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Bifurcation analysis and multiscale modelling of a bistable liquid crystal device

Martin Robinson*

martin.robinson@maths.ox.ac.uk;martinjrobins@gmail.com

We simulate a square planar bistable liquid crystal device, reported in Tsakonas *et al.* [Appl. Phys. Lett. **90**, 111913 (2007)], using three different modelling frameworks each aimed at probing the material at different length scales. At the microscale we use an off-lattice model comprising individual elliptical particles interacting via either a hard-sphere (HS) or Gay-Berne (GB) potential. This is compared with a mesoscale on-lattice model using the Lebwohl—Lasher (LL) potential, as well as a macroscale PDE model using the Landau-de Gennes (LdG) theory for nematic liquid crystals. In each case, we propose a Dirichlet boundary condition that mimics the experimentally imposed tangent boundary conditions.

Each of the three model types provide different and complimentary data analysis. In general we obtain six different classes of equilibrium profiles and these profiles are classified as diagonal or rotated solutions, with defects in each corner of the square domain. We report on the effect of temperature and device size on these solutions and show that the lack of rotated solutions in the microscopic models (HS and GB) can be explained by unstable rotated solutions at small device sizes. We compare the defect structure from the microscopic HS and GB models to that obtained from the LL and LdG models. From the LdG model we calculate the bifurcations that lead from the single solution at small device sizes to the six stable solutions, and more than 80 unstable solutions, at larger sizes.

This is joint work with Radek Erban (Mathematical Institute, University of Oxford, United Kingdom) and Apala Majumdar (Department of Mathematical Sciences, University of Bath, United Kingdom).

*OCCAM, Mathematical Institute, University of Oxford, 24–29 St Giles', Oxford, OX1 3LB, UNITED KINGDOM.