects the radial nanostruturation.

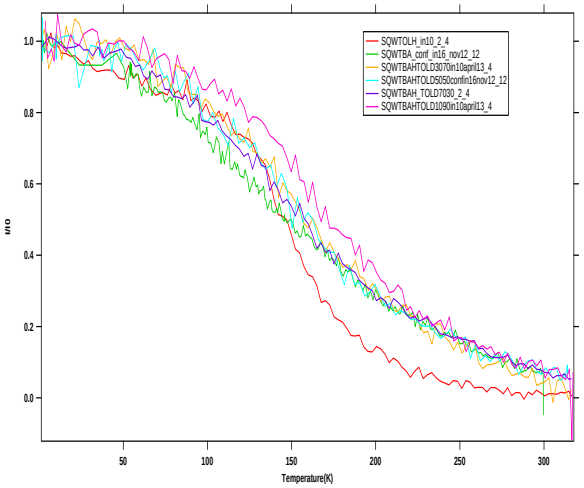

Fig.2. Fixed window elastic scans of different TBAH/TOLD mixtures confined in MCM-41.