Computer Simulation of Nematic Liquid Crystals formed by Monoclinic Molecules

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In recent years, the thermotropic biaxial nematic phase has been claimed to have been observed in experimental studies [1], following its prediction made more than 40 years ago by Freiser [2]. In addition to scholarly interest, the biaxial nematic phase has the potential for applications in fast switching devices [3, 4] compared to those created from the conventional twisted nematic and ferroelectric smectic liquid crystal materials. These new applications are, in turn, expected to encourage further developments of the theory as well as of the molecular models studied by computer simulation.

For example, the original prediction by Freiser [2] attributed, albeit implicitly, a D_{2h} point group symmetry to the biaxial nematic phase, in keeping with the assumed molecular symmetry. However, it has long been recognized that the molecules forming calamitic liquid crystals have a lower symmetry than this. One consequence is that, in addition, to the biaxial nematic phase with D_{2h} symmetry we might also expect to find phases with C_{2h} and C_i symmetry exhibited by the same liquid crystal [5, 6]. In order to investigate the phase behaviour of molecules with low symmetry a system of molecules with C_{2h}, or monoclinic, point group symmetry has been investigated using molecular field theory based on a truncated potential of mean torque [7] which is an extension to that for molecules with D_{2h} point group symmetry [8]. This proves to exhibit a rich and intriguing phase behaviour.

We have investigated this low symmetry truncated model more rigorously by using Monte Carlo simulations based on an analogous pair potential. These simulations pose a number of challenging problems. These include the introduction of MC-moves to facilitate the transition between the C_{2h} and D_{2h} biaxial nematics and the identification of the biaxial nematic phase with C_{2h} symmetry especially as only one director is uniquely defined for this phase. Ways of addressing these problems have been developed. For example, the phase identification is based on the invariants defining orientational correlation functions and so independent of the location of the directors. Knowledge of these has allowed us to confirm the novel methodology used to determine the order parameter needed to characterize the biaxial nematic with C_{2h} point group symmetry. Our simulations have confirmed the predictions of the molecular field theory [7] and have shown that in the two orthorhombic biaxial nematics molecules are arranged in clusters with their symmetry axes parallel.

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