Simulation and experimental study of block copolymers self-assembling under spherical confinement

A relatively new, but conceptually simple experimental procedure makes it possible to form spherically confined nano-particles out of block copolymers by a clever evaporation of mixed good and bad solvent for the polymers. A new simulation setup allows to simulate such spherically confined systems of arbitrary mixtures of block copolymers which reproduce existing experimental results for diblock copolymers. In this project the idea is to investigate the effect of confinement on new metal containing diblocks and/or ABC star polymeric systems which in the melt state form many complex structures already.

Prerequisites:

✓ Basic lab experience

As a student you will:

✓ prepare block copolymer nanoparticles at DTU Nanotech ✓ do simulations as in the figure using Dissipative Particle Dynamics ✓ do structural analysis of particles: scattering and electron microscopy ✓ invent new relevant computational analysis methods? ✓ learn about polymer physics/chemistry and complex self-assembly

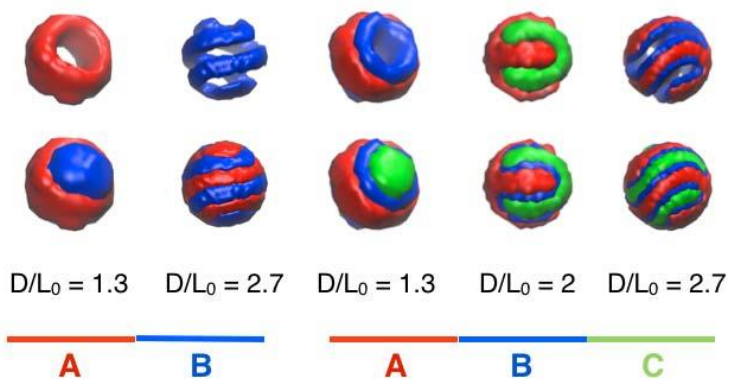

Figure: Simulation results from spherically confined linear AB diblocks and ABC triblocks as a function of the D/L_0 ratio, where D and L_0 correspond to the particle diameter and the period of lamellar structure in the films, respectively.

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Reference: Kirkensgaard, JJK, Soft Matter, 2010, DOI: 10.1039/c0sm00358a