Master 2 Matière Condensée et Nanophysique: Internship projects

Surface tension of polymer films

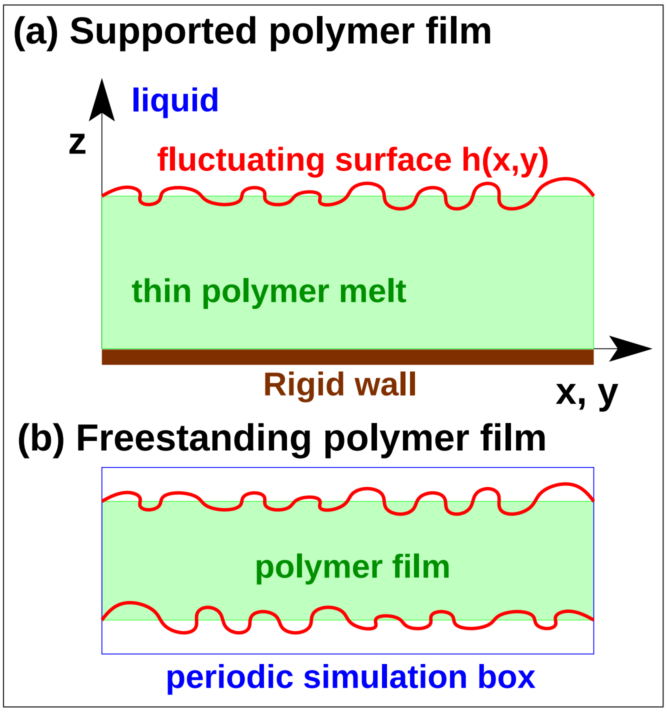
H. Meyer, O. Benzerara, J. P. Wittmer
Institut Charles Sadron, Équipe de Théorie & de Simulation des Polymères
Phone: 03 88 41 40 55, Email: joachim.wittmer@ics-cnrs.unistra.fr

Research context:

Our research group at the ICS is interested quite generally in the statistical physics of soft matter and the rheology of complex fluids with a particular emphasis on systems involving polymers [1]. Using simple coarse-grained models many fundamental and generic aspects of such systems can be investigated by means of Monte Carlo (MC) or molecular dynamics simulations [2-4]. One central research axis of the group focuses on polymer melts in strictly two dimensions and on thin films of finite width [5].

Project description:

Thin films of polymer melts may be either *supported* (adsorbed on a rigid wall) [6] or *free-standing* (confined between two free interfaces) [7] as shown in the figure. The detailed numerical characterization of the static (conformational, thermodynamic) and relaxational properties of such (often glass-like) films is currently of highest relevance for us for both physical and algorithmic-technical reasons. A key parameter for the understanding of the intricate surface processes is the surface tension γ. We remind that quite generally the surface tension is the elastic tendency of a fluid surface to acquire the least surface possible. The aim of the proposed project is to determine precisely the surface tensions of (already simulated and stored) polymer films by comparing two independent measurements.



Required tasks and workflow:

1. Get acquainted to the LAMMPS code [2];
2. Reading of existing ensemble of polymer films and small tests: center of mass of film (used as the origin of the coordinates x, y and z), average radius of gyration of chains, film thickness $\overline{h}$, total pressure tensor $\overline{P}_{\alpha\beta}$ using the Kirwood expression [3];
3. Computation of density profile $\rho(x, y)$ and from this the instantaneous film height $h(x, y)$;
4. Computation of the instantaneous local pressure tensor $P_{\alpha\beta}(z)$ comparing different operational expressions [2,3,9];
5. Fourier transforming of $h(x, y)$. Obtain γ by means of the equipartition theorem;

$$k_{\mathrm{B}}T/q^2 \left\langle |\hat{h}(\underline{q})|^2 \right\rangle \rightarrow \gamma$$

in the limit of small wavevectors q.

6. Obtain γ from the integrated difference of vertical and parallel normal pressure contributions:
$$\gamma = \int_{z=0}^{\infty} \mathrm{dz}\,[\mathrm{P_{zz}(z)} - (\mathrm{P_{xx}(z)} + \mathrm{P_{yy}(z)})/2]$$
7. Compare the precision of both methods;
8. How does γ depend on the chain length N, temperature T and on the preparation protocol ?
9. Preparation of internship report and talk.

References:

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[5] J. Baschnagel *et al.*, *Semiflexible Chains at Surfaces: Worm-Like Chains and beyond*, Polymers **8**, 286 (2016).

[6] T. Salez, E. Raphael, *La transition vitreuse aux interfaces*, Reflets de la Physique, **46**, 24 (2015).

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