Abstract

Using molecular dynamics (MD) we study interactions between elongated colloidal particles aligned to aspect ratio $>1$ in a nematic host. Our simulations show that, for small colloidal particles, depletion interactions are dominating. We measure elastic contributions to the interaction, which deviation from the quadrupolar at small separations. MD simulation results are then compared to the results of the minimization of the Landau-de Gennes elastic free energy.

What are nematic colloids?

If particles of a host fluid have anisotropic shape and are, on average, elongated along some axis (called a director), then the host liquid has long-range orientational ordering. Translational ordering is still short-ranged (i.e. it is still a liquid, not a solid). In this case the host liquid forms a nematic phase and we call the colloidal system a liquid crystal colloid (see Fig. 1).

What differs liquid crystal colloids from usual colloidal systems? Why do we consider them separately from ordinary colloids? There are several reasons for doing this.

Long-range elastic forces

Orientational ordering of liquid crystals is long-ranged. If we distort average molecular orientation (the director) then this distortion vanishes on the scale much larger than the molecular scale. The order parameter map shows that the core region is elongated and the region occupied by the disclination core is quite large (Fig. 4).

Topological defects

Director field is a vector field. Colloidal particles provide some orientation of the director at the particle surface. Sufficiently strong homotopic anchoring (that is, normal to the particle surface) induces a radial point (hedgehog) defect with topological charge +1. If the director field is uniform far from the particle, i.e. the total topological charge of the whole system is zero, then an additional defect must be created to compensate the radial hedgehog.

Saturn ring defect

For all studied radii ($R = 3-15$) the ring defect appears immediately after equilibration of the system starting from the isotropic phase (Fig. 3). This type of the defect is energetically more favorable for the chosen (small) depletion force.

The ring defect does not have very long director distortions. Its core region is located very close to the droplet surface and the director distortion vanishes very quickly in the liquid crystal bulk (Fig. 3). This is in agreement with quadrupolar nature of the defect. This type of the defect can be studied using comparatively small number of particles.

Satellite (dipole)

In case of satellite defect director distortion extends much further than that of the ring defect (Fig. 4). This reflects the dipolar symmetry of the director distribution. Therefore, to study satellite defect, one needs very large systems. Another reason for using such a big system is that satellite defect is stable only for large particles (Fig. 5).

The order-parameter map shows that the core region is elongated and the region occupied by the disclination core is quite large (Fig. 4).

Elongated particles

For elongated colloidal particles the director distribution is not axially symmetric. As rod rotates, the director field becomes less and less frustrated and finally we have a stable orientation of the rod perpendicular to the director (Fig. 6).

Molecular model

Host liquid (nematic liquid crystal) was modelled as a sea of ellipsoids interacting through the soft repulsive potential. For a given temperature ($T = 1.5$ in dimensionless units) this can be thought as harmonious $\varepsilon = 5$.

The interaction of molecules with colloidal particles and walls was given through the so-called force per particle acting on the particle. Due to long-range director distortions around the colloidal particles we used systems of 8,000 - 12,000 particles.

Acknowledgements

D.A. is grateful to the Alexander von Humboldt foundation.

Interaction between elongated particles

We consider interaction of two long rods aligned perpendicular to the director and parallel to each other (Fig. 8). The defect configuration is known: each particle has two 1/2, 3/2 disclinations lines. Therefore, we expect quadrupolar interaction between the particles.

Conclusions

Spherical particles

- Two types of defects: satellite of strength $-1$ and Saturn ring of strength $-1/2$.
- Complex defect core structure (blurred with density modulation).

Elongated particles

- Orient perpendicular to the director.
- Two $-1/2$ strength defect lines.
- Nonlinear effects (change in the position of defects) for small separations influence inter-particle interaction.
- Depletion interaction dominates for the MD accessible particle sizes.

References