Formation and Dynamics of Smectic-A Liquid Crystals

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Over the past several decades many disruptive technological advancements have been enabled through applications of liquid crystals. The majority of these applications utilize nematic liquid crystals (NLCs), which have some degree of orientational order. Continuing this technological trend requires an increased understanding of LC properties and, ideally, the ability to predict and control them to achieve desired device function. In our work, simulation-based approaches are pursued to enable new classes of LC devices. High-order smectic liquid crystals (SLCs), which exhibit translational in addition to orientational order, are targeted in that they present additional challenges compared to NLCs.

Simulations of the isotropic/smectic-A transition using a high-order phenomenological Landau-de Gennes (LdG) model [1] will be presented. This model includes energetic couplings of nematic and smectic order; both bulk order and coupling of the nematic director and smectic wave vector. Simulation results show consistent agreement with experimental observations while providing new insights into nanoscale SLC phenomena. Simulations capture the formation and dynamics of "giant" dislocations [2] and the delicate balance between orientational and translational order in the vicinity of defects.

Finally, simulation results of SLC domains in shallow undercooling conditions are shown using a non-isothermal extension to the LdG model [3]. This extended model correctly predicts diffusion-limited growth kinetics and novel nonmonotonic growth kinetics in regimes where orientational (nematic) pre-ordering present [4].

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