

ANALYSIS ON PORO COMPLEX FLUID DYNAMICS

S. Aruna, G. Shantha

Department of Mathematics & Humanities, Mahatma Gandhi Institute of Technology, Hyderabad

Corresponding Author: aruna_siripurapu@yahoo.com

ABSTRACT

A growing amount of experimental and theoretical research reveals the key importance of supercooled and glassy states in comprehending liquid water, and provides a foundation for a coherent interpretation of its properties in the future. This talk will focus on a new study that uses molecular dynamics simulations to investigate the spatially heterogeneous dynamics of the SPC/E model of water. Our work shows how the average mass n^* of mobile particle clusters can be related to the diffusion constant and the configurational entropy, in particular: N^* can be understood as the mass of "cooperatively rearranging areas" that constitute the basis of Adam-Gibbs' theory of the dynamics of supercooled liquids, n^* .

1. INTRODUCTION

1.1 complex fluids

A material composed of a liquid base within which supra molecular structures such as polymers, droplets, particles whose physical attributes are between solids and liquids [1] can be described as complex fluids. These materials are neither purely elastic nor purely viscous but viscoelastic. In such materials, energy is stored and dissipated in a frequency dependent way in a way are similar to deformable solids. We come across several examples of complex fluids in everyday life, such as polymer materials, living biological cells, Micells, cytoplasm, corn starch, liquid crystals, ferro fluids etc.,. Among complex fluids, materials like liquid crystals exhibit local spatial homogeneity but also have a preferred orientation, and leads to anisotropic diffusivity; these are anisotropic complex fluids. But, materials like cytoplasm, micells are inhomogeneous and do not have preferred direction in the alignment. The peculiarities of the complex fluids stem from their complex

structures and dynamics with their dynamical variations at micro and nano length scales and possessing slow dynamical variations on small time scales. Important technological applications like fast switching operations in LCD (liquid crystal displays), medical applications like drug deliveries, paints, food, cosmetics industry, coolants, oil recovery, processing of plastics are few examples that shows the necessity of understanding of dynamics of complex fluids.

In this thesis, anisotropic complex fluids that possess a particular alignment of particulate and the concerned dynamics are of criteria to study . In particular, slow diffusion dynamics of 8CB (4-cyano 4 Octyl biphenyl) liquid crystals with phase transition temperatures as : Crystalline 21.5°C Smectic A 33.5°C Nematic 40.5°C Isotropic. A131 bent core liquid crystals (BCN) with phase transition temperatures as : 82.5°C Crystalline 93.5°C Smectic Y 104.3°C Smectic X 118.5°C biaxial

nematic Nb 149°C uniaxial nematic Nu 176.5 °C Isotropic and Mn_{0.75}Zn_{0.25}Fe₂O₄ super paramagnetic fluids are studied. Normally, in liquid crystals, molecules are aligned in a particular direction called nematic director (\hat{n}) [2]. In this thesis, we present our study of three specific complex fluids and their dynamical behaviour. Two types of liquid crystals, viz., 8CB liquid crystals, and bent core A131 and a ferrofluid composed of Mn_{0.75}Zn_{0.25}Fe₂O₄ are the fluids chosen for our study. All the three exhibit a preferred orientational direction, which can be obtained either by chemical coating on to the surfaces of the sample cell as in case of liquid crystals, or by application of external magnetic field as in case of ferro fluids. All the three materials show very interesting dynamics, by virtue of the fact that they are complex fluids.

1.2 liquid crystals

A state of matter intermediate between that of a crystalline solid and isotropic liquid are called Liquid crystals (LCs). These organic compounds exhibits many of mechanical properties which are liquid like such as viscosity, surface tension, inability to support shear (shear thinning). Anisotropy in optical, electrical and magnetic properties are similar to crystals.

Frederic Reinitzer first discovered this state of matter in 1888, Lehmann in 1889 characterized and suggested the name 'liquid crystal'. There exist two types of liquid crystals:

- thermotropic (liquid crystalline phase is manifested by virtue of temperature)
- lyotropic (liquid crystalline phase is manifested by virtue of concentration) In this thesis we study the dynamically varying micro structural and micro

mechanical properties of thermotropic liquid crystals.

2. BROWNIAN MOTION OF COLLOIDAL PARTICLE IN LIQUID CRYSTALS

2.1 colloids in liquid crystals

In nematic liquid crystals (NLC), liquid crystal molecules are orientationally ordered complex fluids. These molecules are aligned spontaneously along the nematic director \hat{n} [1],[2]. Oriented molecules in certain direction leads to anisotropy. This orientation of NLC can be manipulated by anisotropic surfaces, electric and magnetic fields. A colloidal particle introduced into NLC disturbs the local orientation of nematic molecules [3]. Because, these NLC molecules interacts with the surfaces of colloidal particle. This disturbance can be considered as an elastic deformation of the NLC and it spreads on a micrometer scale. This deformation depends on the confinement, size of colloidal particles, strength of anchoring at the surfaces [4].

In this thesis, colloids dispersed in liquid crystals were treated with DMOAP (Sigma-Aldrich) to induce perpendicular surface orientation (homeotropic alignment) of the liquid crystal molecules. But, the surfaces of the cell that confines the liquid crystal were chemically treated with polyamide AL 1254 to induce parallel orientation (planar alignment). This kind of alignment on colloidal sphere and on surfaces of cell results in elastic distortions. This leads to repulsive interaction between the colloids and the walls of the cell. Hence, this configuration of alignment leads to elastically stabilizing the colloids in the middle of the NLC layer. Also, this anisotropy in energies of interaction leads to anisotropy in the mobility properties. In general, the parallel

and perpendicular direction mobilities of liquid crystal molecules are different from each other. Which induces the relative diffusion of the colloidal particle with respect to \hat{n} [5].

2.1.1 Topological defects with colloids in liquid crystals

An ordered medium is generally free of defects. Defects in liquid crystals can be simply defined as localized spots with ill defined order parameter and hence the director orientation is also not defined (singular point or disordered spot) [6]. These defects alters the physical properties of NLC locally and increases the overall free energy. However, the influence of surfaces, lowering of the symmetry during

phase transitions, external field applications can spontaneously or controllably generate and stabilize topological defects. The director lines meet at a central point with radial symmetry in the far field, resulting in the topological defect. Simply, topological defects abound systems with broken symmetries. Colloidal particle with homeotropic anchoring is a source to a topological defect called as radial hedgehog. Hedgehogs are point defects in which the director \hat{n} sweeps out all directions on a unit sphere an integer number of times on a spherical surface enclosing the defect. Characterization of these defects is generally done by topological charge.

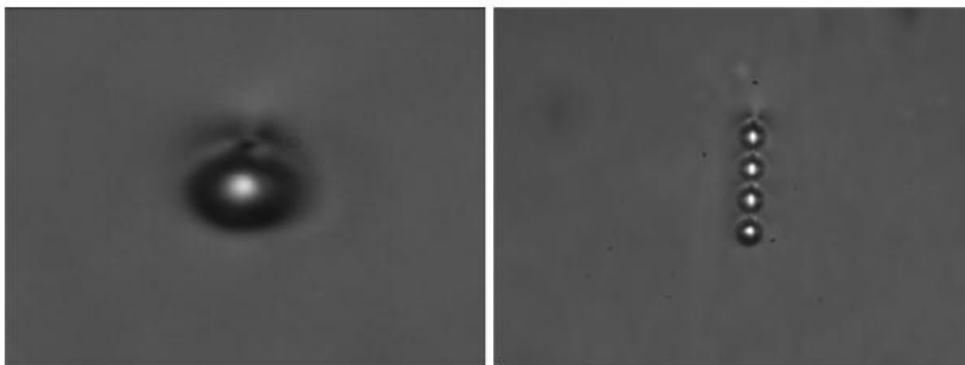


Figure 2.1: In the above figure left picture represents dipole defect with $0.98\mu\text{ m}$ colloidal particle picture on right is a chain of collodial particles with dipole defects

In case of homeotropic anchoring for a spherical colloidal particle embedded in a nematic cell, this particle imposes the director at its surface and this tends to align the director field with the normal of the bead. Here, the bead is a source of singularity for the director field. Because

of the uniform far-field director in the cell and the conservation of the topological charge, a topological defect appears in the close vicinity of the director field [8]. colloidal particles with homeotropic anchoring possess two types of topological defects as shown in figures 2.1, 2.2.

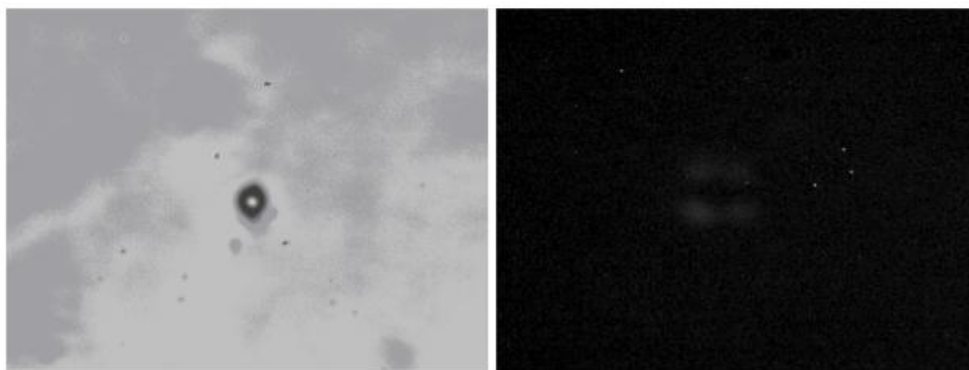


Figure 2.2: Quadrupole defect with $0.98\mu\text{ m}$ colloidal particle

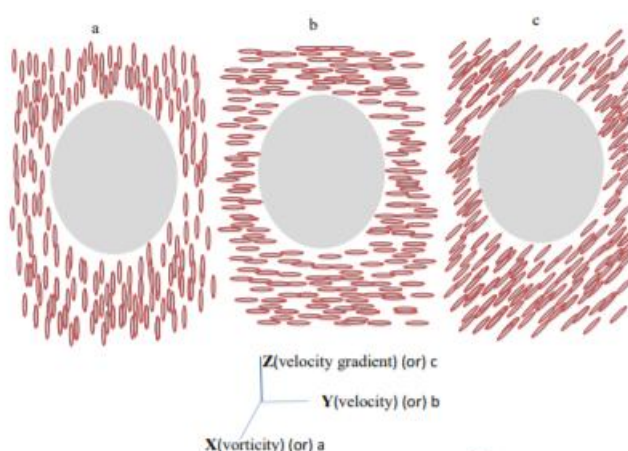


Figure 2.3: a,b,c structures in nematic phase of liquid crystals represent vorticity(x), velocity(y), and velocity gradient(z) directions

The first calculations on diffusion of colloids in nematic solvents are by Ruhwandl and Terentjev [24] who concentrated on the Saturn ring configuration. Later, Stark and Venzki concentrated on the dipole configuration, who treated the dynamics explicitly by relaxing the constraint of a fixed director field.

3. PASSIVE VISCOSITIES OF BENT-CORE NEMATIC LIQUID CRYSTALS

3.1 introduction

The viscosity of liquid crystals strongly depends on the microscopic structures of

the constituent molecules and the mesophases. There are several theoretical and experimental studies of the low molecular weight liquid crystals where the molecules have mostly cylindrical symmetry[[1],[2],[3]]. The nematic(N) phase of liquid crystals has three principal viscosities called Miesowicz viscosities, namely η_1 , η_2 , and η_3 , depending on the direction of the shear and the orientation of the liquid crystal director(The average alignment direction of the long axes of the molecules). A schematic representation of the director orientation in a calamatic (rodlike) nematic liquid crystals is represented as shown in fig.3.1.

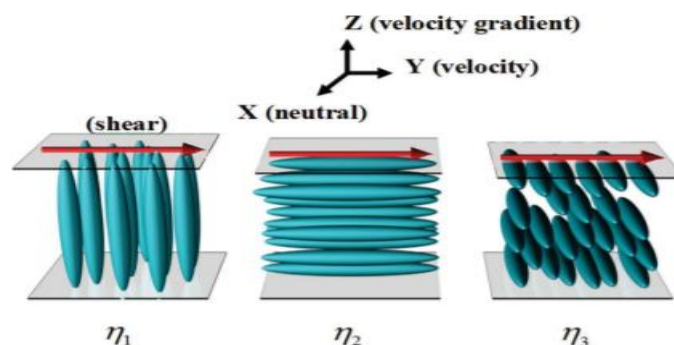


Figure 3.1: Schematic representation of the three fundamental director orientations in the nematic phase. Miesowicz viscosities corresponding to each orientation are designated by η_1 , η_2 , η_3 respectively.

3.2 the experiment

The chemical structure and the phase transition temperatures of the bent-core nematic (BCN) are shown in figure, which exhibits the following phase transitions (cooling): I at 178.5 °C to N at 120°C to Sm-C at 101.3 °C to Sm-X at 90.4 °C to Sm-Y at 60.2 °C in cr. The purity of the compound was confirmed by the high-performance chromatography and other techniques. The single particle tracking technique using video microscopy is used to measure the self diffusion coefficients of a tiny silica microsphere (with a diameter of 0.98 μm and hence the passive viscosities of the sample parallel and

perpendicular to the director. To promote a specific alignment on the surface, the silica microspheres were coated with octadecyldimethyl (3-trimethoxysilylpropyl) ammonium chloride (DMOAP) before mixing with the liquid crystal. Details of the coating of the DMOAP alignment layer is done. The Brownian fluctuations of an isolated microsphere in a planar cell ($d = 23 \mu\text{m}$) was recorded and the position was determined with the help of a commercial software programme.

4. RESULTS AND DISCUSSION

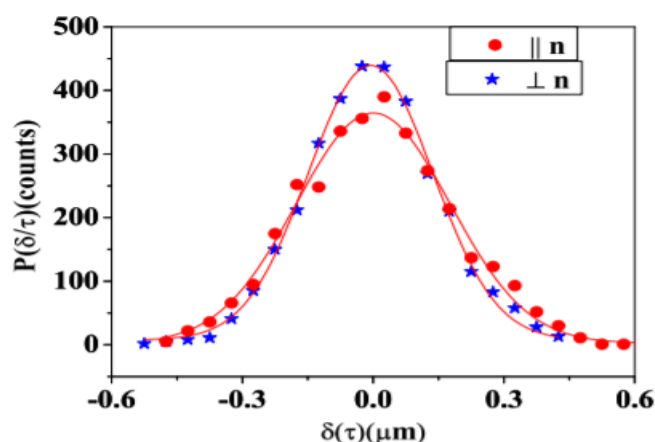


Figure 4.1: Histogram of particle displacements parallel(circles) and perpendicular(stars) to the director for $\tau = 1$ S. The solid lines are Gaussian fits.

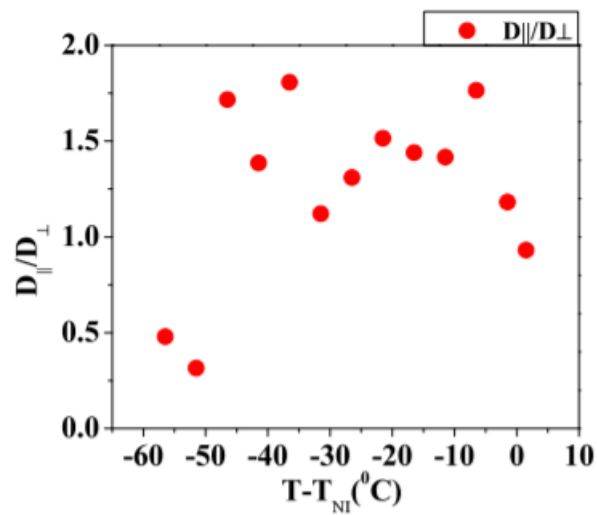


Figure 4.2: Diffusion ratio $D_{\parallel} > D_{\perp}$ for every 5°C difference in temperature. Average of this ratio is at 1.6

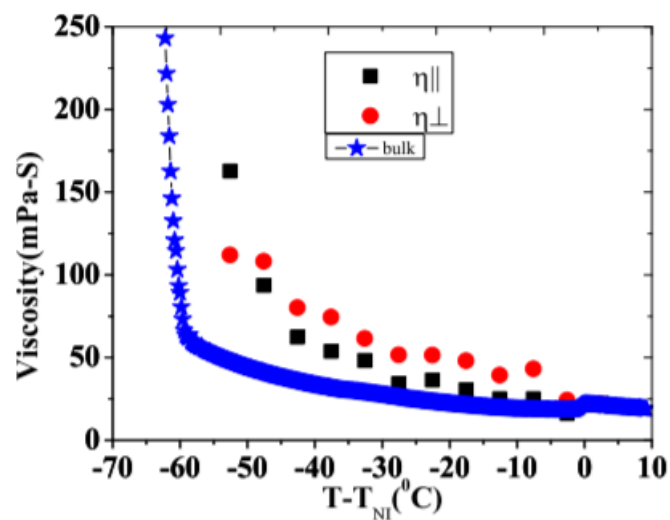


Figure 4.3: Variation of η_{eff} (stars), η_{\parallel} (squares), and η_{\perp} as a function of shifted temperature.

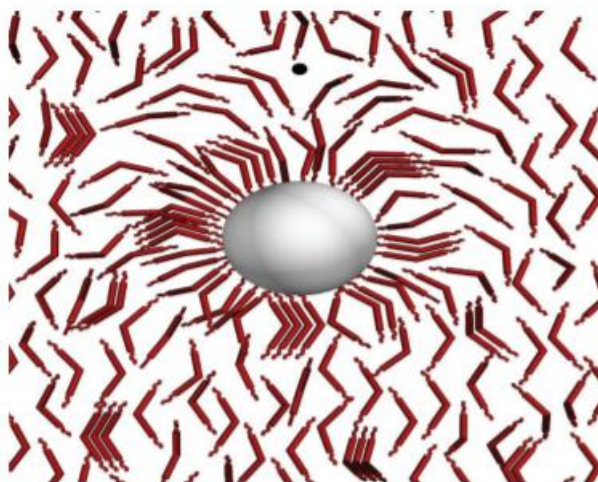


Figure 4.4: Schematic molecular orientation around the microsphere with a dipolar defect configuration.

As a result, the hydrodynamic radius of the microsphere could be significantly larger than the actual radius due to the large cloud of the distorted nematic around the microsphere. Assuming $\eta_k = \eta_e f f = 21.6$ mPa s near the N-I transition ($T - T_{N-I} = -180^\circ\text{C}$), the estimated hydrodynamic radius of the microsphere is $0.68\mu\text{m}$, which is about $0.2\mu\text{m}$ larger than actual radius. A schematic molecular orientation of bent-core molecules and some clusters around the microsphere with a dipolar defect is shown in figure 4.4.

conclusions We report the measurements of passive viscosities of a bent-core nematic liquid crystals. In this single particle tracking experiment, passive viscosities are measured by measuring the self-diffusion coefficient of a microsphere in the aligned sample. The anisotropy in the self-diffusion is observed. The temperature dependence of passive viscosities is stronger than that of active (bulk rheology measurement) viscosity. The effect of presmectic fluctuations are observed much higher than the Nsm-C transition temperature than commonly seen in calamitic liquid crystals. The study of

Brownian motion is useful to understand the smectic fluctuations in bent-core nematic liquid crystals.

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