Dynamic Monte Carlo simulations of nanocubes in an electric field: Structure, dynamics and rheology of an electrorheological fluid.

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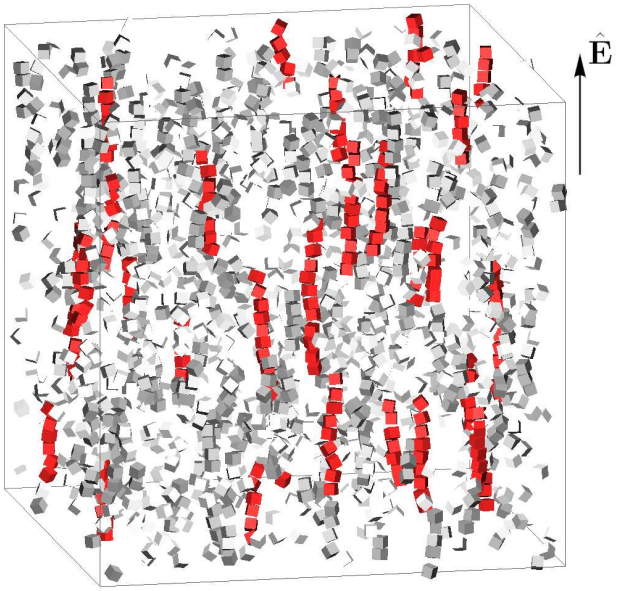

Fig. 1. Snapshot of an equilibrated suspension of cubic particles under the application of an external electric field $\hat{\mathbf{E}}$. Red particles belong to chains made of at least 6 cubes. Arrow on the top right indicates the orientation of the external field.

Colloids are biphasic systems comprising a dispersed phase and a dispersing medium. The former can consist of solid particles, liquid droplets or gas bubbles, whose size is generally between a few nanometers and a few microns. If the dispersed phase comprises solid particles and the dispersing medium is a liquid, these systems are referred to as colloidal suspensions or simply sols. Sols are especially relevant in formulation science as they form the basis for a number of products of daily usage, including detergents, paints, coatings and foods.

The phase behaviour of colloids can be altered by very mild energy changes of the order of thermal fluctuations, namely few k_BT per particle, where k_B is the Boltzmann constant and T the absolute temperature. When an external electric field is applied to a sol, the colloidal particles are polarised due to a difference in permittivity between the dispersed phase and the surrounding medium. The induced dipoles generated by external fields enhance particles attraction, which cause microscopic reorganization of the dispersed phase and the formation of oriented string-like clusters or chains. These chains, whose length strongly depends on the intensity of the applied field, have been observed in suspensions of both spherical [1] and anisotropic dielectric particles [2]. Such a directed self-assembly has relevant consequences in the rheological properties of the entire suspension. Under some specific conditions, where volume fraction, dielectric properties and field intensity play a crucial role, the viscosity of the colloidal suspension can change drastically with the overall system behaving like a Bingham plastic [3]. These very intriguing electrorheological (ER) fluids are especially attractive in technology applications where controlling viscosity is especially relevant, such as in vibration suppression and motion control of vehicles.

In this work, we report on Dynamic Monte Carlo simulations of ER colloidal suspensions of polarisable nanocubes and investigate the kinetics of formation of chain-like clusters. Our interest is estimating the response time of chain formation upon switching the field on and chain disruption upon switching the field off. Additionally, we investigate the main structural properties of the chains that are formed and how they influence the viscoelastic response of the system. More specifically, we apply passive microrheology [4] to compute the viscous and elastic moduli along the direction of the field and perpendicularly to it. Our results clarify the role of chains in determining a change in viscosity and open up a path to evaluate the viscoelastic response of ER fluids by applying efficient simulation methods.

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