P.41 Dynamical Landau theory for the assembly and disassembly kinetics of supramolecular polymers

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Theoretical studies of the kinetics of supramolecular self-assembly are in general based on reaction-rate master equations, which are usually nonlinear and very difficult to solve analytically.

Hence, we attempt to describe these processes in a different way using only two moments of the full distribution of sizes of the assemblies.

For co-operative self-assembly these moments show very large yet not quite diverging susceptibilities, allowing us to write down a Landau-type free energy function satisfying conditions obtained from equilibrium statistical mechanics of self-assembled supramolecules. This free energy function then naturally leads us to evolution equations for the relevant order parameters, which are the two relevant moments of full distribution being the average degree of polymerization and the fraction of active material accounting for nucleated self-assembly.

Solving these differential equations, we are able to describe experimentally observed phenomena, including as overshooting, hysteresis and a lag time to assembly.