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Structuring of polymer gels via catalytic reactions

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Certain biopolymers transform into a gel because of a catalytic reaction in which freely moving catalysts, called enzymes, convert repulsive monomers of the polymers into attractive ones. These attractive monomers stick to each other and make that the polymer sol slowly transforms into a gel. Important examples for such systems occur in plant cell walls where some polysaccharides (pectins) undergo gelation due to the presence of an enzyme (pectin methylesterase) [1].

We have developed a simple model (bead-spring polymers+soft particles) that can serve to describe such systems. Using large scale computer simulations we study how the polymer sol ($t_B = 0$ in Fig. 1) becomes unstable due to the increasing fraction of attractive monomers and transforms at high temperatures into a dense liquid (i.e. phase separation, $t_B \approx 7.10^4$) or into a gel at low temperatures ($t_B \approx 3.10^3$).

We find that before the system reaches at long times one of these two phases, it forms at intermediate times a rather regular cluster phase ($t_B \approx 10^2$). We rationalize this finding by a competition between two mechanisms: Nucleation of the attractive particles to form clusters and the slow relaxation dynamics of the coarsening of the polymer sol. We show that the temperature dependence of the time scale of these two processes can be understood semi-quantitatively from the bare potential between the constituent particles, i.e., monomers and catalysts, which governs the reactions. Finally we discuss how this cluster phase can be stabilized, thus giving rise to a gel with a non-trivial internal structure.

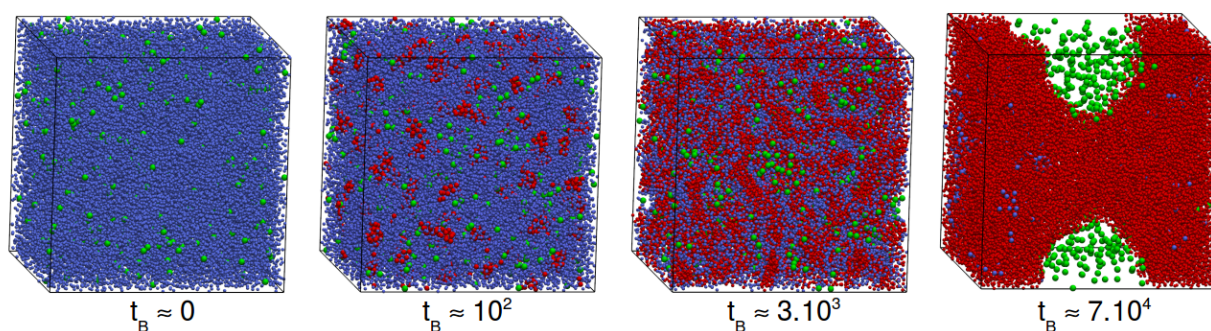


Fig. 1: Time evolution of the polymer structure
 (catalysts: green beads; repulsive monomers: blue beads; attractive monomers: red beads)

[1]. D.J. Cosgrove, *Nature Rev. Mol. Cell. Biol.* **2005**, 6, 850-861.