Cellulose in fluid form: dispersions and solutions,

Webinaire du GDR DUMBIO, on 9 of December, 14:30

- broadcasted via Zoom,
- held at Laboratoire Léon Brillouin, Salle 16 or Rossat-Mignot, CEA- Paris-Saclay*.

/!\ avis de rendez-vous nécessaire sans badge d'entrée : Llb-sec@cea.fr, francois.boue@cea.fr

Cellulose is an abundant and sustainable polymer. It is mostly used in its crystalline forms, but cannot be melted, which means its processing largely depends on making it in a liquid form, followed by shaping processes. This is one of the main challenges for cellulose-based materials. Despite its polar structure, cellulose is well known to have an extremely low solubility in pure water, due to a combination of entropy, van der Waals interactions, a potential network of hydrogen bonds, and hydrophobic interactions.
Beyond the dispersion in the form of Cellulose NanoCrystals (CNC), which will be addressed here by one communication, real solutions and di or multi phasic systems will be considered, in different solvents. In such cases, a further step, to obtain a solid material, is for the cellulose to be re-crystallized ("regenerated"). The obtained properties are then closely linked to the dissolution step.

Program:

14:30, Prof. Ruigang LIU, Institute of Chemistry - Chinese Academy of Sciences

Understanding the dissolution and regeneration of cellulose in different solvents

Abstract: Cellulose is one of the abundant renewable biopolymer on the earth. The chain stereoregularity and the abundant hydroxy groups on cellulose chains lead to the strong inter- and intra-molecular hydrogen bonds, which made it difficult in processing to produce cellulose materials and chemical functionalization of cellulose. In this talk, the interactions between cellulose and solvents in direct solvent systems, including DMAc/LiCl, low temperature NaOH/urea aqueous system, and deep eutectic solvents, will be discussed. Furthermore, the regeneration process will also be discussed. The purpose of our researches is to develop the efficient approach to find new cellulose solvents and develop new platforms for cellulose processing and functionalization.

14:55 Questions

15:05 Yoshi NISHIYAMA, CERMAV, Grenoble

Water-induced crystallization and nano-scale spinodal decomposition of cellulose in NMMO and ionic liquid dope.

- *Abstract* We followed the cellulose structure formation induced by water diffusion into Lyocell dopes based on both N-Methylmorpholine N-oxide (NMMO) and 1,5-diazabicyclo[4.3.0]non-5-ene acetate ([DBNH][OAc], by using scanning simultaneous small- and wide-angle scattering (SAXS-WAXS) experiment along the diffusion gradient. In the case of the cellulose solution in NMMO monohydrate, diffraction peaks corresponding to cellulose II appeared concomitantly with the increase in small angle scattering features indicative of nanofibril formation. In the cellulose solution in the ionic liquid, an increase in small angle scattering intensity with the progression of water content appeared corresponding to a correlation length of about 40 nm, indicative of nanometric spinodal decomposition preceding the coagulation process, though no crystalline peak appeared in the wide-angle scattering.

15:25 Questions

15:35 I. Capron, BIA-INRAE, Nantes

- *Title to be announced*
- *Abstract*

15:55 Questions

16:05 Qiang ZHANG, François BOUÉ, LLB, Saclay

Cellulose in solution in Ionic Liquids: conformation and inter-chains correlations.

Abstract Ionic liquids (ILs) emerged as a non-polluting solvent that can dissolve cellulose effectively. The solvation mechanism is slightly controversial. In studies of such solutions using SAXS, in spite of low contrast and thin chain conformation giving very low intensity,

- we extracted a form factor of core-shell semiflexible chain.
- increasing concentration on a wide range (0.0005 - 0.3 g/g), we unveiled interchain effects:
- in well dissolved cases, a structure factor can be proposed for independent softly aligned cellulose chains
- at higher concentration, or in presence of a small percentage of water, a stronger scattering is observed suggesting biphasic structures, which can be useful to understand the first stages of the "regeneration"
- analysis of bacterial cellulose scattering evidences identical chain whereas aggregates additional low q scattering can be subtracted. This widens the way to neutron scattering experiments using deuteriated bacterial chains.

16:20 Questions

16:30 End of the DUMBIO seminar