

Shear-stress relaxation modulus in simulated polymer melts with connectivity altering double-bridging moves

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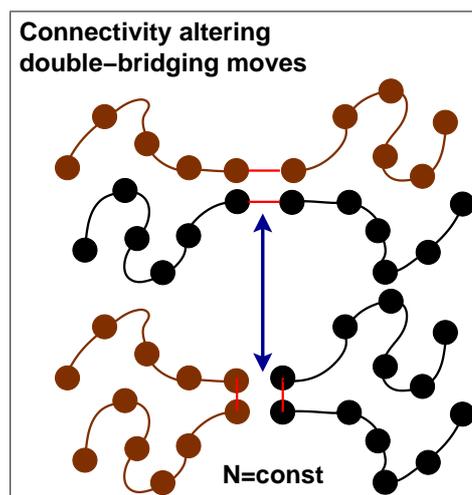


Research context:

Our research group at the ICS is interested quite generally in the statistical physics and rheology of soft matter 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]. The continued development of more efficient algorithms, especially for dense polymer systems with increasing long chains, is one of the main interests and challenges of the group [5]. A very promising algorithm in this respect is the double-bridging algorithm investigated in the presented proposal.

Project description:

Generic aspects of polymer melts [1] may be successfully modeled by means of coarse-grained bead-spring models such as the Kremer-Grest Hamiltonian [2]. Such systems can be investigated numerically by means of standard Langevin molecular dynamics or off-lattice Monte Carlos (MC) with local jump attempts [3,4]. Assuming short chains topological effects are negligible and the dynamics becomes of Rouse type [1]. The shear-stress relaxation function $G(t)$ thus decay algebraically as $G(t) \sim 1/t^{1/2}$ with time t . This should be dramatically changed if so-called double-bridging connectivity altering MC moves [5] are added with a finite frequency f . See the figure for a sketch of such MC moves.



Key question:

One expects from the stress relaxation of equilibrium polymers [6] and so-called vitrimers [7] that the shear-stress relaxation function $G(t)$ should decay strictly exponentially beyond a relaxation $t_*(f) \sim 1/f$. The aim of the proposed study is to verify this claim.

Required tasks and workflow:

1. Get acquainted with existing MC algorithm recently included into the LAMMPS framework for polymer chains with short-range interactions [3];
2. Create a small test configuration and create an ensemble of m equilibrated configurations;
3. Determine standard thermodynamic properties, such as the instantaneous stress tensor [2], and conformational properties such as the radius of gyration [1];
4. Determine the shear-stress relaxation function $G(t, f = 0)$ using the methods of Ref. [5];

5. Include connectivity altering MC double-bridging moves respecting the chain monodispersity [4];
6. Verify that all static properties remain unchanged irrespective of the frequency f of the DB MC moves;
7. Verify simple dynamical properties such as the monomer mean-square displacements. How does the diffusion coefficient increase with f ?
8. Determine the shear-stress relaxation function $G(t, f)$ for several frequencies f ; Try to understand the scaling: Does it decay exponentially as in vitrimer systems [6] ? How does the relaxation time depend on f ?
9. Preparation of internship report and talk.

References:

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