Multiscale models of liquid crystals dispersions of nanoparticles

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Suspension of nanoparticles in liquid crystals have been modelled on a range of scales, from molecular simulations[1] to macroscopic models[2]. The former are computationally expensive and only a few particles can be modelled. The second rely on macroscopic parameters whose values are not determined self-consistently.

Here we use homogenization theory[3] to bridge the microscopic and macroscopic scales. This method captures the underlying microscopic geometry through a series of representative cell problems derived from the underlying liquid crystal equations. These describe the local effect of a single nanoparticle on the liquid crystal alignment based on the assumption that the nanoparticles are evenly distributed and, hence, the underlying geometry is approximately periodic. By combining the results from the cell problem with the underlying microscopic equations and averaging we obtain a set of approximate macroscopic equations.

We consider two regimes of nanoparticle–liquid crystal interaction, strong and weak. In the former, characterised by high nanoparticle density and/or large anchoring energy at their surface, the nanoparticles are the dominant factor in determining the alignment of the liquid crystal.

In the weakly interacting regime, i.e. small anchoring energy and/or low concentrations, the liquid crystal director is determined by a balance between the bulk forces in the liquid crystal and the alignment at the boundary of the device and at the nanoparticles. In this regime, the macroscopic equations for the director alignment contain two key differences with respect to those for a pure liquid crystal: (i) the elastic constants are in general smaller, and (ii) there is a forcing term proportional to the anisotropy of the particles. Figure 1 shows the effect of the anisotropy on the Frederiks threshold for a 2D planar cell with elliptical nanoparticles of aspect ratio 3. As the particles are rotated with respect to the cell boundary the Frederiks threshold is shifted: even though the reduction in the elastic constant tends naturally to reduce the value of the threshold, the forcing term induced by the anisotropy of the particles can ultimately increase its value and make it larger than for a pure liquid crystal.

We discuss the derivation of these equations and the validity of the assumptions. Finally we compare the different macroscopic properties observed in the two different cases and how these equations can be used to model liquid crystal-nanoparticle suspensions capturing both the micro and macroscopic scales.

References:

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