# Ferroelectric phenomena in soft matter systems

organized by
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Workshop Summary

## 1. Topics of the workshop

The main theme of the workshop was to study the interaction between applied electric field and flow in ferroelectric liquid crystals, and specifically, to obtain predictions on the flow generated by an applied voltage, and vice-versa, the distribution of polarization resulted from the flow. An ultimate goal of such a study, and with possible industrial implications, is the design and manufacturing of soft devices such as valves.

The study of the ferroelectric flow involves several components: modeling and analysis of the governing system of partial differential equations, numerical studies of the discretized system and simulations. The lectures during the workshop and the follow-up discussion groups addressed several aspects of the project.

We list below the main topics that were discussed and their roles in the ferroelectric liquid crystal flow project.

**1.1 Modeling** A main objective of the workshop was to develop flow equations for such materials. The first two days of the workshop were devoted to providing background materials for the ferroelectric liquid crystal flows. The following lectures covered a wide range of issues related to the experiments and modeling of such flows:

- Jonathan Selinger, *Liquid crystal molecules, phases and polarization properties*
- Chuck Gartland, *Energetics of liquid crystals*
- Carme Calderer, *Modeling of ferroelectric liquid crystal flow*
- Antal Jakli, *Rheology and properties of bent core liquid crystals*
- Qi Wang, *Order tensor models of nematic liquid crystals*

Starting from the Second Law of Thermodynamics, a standard procedure provides the expressions of the reversible parts of forces and stresses of the system, and also yields the dissipative inequalities to be satisfied by the non-reversible force and stress contributions. On the other hand, one also needs to sort out the symmetries satisfied by the system. Using the previous results on the Leslie-Ericksen system for nematic liquid crystals, we derived anisotropic forms of the stresses consistent with the shape of the molecules and the polar property. The system of partial differential equations consists of balance laws of linear momentum and angular momentum. The latter includes an equation for the main director of the molecule and also an equation for the polarization field. In addition, these equations are coupled with the Maxwell's equations of electromagnetism.

The explicit form of these equations for a special geometry (shear geometry, with the material confined between parallel plates, with either an imposed pressure gradient or a relative speed of displacement of the plates) took shape during the discussion group in the Thursday afternoon. This particular geometry is useful from two points of view:

- It corresponds to the experiments carried out at the Kent State Liquid Crystal Institute. These experiments provide realistic parameter values of the coefficients of the system, and allow for comparison with mathematical analysis and numerical simulation.
- It simplifies significantly the system of equations. In fact, The equations reduce to a one-dimensional system of partial differential equations that are of first order in time and second order in space.

At the end of Thursday's discussion, mathematical features of these equations in the shear flow regime had been identified, in particular:

- Specification of boundary conditions for the flow and electric polarization.
- Formulation of the energy dissipation for the flow system: This by no means guarantees well-posedness of the system but it is definitely an important first step in the analysis.

**1.2 Numerical themes** Another main goal of the workshop was to develop efficient numerical methods for the proposed ferroelectric liquid crystal flow. The lectures in Wednesday morning were devoted to the numerical issues:

- A summary of numerical methods was discussed by Jie Shen in his lecture. He devoted special attention to the *phase field methods* that have proven particularly successful in simulations of free surface flows (e.g. nematic droplet in fluid). His lecture provided understanding on how such a method may be applied to the numerical simulation of ferroelectric liquid crystal flow.
- In his presentation, Xiobing Feng addressed theoretical challenges encountered in the numerical discretization of liquid crystal systems.
- Allison Ramage presented numerical methods for liquid crystal flow, but in the case that the anisotropy is modeled with the order tensor rather than the nematic director. Her presentation was the numerical complement of Qi Wang's talk on liquid crystals with order tensor.

Overall, the problems and case study topics presented by Shen, Feng and Ramage provide the basic background to future numerical study of ferroelectric liquid crystal flow.

## 2. Related topics

Although the main thrusts of the workshop were the modeling and numerical simulation of ferroelectric liquid crystal flow, a parallel line of work and discussion on related topics took place on Thursday and Friday.

- Robin Selinger did a simultaneous translation of fluid modeling into solids. Although bent core molecule liquid crystals are well understood as liquids, materials made of cross-linked polymers and with permanent polarization are also of current interest. Robin's research is on such solids (*liquid crystal elastomers*, although currently neglecting electrostatic effects).

- Patricia Bauman presented a lecture on her recent joint work with Dan Phillips on the mathematical analysis of bent core filaments.
- Marie Rognes gave a presentation (Thursday) on an open source *finite element software* and showed *in real time* how one can use it to solve dynamical flow problems.
- Keith Promislow was attracted to the workshop in his quest of searching for modeling tools of electric effects in matter. He presented a lecture on *fuel cells and renewable energies.*
- Jonathan Robbins presented the research conducted by the Bristol-HP group on liquid crystal defects in domains with corners.

## 3. Conclusions

We conducted in this workshop a case study of ferroelectric flow in the shear geometry with the permanent polarization of the liquid crystal being of flexoelectric type. We developed a system of partial differential equations which possesses dissipation properties and exhibits the interaction mechanism between electric and flow effects that are required in the push-pull effect. Development of such a system would have proved very difficult without a team effort of mathematicians (numerical methods and analysis) and physicists (modeling and experimental). Two postdocs, Sookyung Joo and Jinhae Park, are pursuing the analysis in collaboration with other participants (Calderer, Shen, Wang, in consultation with Jakli). Although the duration of the workshop did not allow for the numerical exploration of the problem, the lectures and discussions prepared the ground for carrying out this task. There will be further discussions among workshop participants as the work progresses.