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Polymer particulate nanocomposites (PNCs) have many industrial and military applications. They can achieve very high mechanical modulus and possess superior transport or barrier properties. The project aimed to study the mesoscopic structure formation during flow processing and the corresponding rheological consequence leading to characterization of material properties in solid states. Significant progress has been made to model the materials and to understand their rheological properties in melt or solution processing during the project year. In addition, the anisotropic molecular configuration in bent-core liquid crystals and its impact to the macroscopic material properties are investigated; applications of the modeling and numerical tools developed for complex fluids are used to important biological applications.

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THEORETICAL AND NUMERICAL INVESTIGATION OF POLYMER-PARTICLE NANOCOMPOSITES AND THEIR EFFECTIVE MATERIALS PROPERTIES

Final Technical Report

AFOSR *(FA9550-08-1-0107)*,

(Dec. 1, 2007-Nov. 11, 2008)

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Abstract

Polymer particulate nanocomposites (PNCs) have many industrial and military applications. They can achieve very high mechanical modulus and possess superior transport or barrier properties. The project aimed to study the mesoscopic structure formation during flow processing and the corresponding rheological consequence leading to characterization of material properties in solid states. Significant progress has been made to model the materials and to understand their rheological properties in melt or solution processing during the project year. In addition, the anisotropic molecular configuration in bent-core liquid crystals and its impact to the macroscopic material properties are investigated; applications of the modeling and numerical tools developed for complex fluids are used to important biological applications.

The objective of the project is to develop a suite of multiscale models and simulation tools to probe the flowing and solid-state properties of liquid crystal polymer (LCP) and polymer nano-particle (anisotropic particle in particular) composite (PNC) materials guided by Air Force contact Dr. Richard Vaia of material directorate WPAFB. The grant began on December 1, 2007 and ended on Nov. 30, 2008 due to my transfer from Florida State University to University of South Carolina. The research activities included developing kinetic theories for blends of rigid liquid crystal polymers and flexible polymers as well as theories for biaxial liquid crystals and nano-particle dispersions; multiphase flows of rigid LCPs in viscous or polymeric matrices; application of the complex fluids theories and simulation tools to biological settings like biofilm modeling and simulation. In the following, I summarize the completed work and list the publications and synergistic activities during the period. For more technical details, please refer to our publications.

Structure formation and defect evolution in shear flows of liquid crystal polymers

The Pi and his collaborators (M. G. Forest, and X Yang of UNC-CH) continued the refined analysis on the extended Doi-Hess kinetic theory for shear flows of inhomogeneous liquid crystal polymers. The aim here is to provide a comprehensive understanding of the poly-domain flow behavior as well as the mesoscale structures governed by the kinetic theory and closure models for inhomogeneous LCPs. We focused on multidimensional phenomena where the defect formation and annihilation dominates the mesoscale morphology leading to the experimentally observed optical turbulence. A spatially 2-D tensor based solver is developed to study the multiscale phenomena. Following the monodomain road map, we have identified a variety of temporal-spatial structures and patterns in sheared nematic LCPs of inhomogeneous flows. A new diagnostic is developed to detect and monitor the defect dynamics in time and space. Various spatial-temporal phenomena in the sheared nematic system are explored and reported, improving one's understanding of defect dynamics and their rheological and fluid mechanics consequence.

## Multiscale kinetic theories for flows of biaxial liquid crystal polymers

Given the rising interests in the modeling of nanofluids of biaxial constituents such as the bent-core liquid crystal polymers, my graduate student Sarthok Sircar and I developed hydrodynamic theories for the biaxial liquid crystal polymer by modeling it as an ellipsoid or a V-shaped rigid body suspended in viscous solvent. The excluded volume interaction potential is calculated from the first principle. The probability density function is sought by a spectral method for the Smoluchowski equation based on the Wigner function expansion. Lower-dimensional approximation to the second moment space or reduced order models is also attempted to resolve the coarse-scale dynamics. We have studied the flow-induced structure transition with a general excluded volume potential and the monodomain structure in sheared biaxial liquid crystals. In the case ellipsoidal biaxial lcps, two time-periodic motions are identified along with the chaotic motion. While the chaotic motion is apparently absent in the bent-core liquid crystal system in steady shear. The picture below shows one of the time-periodic motion observed in sheared ellipsoidal and bent-core biaxial LCPs, called fluttering motion.

(b)
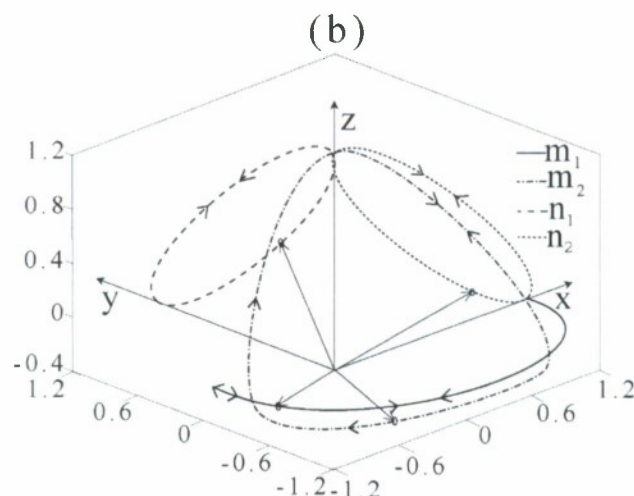
Kinetic theories and rheological prediction for polymer nano-particle composites

The PI along with his collaborators have developed a new set of kinetic theories for polymer nano-particle composites accounting for the semiflexibility of the nano-particles such as nanoclays, silicones, etc. as well as the contact interaction between flexible polymers and the nano-particles. These nano-particles can be semiflexible rods or thin platelets. The effect of the semiflexibility and surface contact interaction between the nanoparticle and the host polymer matrix influences the equilibrium phase as well as the shear flow induced phase significantly. The first figure below depicts the shear viscosity prediction at a set of selected shear rates. The prediction qualitatively matches the experimental data.

In the next figure, the semiflexibility of the "nanoparticles" or inclusions also affects the phase behavior of the nanocomposites, where r_f denotes the degree of semiflexibility of the nanoparticles ($r=0$ corresponds to the fully rigid limit). The details are summarized in two papers either accepted or submitted.

NN=30, β= 10, r_f= 0.5, a= 0.98, λ= 5, D_r=1

$0 \leq T \leq 200$

β = 5, a= 0.98, λ= 5, D_r=1, ϕ=0.94
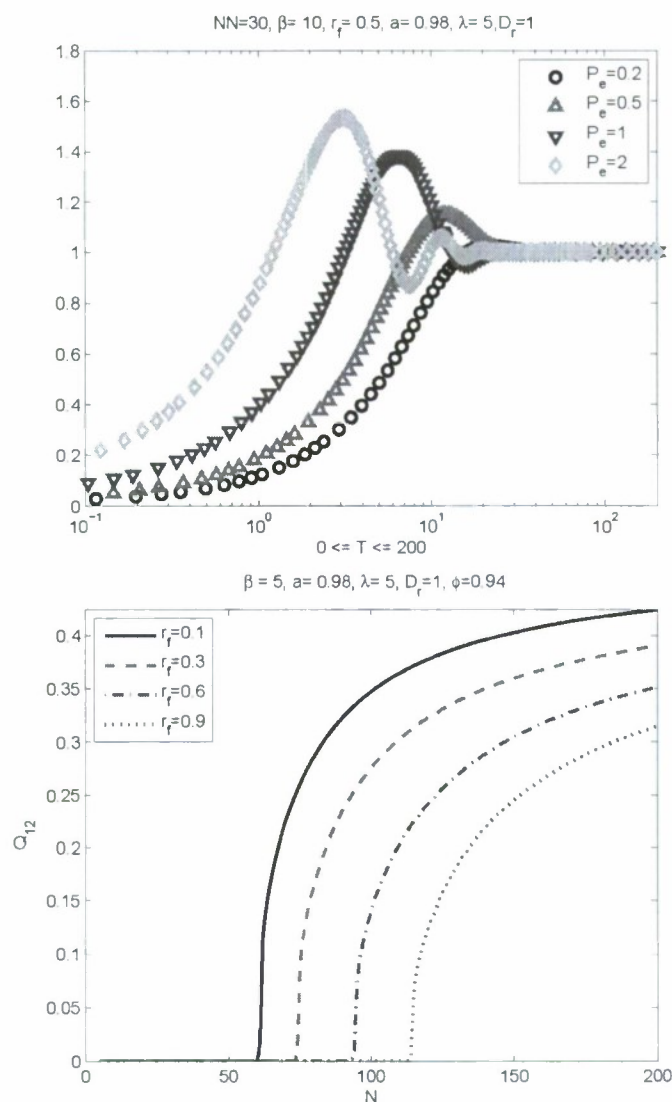
Modeling blends of liquid crystal polymers and flexible polymers

In collaboration with Prof. Ping Lin of National University of Singapore, we are conducting a series studies on the blends of immiscible liquid crystal polymers and viscous fluids or flexible polymer fluids. Various combinations of the constitutive models for the flexible polymers can be incorporated into the phase-field model for the blends. The goal is to understand the motion of liquid crystal droplets in viscoelastic matrix subject to external shear or pressure. This study would shed light on the mixing of liquid crystal polymers in polymer matrices through external stirring motion. A finite element solver for the flow problem has been implemented and preliminary numerical results are obtained.

Applications to biofilm modeling

The experience and expertise acquired during our studies of complex fluids, especially, the liquid crystal polymer and flowing nanocomposites has enabled us to model multiphase complex fluids both theoretically and numerically using the phase field approach. We have found applications of our models and methodologies in biofilms, amixtures of polymeric network and viscous fluid components comprising of bacteria and nutrient-rich solvent, cell motility, etc. The 2-D and 3-D simulation code have been developed and being paralellized presently. We are applying a coarse-grain dynamical model for semi-flexible polymers to study the self-assembly phenomena in F-actin solution. This could have a potential impact on tissue regeneration for wounded soldiers and fabrication of high performance materials. Figure below depicts the detachment of a biofilm in shear flows in a 2-D simulation.
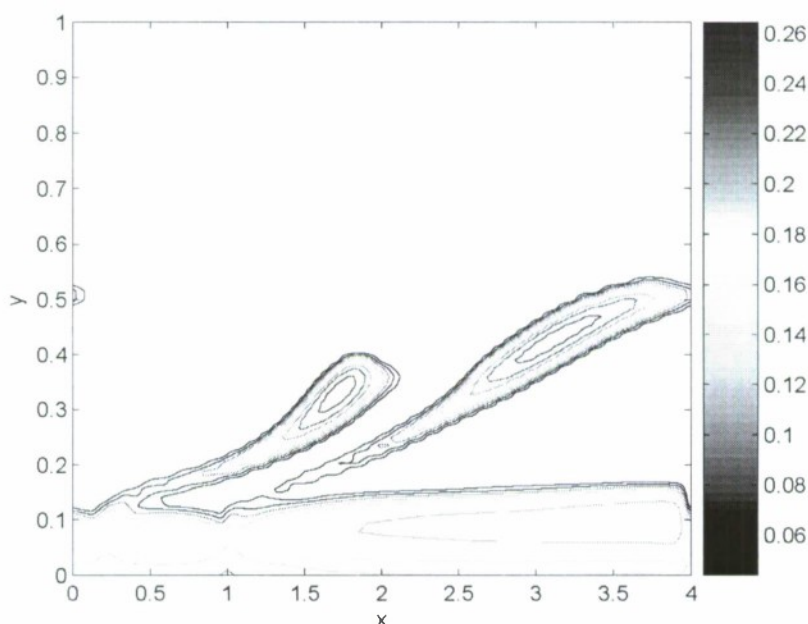
The research activities on the project funded by the award proceeded smoothly according to the plan. Additional projects closely related to the originally proposed were identified and added to our research activities (like actin self-assembly study and applications to biofilms etc.). The slightly expanded scope of research facilitated our efforts for the overall objective as well as addressing the need of the Air Force.

Personnel Supported through the grant

Mr. Sarthok Sircar	Ph. D candidate, Florida State University, Ph. D. expected date: May, 2009
Dr. Guanghua Ji	Postdoc Associate, Florida State University

Point of Contact

Dr. Richard Vaia, AFRL/MLBP, WPAFB, OH, Phone: 937-255-9184. The last time we met was in the contractor's meeting held at WPAFB, Dayton, OH, August, 2008.

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