Study of polymer dynamics in confinement by computer simulations

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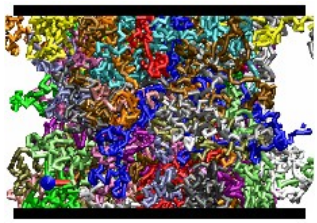
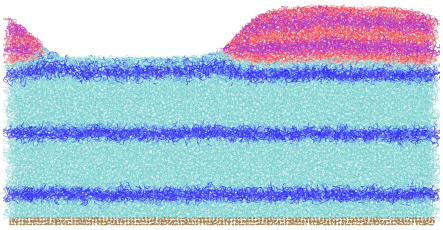
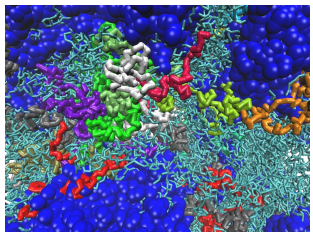
Polymers have fascinating properties because of their broad spectrum of internal relaxation modes. In a multichain system as a polymer melt, the chains couple in addition to each other. Contrary to textbook knowledge, we have recently shown that hydrodynamic interactions are not immediately screened in polymer melts, and that their combination with the viscoelastic properties of the melt can explain different regimes of anomalous center-of-mass motion of the chain [1,2]. In the present work, we want to analyse these effects for confined polymer systems and for polymer models of different rigidity. Starting from thin films confined between flat walls [3], the influence of wall rugosity should be taken into account, e.g. by grafted chains. In the following, different orientations of the thesis work are possible according to the taste of the candidate: study polymer melts confined between rough nanoparticles in the melt, or study the effect of temperature while approaching the supercooled regime [4] for these more complex confinements.

The candidate should have a good background in statistical physics and the taste of working with the computer as the main tool. Some knowledge of programming with C or Python is expected. Coarse-grained molecular dynamics simulations will be performed with the LAMMPS code, but the analysis will need reprogramming of existing tools to obtain locally resolved observables necessary for this study.

[1] J. Farago, H. Meyer, and A.N. Semenov; A*nomalous Diffusion of a Polymer Chain in an Unentangled Melt* Phys. Rev. Lett. **107** (2011) 178301. J. Farago, H. Meyer, J. Baschnagel, and A.N. Semenov; *Mode-coupling approach to polymer diffusion in an unentangled melt: II. The effect of viscoelastic hydrodynamic interactions,* Phys. Rev. E **85** (2012) 051807.
[2] A.N. Semenov and H. Meyer; *Anomalous diffusion in polymer monolayers*, Soft Matter **9** (2013) 4249.
[3] H. Meyer, T. Kreer, A. Cavallo, J.P. Wittmer, and J. Baschnagel; *On the Dynamics and Disentanglement in Thin and Two-Dimensional Polymer Films*, Eur. Phys. J. Special Topics **141** (2007) 167. Nam-Kyung Lee, D. Diddens, H. Meyer, and A. Johner; *Local chain segregation and entanglements in a confined polymer melt*, Phys. Rev. Lett. **118** (2017) 067802.
[4] S. Peter, H. Meyer, and J. Baschnagel; *Thickness-dependent reduction of the glass transition temperature in thin polymer films with a free surface*, J. Polym. Sci. B. **44** (2006) 2951.