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Simulation of Spherulite Growth Using a Comprehensive Approach to Modeling the First-Order Isotropic/Smectic-A Mesophase Transition

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Abstract. A comprehensive modeling and simulation study of the first-order isotropic/smectic-A transition is presented and applied to phase diagram computation and two-dimensional spherulite growth. An approach based on nonlinear optimization, that incorporates experimental data (from 12CB, dodecyl-cyanobiphenyl), is used to determine physically realistic model parameters. These parameters are then used in conjunction with an optimized phase diagram computation method. Additionally, a time-dependent formulation is presented and applied to the study of two-dimensional smectic-A spherulite growth. These results show the growth kinetics and defect dynamics of nanoscale smectic-A spherulite growth in an isotropic phase with an initially radial layer configuration.

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1 Introduction

Liquid crystallinity and other forms of self-organization are key phenomena both technologically and in Nature. Liquid crystalline order ranges from liquids that show some degree of orientational order to those that, in addition, show various types of translational order. The myriad of types of material that exhibit this behavior range from traditional low molecular mass molecules, currently used in display technology, to biological membranes composed of phospholipids [1]. To date, the main focus of liquid crystal research has been on the simplest class of mesophases where some degree of orientational order is

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present: the nematics. Research on mesophases that also show a degree of translational order, including smectics and columnar liquid crystals, has been less abundant. Recognizing the increasing importance of these mesophases, particularly in biological systems, there is a need for practical methods to access the time and length scales at which these phenomena occur.

Experimental work in this general field has made great progress in the basic understanding of translationally ordered liquid crystals [2–6]. Nonetheless, it is currently infeasible to access much of the dynamic phenomena of translational phase-ordering processes. Recent experimental work has begun to address these issues [4,5], but theoretical approaches are currently the only way to access the length scales (nanometers) and time scales (nanoseconds) at which liquid crystal dynamics occur. The use of high-order models in conjunction with advanced numerical simulation techniques has shown a great deal of promise for theoretical study [7–10]. Recent computational advances have allowed for the possibility of simulation in greater detail than ever before.

Utilizing a high-order Landau-de Gennes model of the first-order isotropic/smectic-A mesophase transition [7,11], the objectives of this work are:

- to present a comprehensive approach to modeling and simulation of the first-order isotropic/smectic-A transition.
- to determine phenomenological model parameters through incorporation of experimental data (from 12CB, dodecyl-cyanobiphenyl).
- to efficiently compute the phase diagram predicted by the model and parameter set.
- to study the two-dimensional growth kinetics and defect dynamics of an initially radial textured smectic-A spherulite in an isotropic matrix.

This approach builds upon previous work [12], which incorporates experimental data into the phenomenological model and derives equations for phase diagram computation. A time-dependent formulation [9,10] and the nano-scale growth of an initially radial spherulite are presented. This work is organized as follows: a brief background on relevant types of liquid crystalline order is given (Section 2.1), the model and simulation approach are explained (Sections 2.3-2.6), and simulation results are presented and discussed (Section 3).

2 Background and theory

2.1 Liquid crystalline order

Liquid crystalline phases or mesophases are materials which exhibit partial orientational, or in addition translational order. They are composed of anisotropic molecules which can be disc-like (discotic) or rod-like (calamitic) in shape. Thermotropic liquid crystals are typically pure-component compounds that exhibit mesophase ordering most greatly in response to temperature changes. Lyotropic liquid crystals are mixtures of mesogens