How to stabilize the diblock copolymer networks and tailor their percolation properties?

Diblock copolymer network morphology

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In Short

• Frequency-dependent Onsager coefficient – Is dynamic Self-Consistent Field Theory (SCFT) valid on short time and length scales?

• Evaporation – How does solvent evaporation influence the structure formation of mesoporous nanostructures?

• Diblock copolymer nanofibrils – Explore the morphology and transport properties of diblock copolymer nanofibrils.

• Delivering copolymers to an interface to fabricate a microemulsion – Explore the free-energy barrier of fusing a copolymer micelle with homopolymer interfaces

Scientific background – Diblock copolymers are linear, flexible macromolecules that contain two chemically distinct building blocks. Thermodynamically, the two distinct segment species tend to phase separate but the connectivity of the blocks along the macromolecular backbone prevents the formation of macroscopic domains. Instead, the different segment species arrange into a fascinating variety of periodic, spatially modulated microphases with characteristic sizes of 5-100 nanometers. These have attracted abiding technological interest because their geometry and length scale can be tailored by the macromolecular architecture. On large length scales and within a judiciously selected parameter range, copolymer materials microphase-separate into distinct network mesostructures, showing interesting application properties such as the enhanced electrical transport in copolymer morphologies that percolate.

The overarching goal of our project consists in exploring strategies for fabricating diblock copolymer network morphologies and analyzing their properties. The results will promote the understanding and application of the diblock copolymer network morphologies in modern technologies. Our project is organized into different sub-tasks, each of which focuses on a specific scientific question cf. In Short. Figure 1 exemplifies the interplay between simulation and experiments, investigating the formation of mesoporous nanostructures via a solvent-evaporation induced self-assembly process.

All sub-tasks will use highly coarse-grained models that are characterized by a small number of experimentally measurable parameters – like (i) the molecular size, quantified by the end-to-end distance, $R_e$, of the flexible, chain molecule, (ii) the incompatibility between building blocks, $\chi N$, and (iii) the invariant degree of polymerization, $\bar{N}$ that measures the square of the number of molecules in the volume $R_e^3$. This top-down modeling allows for a direct comparison with experiments.

The development of meaningful coarse-grained models in conjunction with the application of advanced computational techniques, including the Single-Chain-in-Mean-Field (SCMF) simulation algorithm, numerical Self-Consistent Field Theory (SCFT), and parallel computing allows us to address timely and ambitious research topics that involve extraordinarily big systems and long time scales. In all our projects, the systems contain in general a few millions or more soft particles (or interaction centers). The preparation, simulation, and analysis of these systems poses extreme, computational challenges.
Although a careful choice of coarse-grained models and an efficient implementation of algorithms can mitigate some of the high computational cost, the use of parallel computers is crucial for our research projects.

Computational aspects – Although our computational studies employ soft, highly coarse-grained models and advanced analysis techniques, the widespread time and length scales ranging from a highly coarse-grained segment (microsecond and nanometer) to grains of microphase-separated domains or the large distances between defects (hours and micrometers) as well as the stochastic nature of the self-assembly process or the quenched, disordered topology of polymer networks require significant computational resources. Thus the development of advanced simulation and analysis techniques as well as an efficient implementation on modern computer architectures is important. We use a spectrum of computational techniques including Single-Chain-in-Mean-Field (SCMF) simulations of soft, coarse-grained particle based models and numerical self-consistent field theory.

Here, we highlight our recent progress in SCMF simulations that exploit the scale separation between the strong, bonded forces and the weak but computationally expensive, non-bonded forces by approximating the latter ones with quasi-instantaneous fields. This results in an intrinsic, high parallelism of the simulation technique.

Our SCMF code is written in c99 utilizing OpenMP (shared memory), MPI (multiple-nodes) and the HDF5 library (parallel MPI/IO for initialization and analysis) for different layers of parallelism. Each MPI-rank handles a number of independent polymers, which are propagated in time with OpenMP acceleration. If the MPI-rank in heterogeneous con-

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**Figure 2:** Strong scaling performance of our implementation measured in Million Particle monte-carlo Time-steps Per Second (MPTPS). Error bars have been obtained from multiple runs.

**WWW**
http://www.theorie.physik.uni-goettingen.de/forschung/mm/

**More Information**

**Project Partners**
Soft Matter/Biophysics, University of Göttingen

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