



HAL
open science

Cluster Phase in enzyme-induced Gelation of Polymers

Virginie Hugouvieux, Walter Kob

► **To cite this version:**

Virginie Hugouvieux, Walter Kob. Cluster Phase in enzyme-induced Gelation of Polymers. International soft matter conference (ISMC), Sep 2016, Grenoble, France. hal-01837806

HAL Id: hal-01837806

<https://hal.science/hal-01837806>

Submitted on 5 Jun 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Cluster Phase in enzyme-induced Gelation of Polymers

Virginie Hugouvieux^a and Walter Kob^b

^a SPO, INRA, Montpellier SupAgro, Université Montpellier, 34060 Montpellier, France

^b Laboratoire Charles Coulomb, CNRS, Université Montpellier, 34095 Montpellier, France

* Corresponding author: virginie.hugouvieux@supagro.inra.fr

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 becomes unstable due to the increasing fraction of attractive monomers and transforms at high temperatures into a dense liquid (i.e. phase separation) or into a gel at low temperatures. 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. 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.

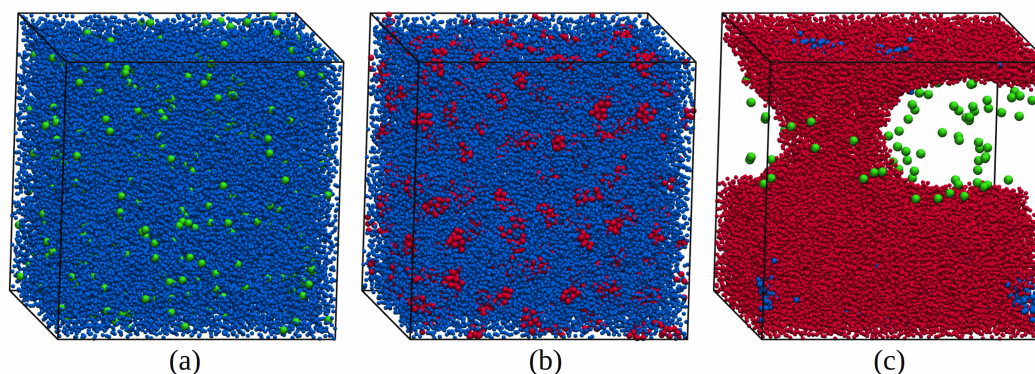


Figure: Typical evolution of the system from (a) a homogeneous solution of enzymes (green) and repulsive (blue) homopolymers, to (b) a gel containing clusters of attractive (red) monomers (enzymes not shown), and (c) a macroscopic phase separation.