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Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics

Publication details, including instructions for authors and subscription information:
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Version of record first published: 13 Dec 2006.

To cite this article: D. J. Reynolds , A. Hoare & M. C. Holmes (1987): A Monte-Carlo Study of a System of Anisometrically Interacting Particles, Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 152:1, 113-119

To link to this article: http://dx.doi.org/10.1080/00268948708070946

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Mol. Cryst. Liq. Cryst., 1987, Vol. 152 pp. 113-119
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A MONTE-CARLO STUDY OF A SYSTEM OF ANISOMETRICALLY INTERACTING PARTICLES

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Abstract We report preliminary results of a three dimensional Monte-Carlo study of a system of anisometrically interacting particles possessing both translational and orientational freedom. A simple interaction potential has been used to generate equilibrium values for the translational order parameter in addition to the long and short range orientational order parameters.

INTRODUCTION

In order to evaluate the thermodynamic parameters of a complex system such as a liquid crystal it is necessary either to resort to approximate analytical theories or to use computer simulation.

The use of Monte-Carlo techniques to investigate systems of anisometric particles is not new and has successfully been carried out in the past by the use of lattice site models in which the particles are allowed only orientational freedom[1]. Whilst these are effective at evaluating the long and short range orientational order parameters they are unable to offer any information on the translational behaviour of such a system. A three dimensional model offering both orientational and translational freedom to a fluid of thin hard discs has bee used[2] but only the orientational behaviour of the system was examined.

Current ideas of the smectic-nematic transition require that the significant translational order of the smectic phase

must vanish when the nematic is entered. Therefore any proposed model must satisfy this criteria in order to be successful.

The purpose of this paper is to report the preliminary results of a computer simulation of one thousand anisometric particles possessing both translational and orientational freedom interacting via a simple interaction. In addition to the orientational order parameter the translational order parameter has been evaluated.

THEORY

In this simulation the method of Metropolis et al[3] is used. This method involves the use of random numbers to generate changes in particle parameters, once a particle has randomly changed its configuration the new energy of the system is calculated. If the energy is lowered then the move is accepted otherwise it is subject to a Boltzmann energy criteria:

$$P(x)=A\exp(-B(Uf-Ui))$$

where $P(x)$ is the probability of move acceptance,

Uf is the energy of the final state,

Ui is the energy of the initial state,

B has its usual meaning

A is a normalising constant

In practice this is achieved by comparison of $P(x)$ with a random number between zero and unity.

The potential chosen to represent the particle interaction is of the type used by McMillan in his mean field approach[4]:

$$E_{i,j} = f(r_{i,j})(P2(\cos\theta_{i,j})-d)$$

where $E_{i,j}$ is the pair potential between the particles,

$r_{i,j}$ is the centre to centre distance,

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d is an interaction constant for the scalar interaction

$\theta_{i,j}$ is the angle between the principle axes of the ellipsoids.

The form of f(r) chosen was C/r, this is because it is simplest form of distance dependence that has the desired property of decrease with increasing r.

A spherical excluded volume has been used so far because it is the simplest ellipsoid and it is intended to use ellipsoids to approximate both rods and discs in a study of the effect of shape.

To characterise the behaviour of the system we use three order parameters: the short range orientational order parameter, <P2>, which is merely the local average of $P2(\cos\theta_i)$; the long range orientational order parameter, S, is merely the average of the local directors; and the translational order parameter, T, is given by the expression below:

$$T=\langle\cos(2\pi z/d)\rangle$$

where z is the distance along the z axis (parallel to n)

d is the statistical average layer repeat unit.

Experimental and Results

Initially it was decided to set both the excluded volume and the scalar component of the interaction potential to zero and using an arbitrary interaction constant of C=50.0 investigate the behaviour of the order parameters with temperature. It can be seen from Figure 1. that the long range orientational order parameter decreases slowly at low temperature and exhibits a sharp transition to an isotropic phase with S<0.1 at 10KT. The short range orientational order parameter shows a sigmoid behaviour associated with the transition reaching a plateau value of ~0.35 in the

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isotropic phase. This plateau value indicates that considerable short range correlation exists in the isotropic phase.

The translational order parameter does not exhibit and temperature dependence remains constant at 0.03.

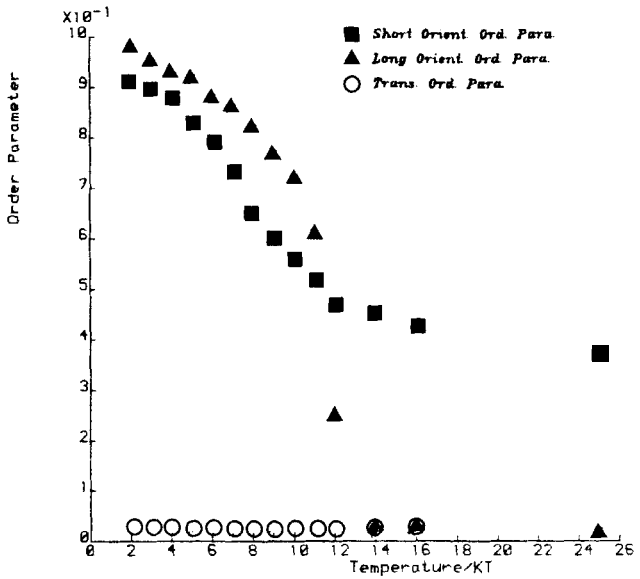

Figure 1.

Having determined that the orientational behaviour of the system was reasonably consistent with fixed site lattice simulations it was decided to introduce an excluded volume in an attempt to induce translational phase behaviour. As can be seen from Figure 2. with a volume fraction of 0.27 the translational order is considerably improved but there is again no temperature dependence nor does this situation improve with an increase in volume fraction to 0.40.

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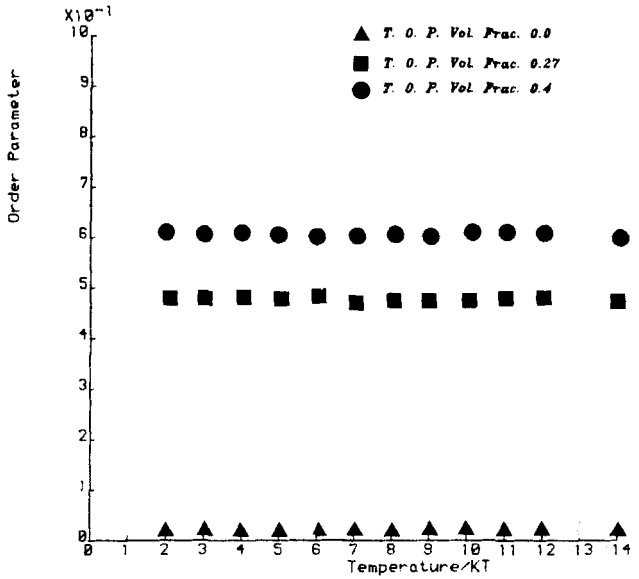

Figure 2.

It was now evident that a scalar component is required to give a temperature dependence to the translational order of the system. With its addition to the interparticle potential it can be seen that a small but definite step change occurs at 2KT with the translational order parameter dropping from 0.104 to 0.061 over a range of 1KT, see Figure 3.

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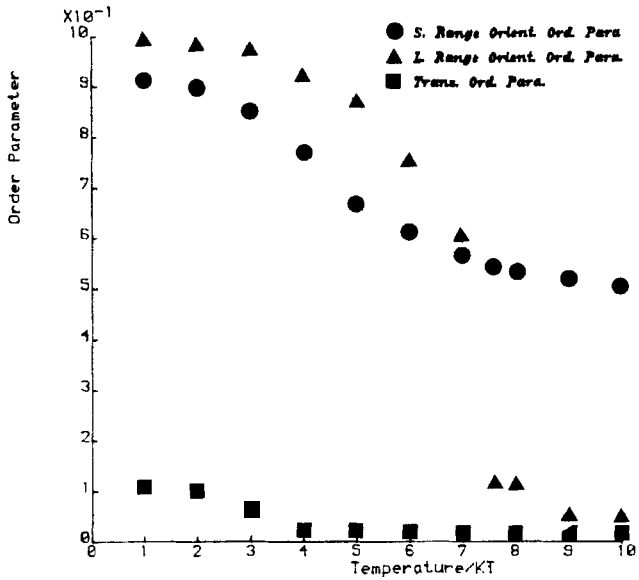

Figure 3.

Conclusion

The results so far obtained from this simulation indicate that it is possible to obtain a 'smectic' phase behaviour. The phases obtained are crude analogues of a low temperature smectic phase exhibiting: a high orientational order and significant translational order; an intermediate nematic phase with high orientational order and no significant translational order; and an isotropic phase possessing no long range orientational order or translational order but still possessed of considerable short range orientational correlation indicative of nematic clusters.

However, the translational order is still very low even

at low temperature and while it is expected that it will increase as the translational interaction constant is increased this has not yet been tested. Also the effects of excluded volume and shape have not yet been investigated and it is expected that these factors will significantly alter the behaviour of the sample.

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