COMPUTER SIMULATION STUDY OF THE DYNAMICS IN POLYMER LATEX FILMS WITH NANOFILLERS

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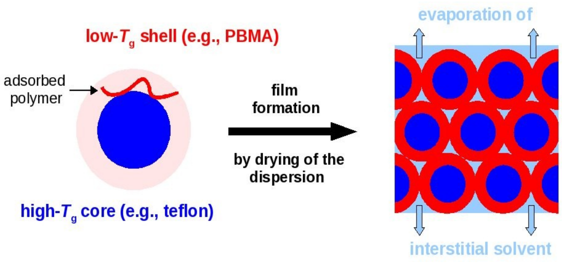
Cette thèse numérique se déroulera dans le cadre de l'IRTG “Soft Matter” Strasbourg-Freiburg en collaboration avec l'équipe expérimentale du prof. E. Bartsch.

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 solution to this problem has come from transfering 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 [2,3]. Experimental studies of such systems are performed in the group of Prof. E. Bartsch (Freiburg) in collaboration with Y. Holl and C. Gauthier (Strasbourg).

In the proposed project the film formation from core-shell latexes and the properties of the final films will be studied by a combination of tracer and polymer diffusion experiments, computer simulations of solvent and polymer motion near rigid spherical substrates, and experiments monitoring the distribution of surfactants and water during drying and in the final films as well as the mechanical properties of the films.



The work of this thesis 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 [4,5]. The main goal is to implement a data analysis in the same way as done in the forced Rayleigh scattering (FRS) technique performed in Freiburg and to obtain a correlation of the experimentally observed signal with a molecular picture of the dynamic processes in the film. In a second stage, advanced simulations techniques [6] shall be implemented to characterize the mechanical properties of multicomponent films.

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