COMPUTER SIMULATION STUDY OF THE DYNAMICS IN CONCENTRATED POLYMER SOLUTIONS WITH NANOFILLERS (COOPÉRATION INTERNATIONALE 2013)

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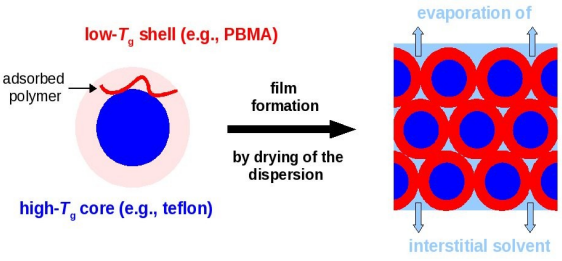
This PhD project is proposed in the framework of the IRTG "Soft Matter Science" between Freiburg and Strasbourg in collaboration with the experimental group of Prof. E. Bartsch from Freiburg (http://www.softmattergraduate.uni-freiburg.de/project/B3).

Scientific context: High-performance coatings are increasingly produced via the drying of water-based polymer ("latex") dispersions which replace polymer films from solvent-casting due to environmental reasons. An ongoing challenge in the field of latex film formation is posed by two conflicting requirements: sufficient viscoelasticity of the polymer material during film formation and high mechanical strength of the final film [1]. A recent advance has come from transferring the concept of nanofillers, i.e. reinforcing polymer films with nanoparticles, to latex films either via polymer-latex blends composed of high-T_g and low-T_g components or via core-shell polymer latexes with a high-T_g core and a low-T_g shell [2-4]. Experimental studies of such systems are performed in the group of Prof. E. Bartsch (Physical Chemistry, Freiburg) in collaboration with Y. Holl and C. Gauthier (ICS, Strasbourg). An important issue for the improvement of the film formation process is the understanding of the dynamics of the various components at different concentrations.



Outline of the PhD project: This work consists in large scale molecular dynamics simulations of multicomponent systems of nanofillers, polymer, solvent and tracer (dye) particles. The mobility of the different components shall be analyzed for different concentrations of polymer and solvent. This can build on previous work on pure polymer films and polymer-solvent systems [5,6]; the role of viscoelastic hydrodynamic interactions recently characterized for polymer melts [7] should be analyzed for the concentrated solutions with fillers. The main goal of the PhD work is to implement a data analysis as done in the forced Rayleigh scattering (FRS) performed in Freiburg and to obtain a correlation of the experimentally observed signal with a molecular picture of the dynamic processes in the film, which is lacking so far to explain the length scale dependent diffusion properties [3,4]. For this, several stays (at least 3 months) in Freiburg are planned to learn about the FRS technique and the data analysis to be implemented, and to exchange on the relative length scales involved in the problem to optimize the parameters of the simulated systems. By this collaboration between simulation and experiment we hope to improve our understanding of the diffusion processes taking place during the film formation process.

Required profile of the candidate. The candidates should have a master degree in physics (or theoretical chemistry). A specialization in polymer, condensed matter and statistical physics is highly welcome. The candidate must perform extensive computer simulations and data analysis. A disposition for numerical work and programming is required as well as a strong will to collaborate with the German partner. Proficiency in English is important.

[1] J. L. Keddie, Mater. Sci. Eng. **R21**, 101 (1997).
[2] P. A. Steward, J. Hearn, M. C. Wilkinson, Adv. Colloid Interf. Sci. 86, 195 (2000).
[3] A. Vanieminov, T. Jahr, H. Sillescu, E. Bartsch, Macromolecules **35**, 808 (2002)
[4] K.I. Suresh, A. Veniaminov, E. Bartsch, J. Polym. Sci. B **45**, 2823 (2007).
[5] S. Peter, S. Napolitano, H. Meyer, M. Wübbenhorst, J. Baschnagel, Macromolecules **41**, 7729 (2008).
[6] S. Peter, H. Meyer, J. Baschnagel, J. Chem. Phys. **131**, 014902 (2009).
[7] J. Farago, H. Meyer, A.N. Semenov, Phys. Rev. Lett. **107**, 178301 (2011).