Shear effects in the induction of the kinetic phase transformations in depletion driven colloids

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The general problem of how a dispersed phase, such as colloids in solution, come together when destabilized to form a condensed phase, like gels or crystalline solids, is of fundamental importance to control the assembly of the dispersed phase into a useful material. Colloidal solutions can display a rich series of phase transitions that are controlled by the interacting potential between the dispersed components and the kinetics of the phase transformation. Recent Brownian dynamics simulations¹ of a 2D model of polymer depletion-driven colloids have shown a transition from a dispersed colloidal phase to a coexistence of dispersed-phase and solid-phase for increasing depth of the depletion potential well. Near the transition point the formation of clusters with a round shape is observed. As the well depth is increased further, elongated clusters first, and then fractal aggregates are obtained. The effect of shear in crystal nucleation has been considered quite recently, however, while some authors predict a shear-induced ordering of the liquid which enhances the nucleation rate²⁻⁴, others predict that shear induces the suppression of crystallization⁵⁻⁷, even at very low shear rates.

In this study, we shall present extensive 2D Brownian Dynamics computer simulations to characterize the effect of shear on the nucleation and crystal growth in two different kinds of colloidal systems: a repulsive-stabilized dense suspension modeled by a Yukawa repulsive pair potential, and a polymer depletion-driven system modeled by an attractive Asakura-Oosawa potential. In both systems, it has been found that small and moderate shear rates do not affect crystall growth (the transition takes place at the same critical value of the potential depth), however, for shallow quenches in the two phase region, low shear rates are observed to speed up the process of nucleation, whereas large shear rates produce the opposite effect. In the limit of very large shear rates the system virtually reverts into a single phase. We provide a plausible explanation for the dual nature of shear during the aggregation process: the weakening of the effective interaction among particles due to the shear compete with the induction of an extra flux of matter that increases the frequency of collisions that contributes to speed up the aggregation process.

Figura 1. Nucleation proceeds from round shaped clusters (a) to fractal structures (b) for increasing potential depth. Hexagonals crystalline ordering is found at small scales

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