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An Idea of Molecular Dynamic Simulation on Liquid Crystals: An Exotic Material

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The study of liquid crystals (LCs) belongs to the wider field of soft condensed matter physics, an area growing in importance because of new physics being discovered and the possibility of various technological applications being developed. Impact of liquid crystalline materials on the modern science, technology, industry and medicine has been very profound. The research activities in this area are undergoing a modern-day renaissance. It is now a subject of a well established and mature field of science. It is well known that liquid crystallinity is relevant to a wide range of branches of science and engineering: from cell membrane to display technology, from biological systems to polymer networks, from cosmetics to telecommunications, from paints to optical information processing, etc. Liquid crystals are of interest to chemists, physicists, biologists, mathematicians and engineers. In recent years, the incorporation of dyes, polymers and nanomaterials in LC geometry has provided an effective tool to tailor the material suitable for various applications. It is also becoming helpful in understanding many unsolved problems related to this fascinating subject.

Introduction:

Impact of liquid crystalline materials on the modern science, technology, industry and medicine has been very profound. The research activities in this area are undergoing a modern day renaissance. The research activities in this area are undergoing a modern day renaissance. The subject has come up of age and has acquired the status of being a very exciting interdisciplinary field of science covering chemical structure, physical properties and wide variety of applications. However, there are a large number of questions that remain unaddressed. One of such problems is “Phase ordering dynamics” in liquid crystals which is almost unexplored.

Liquid crystals signify a state of soft condensed matter sharing symmetries and properties that are intermediate between liquids and solids. The various states of matter can be transformed into each other at appropriate thermodynamic conditions. In liquids the particles can vibrate, move about and slide past each other.

Liquid crystal physics, although a field in itself is often included in the larger area called 'soft matter', including polymers, colloids, and surfactant solutions, all of which are highly deformable materials. This property leads to many unique and exciting phenomena not seen in ordinary condensed phases, and possibilities of novel technological applications. Studies of these phases are of importance in a wide range of scientific fields and as such have stimulated considerable theoretical work including computer simulations and experimental efforts over the decades.

The problem of kinetics of phase transition, that is, the evolution of dynamics of a system that is rendered thermodynamically unstable by a rapid change of external parameters (temperature, pressure, etc. quenches), have been the subject of intense research interests during last two decades. In case of liquid crystals (LCs) this area is almost unexplored and constitutes one of the most challenging problems in soft condensed state and statistical physics. The aim of the present work is to undertake some theoretical and Molecular Dynamic (MD) simulations studies of the dynamical properties of the growth of order in nematic liquid crystals. We intend to investigate how their behavior may be simulated and characterized, which involve various phenomena such as nucleation, spinodal decomposition, late stage growth and coarsening. when the external parameters of a homogeneous system are suddenly changed, the system will not be in equilibrium state under the new condition. Such systems are termed as "far-from equilibrium" systems. Their evolution is characterized by nonlinear evolution equations and spatio-temporal pattern formation. Usually, the exact solutions for the time-dependent evolution of the system cannot be obtained. Fortunately, the existence of domain boundaries or defects in these systems provides a convenient method to understand the resultant pattern dynamics. This nonequlibrium evolution is usually known as "kinetics of phase transition" or "phase ordering dynamics" or "domain growth" or "domain coarsening" or "ordering kinetics.

A quantitative characterization of the far-from-equilibrium evolution of the phase ordering systems basically depends on few parameters like domain growth size, statistical properties of the evolution morphology and structure factor.

So many questions related to the growth of nematic domains will still remain unanswered: How various domains grow with time? What growth law they follow? How the order parameter correlation function, structure factor, length scale and other characteristic features vary with time? How the interactions influence the morphology of domains pattern? To answer some of these questions by performing MD simulations.

Order Parameters

As discussed in Sec. 1.2.3, the most basic characteristics of LCs, at least from a macroscopic point of view, is the presence of long-range orientational order while the positional order is limited or absent altogether. Often these correlations are described in terms of order parameters (OPs). Since the phase transitions between different phases are, in general, a symmetry breaking event, an order parameter can measure the extent to which the orientational and positional correlations among molecules in the less symmetric (more ordered) phase differs from that in the more symmetric (less ordered) phase [12, 43, 44]. So we can define an order parameter Q, such that,

(i) **Q**= 0, in more symmetric phase,

(ii) **Q** ≠ 0, in less symmetric phase.

These requirements do not define an order parameter in a unique way. In spite of this arbitrariness, in most of cases the choice follows quite naturally.

Molecular Dynamic Simulations:

The basic Idea: The MD method comprises two general forms: one for systems at equilibrium and another for systems away from equilibrium. The equilibrium molecular dynamics is typically applied to an isolated system containing fixed N and V. As the system is isolated, the total energy is conserved.

MD simulations procedure: To start the simulation, the initial positions and velocities to all particles in the system are assigned. The particle positions are chosen compatible with the structure of the problem. While assigning the initial positions care must be taken to avoid the appreciable overlap of the atomic or molecular cores. Usually the same structure is adopted for this purpose as is done in case of MC simulations. Once the positions have been chosen, we attribute to each velocity component of every particle a value that is drawn from the uniform distribution in the interval [−0.5, 0.5]. Subsequently, all velocities are shifted such that the total momentum is zero, and the resulting velocities are scaled to adjust the mean kinetic energy to the desired value. However, in practice, the velocities themselves are not used in our algorithm to solve the Newton's equation of motion. Rather, the positions of all particles at the present and previous time steps, combined with the information about the force acting on the particles, are chosen to predict the positions at the next time step. At the start of simulation, one bootstraps this procedure by generating approximate previous positions. After initialization, the next task is the calculation of the force acting on every particle. If we assume the pairwise additivity of the interaction potential the contribution to the force on particle i due to all its neighbours has to be accounted. Efficient techniques are available to speed up the evaluation of both the short-range and long-range forces. These techniques apply equally well to both the MC and MD simulations. Once the force calculation is complete, we have to integrate the Newton's equations of motion.

We first intend to analyze the role of range of interaction on the ordering kinetics of a system with interaction potential via MD simulations,

$$H_{LC} = -J \sum_{i<j} \frac{1}{r_{ij}^{n}} P_2(\cos\theta_{ij})$$

Here J signifies the potential strength, superscript n on the r_{ij} characterizes the range of interaction. Using this potential phase ordering dynamics of nematic liquid crystal via Monte-Carlo (MC) simulations has been investigated by Singh et. al (A. Singh, S. Ahmad, S. Puri and S. Singh, EPL 37, 2 2014) diffusive growth law with logarithmic correction has been observed. We want to compare the results of MC and MD simulations. It expected that MD simulations will give many more interesting features than MC one.

Once this is done we will proceed for Gay-Berne type interaction potential to analysis the dynamics of nematic liquid crystal. The **Gay-Berne model** is used extensively in simulations of liquid crystalline systems. The Gay-Berne model is an anisotropic form of the Lennard-Jones 12:6 potential is-

$$U_{ij}^{LJ/GB} = 4\epsilon_0^{LJ/GB}[\epsilon^{LJ/GB}]^{\mu}(\hat{\mathbf{u}}_j, \hat{\mathbf{r}}_{ij}) \times \left[\left(\frac{\sigma_0^{LJ/GB}}{r_{ij} - \sigma^{LJ/GB}(\hat{\mathbf{u}}_j, \hat{\mathbf{r}}_{ij}) + \sigma_0{}^{LJ/GB}} \right)^{12} - \left(\frac{\sigma_0^{LJ/GB}}{r_{ij} - \sigma^{LJ/GB}(\hat{\mathbf{u}}_j, \hat{\mathbf{r}}_{ij}) + \sigma_0{}^{LJ/GB}} \right)^{6} \right],$$

where, in the limit of one of the particles being spherical, gives:

$$\sigma^{LJ/GB}(\hat{\mathbf{u}}_j, \hat{\mathbf{r}}_{ij}) = \sigma_0[1 - \chi\alpha^{-2}(\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_j)^2]^{-1/2}$$

Importance:

The liquid crystals are a state of matter sharing properties that are usually associated with both solids and liquids. Their study belongs to the wider field of soft condensed matter physics, an area growing in importance because of new physics being discovered and the possibility of various applications being developed. The study of liquid crystals constitutes a large science. It covers a wide area: chemical structure, physical properties and technical applications. A better understanding of the structure and properties is important not only because of the exotic nature of their properties, but also because it cuts through conventional boundaries of scientific disciplines. The growing science of molecular biology involves at every stage the properties of liquid crystals, electrolytes and polymer solutions. A better understanding of the process of various phase transitions, and the evolution of a system from one equilibrium state to another via nonequilibrium intermediate states is not only important from the academic point of view but also may be much more important from the point of view of applications in industry, biology and medicine. Recent technological development in display devices, medicinal industry, etc., makes it certain that the understanding at the molecular level of the static and dynamic behavior of liquid crystals, biological membranes, solid solutions may revolutionize these areas. It is desired that any device must be defects free, and so understanding of the kinetics of defects is of immense significance. These instances could be multiplied almost indefinitely to emphasise that the science of liquid crystals will continue to be a very important interdisciplinary area of scientific endeavour.

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