Viscoelasticity of glassy polymer films

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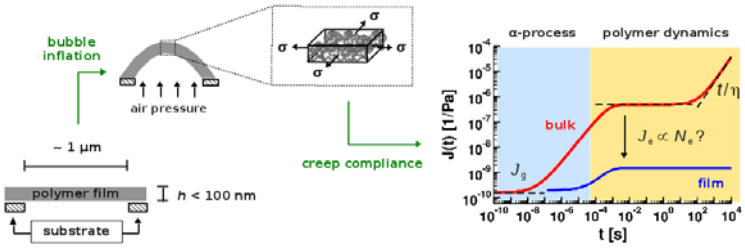
Background. One of the fundamental properties of any poylmer material is its viscoelastic behavior, i.e., the fact that the material can show a solid-like (elastic) or liquid-like (viscous) behavior, depending on the time scale probing its response. However, established methods for bulk polymers to measure the viscoelastic response cannot be applied to polymer films when the films become ultrathin, with thicknesses of 100 nm or below. New techniques adapted to the small size of the system have to be developed. One such technique is the nanobubble inflation method (see Figure on the right) [1]. This method inflates a freely standing polymer film into a bubble by a constant air pressure and infers the viscoelastic response from the creep compliance [$J(t)$], i.e., from the ratio of the measured time-dependent deformation of the film and the imposed (constant) stress. Several polymers were studied by this technique in the past and striking deviations from the bulk behavior were observed (see the pronounced reduction of $J(t)$ for the film relative to the bulk in the Figure). These observations are, however, still fairly controversial in view of other experiments [2]. This state of affairs calls for a comprehensive study of the viscoleastic behavior of nanoscopically thin polymer films.



PhD project. Here we propose such a study combining experiment and numerical modeling. The experiments will be carried out in the group of Prof. Gauthier (ICS). The here proposed complementary numerical PhD project will employ molecular dynamics (MD) simulations of model polymer films [3] to elucidate the underlying phenomena in three ways: *i*) by measuring the experimental observable, the creep compliance, through deformation of the films via a constant stress (see Figure above); *ii*) by characterizing the (linear) viscoelastic response of the films by time-dependent (equilibrium) correlation functions (exploiting the fluctuation-dissipation theorem); *iii*) by performing a "tomographic" analysis of the film, i.e., by studying the film properties locally as a function of the distance from the interfaces. It could also be envisaged to complement the MD simulations by finite-element (FE) calculations [4], which would allow to overcome the restrictions of (small) length and time scales, intrinsic to the MD approach, and so to bridge the gap between modeling and experiment. The FE simulations could be carried out in collaboration with Dr. Le Houérou (also Gauthier group).

Profile. The candidate must have a good background in statistical physics; a specialization in liquid or (soft) condensed matter physics is welcome, but not indispensable. The PhD project involves 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 experimental partner.

[1] P. A. O'Connell, G. B. McKenna, Science **238**, 1676 (2008).
[2] H. Bodiguel, C. Frétigny, Eur. Phys. J. E **19**, 185 (2006).
[3] J.-L. Barrat, J. Baschnagel, A. Lyulin, Soft Matter **6**, 3420 (2010).
[4] M. Solar, H. Meyer, C. Gauthier, O. Benzerara, R. Schirrer, J. Baschnagel, Phys. Rev. E **85**, 021808 (2012).