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A Multiscale Approach for Complex Functional Materials and Nanostructure

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1) the study of the analogy of lattice dynamics in slender nanostructures, and in particular the possibility of tuning the wave speeds through external loads.
2) the development of multiscale methods for quantum mechanical electronic structure of the scattering process at crystalline defects using non-reflecting boundary conditions, and the extension of this method to non-crystalline nanostructures

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Abstract

This is the final report for Grant Number: FA9550-12-1-0350, managed by Dr. Jean-Luc Cambier and formerly by Dr. Fariba Fahroo.

The research objective of this grant is to develop and apply new multiscale methods for complex nanostructures and functional materials. The technical strategy is based on a systematic framework that generalizes crystalline materials using isometry groups (the Objective Structures framework introduced by R D James). In particular, the research includes work that built on, and went beyond, work from a few years ago that developed and applied this framework to perfect nanostructures to inhomogeneous and / or defected nanostructures. The key results include: 1) the study of the analogy of lattice dynamics in slender nanostructures, and in particular the possibility of tuning the wave speeds through external loads. 2) the development of multiscale methods for quantum mechanical electronic structure of the scattering process at crystalline defects using non-reflecting boundary conditions, and the extension of this method to non-crystalline nanostructures 3) the introduction of a new theoretical concept, Quasi Objective Structures, that extends the key ideas of Objective Structures to 2D materials with complex deformations, and the demonstration of their use for graphene and lipid bilayers

Additional related results include new strategies using strain gradient effects at the nanoscale ("flexoelectricity") to achieve temperature-stable electromechanical coupling for high temperatures; the development of new models for defect dynamics in liquid crystals; and the statistical mechanics of non-crystalline functional materials with electromechanical coupling.

The methods will be relevant to many other nanostructures and materials of interest to the Air Force, particularly electronic materials and energy-storage materials.

1 Introduction

This grant extends multiscale methods to complex functional materials and nanostructures, and applies these methods to various systems of current scientific and technological interest. The technical strategy is based on Objective Structures[2]. The key idea of Objective Structures is a combination of structural symmetry and fundamental physical invariances. In particular, James and following works demonstrate the existence of a large class of Objective nanostructures such that every structural subunit "sees" the same environment up to an orthogonal transformation. Such a relation is obvious in a perfect crystal, a subset of Objective Structures, but Objective nanostructures include numerous other systems, for instance some of the most important nanostructures

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[2]*Objective Structures*, R. D. James, J. Mech. Phys. Solids, 2006.

such as carbon nanotubes. The practical consequences of this observation are far-reaching. Based on a systematic approach using isometry groups, one can construct the entire set of Objective nanostructures. Further, one can develop methods to study these systems, drawing on analogies between crystals and Objective Structures.

In previous work (by the PI and his co-workers, as well as other groups), this work has been entirely restricted to perfect nanostructures. In the current grant, we go beyond perfect nanostructures, in particular by drawing on multiscale methods. As in crystals, these methods enable us to study defected and inhomogeneously deformed Objective Structures in realistic settings: e.g., nanostructures with defects subject to complex loads, and so on. In addition, for functional crystalline materials, we examine the behavior of defects when atoms interact both by long-range Coulombic forces as well as standard short-range forces.

The Objective Structures idea of structural symmetry and fundamental physical invariances is also implicitly a central element of many homogenization frameworks. Consequently, there is a direct intellectual connection from Objective Structures to homogenization. For instance, Objective Structures relies on solutions to problems on a unit cell to provide solutions to system-level problems, with similarities to many homogenization approaches. This connection to homogenization also motivates the notion of a defected Objective Structure: defects can be related to departure from a perfect Objective Structure. Hence, our numerical methods use a systematic approximation based on exact solutions to unit cell problems. Consequently, the Objective framework provides a firm basis for future rigorous numerical analysis.

2 Results

1. the study of the analogy of lattice dynamics in slender nanostructures, and in particular the possibility of tuning the wave speeds through external loads.

2. the development of multiscale methods for quantum mechanical electronic structure of the scattering process at crystalline defects using non-reflecting boundary conditions, and the extension of this method to non-crystalline nanostructures

3. the introduction of a new theoretical concept, Quasi Objective Structures, that extends the key ideas of Objective Structures to 2D materials with complex deformations, and the demonstration of their use for graphene and lipid bilayers

4. Additional results include new strategies using strain gradient effects at the nanoscale ("flexoelectricity") to achieve temperature-stable electromechanical coupling for high temperatures; the development of new models for defect dynamics in liquid crystals; and the statistical mechanics of non-crystalline functional materials with electromechanical coupling.

This report is a brief summary of the highlights of our research. More details and further developments can be found in the published papers, PhD theses, and preprints that will be shortly submitted. Preprints and reprints are available at `sites.google.com/site/kaushikdayal/publications`.

2.1 Objective Phonon Analysis of Nanostructures

The characteristics of phonons, i.e. linearized normal modes of vibration, provide important insights into many aspects of crystals, e.g. stability and thermodynamics. We use the Objective Structures framework to make concrete analogies between crystalline phonons and normal modes of vibration in non-crystalline but highly symmetric nanostructures. Our strategy is to use an intermediate linear trans- formation from real-space to an intermediate space in which the Hessian matrix of second derivatives is block-circulant. The block-circulant nature of the Hessian enables us to then follow the procedure to obtain phonons in crystals: namely, we use the Discrete Fourier Transform from this intermediate space to obtain a block-diagonal matrix that is readily diagonalizable. We formulate this for general Objective Structures and then apply it to study carbon nanotubes of various chiralities that are subjected to axial elongation and torsional deformation. We compare the phonon spectra computed in the Objective Framework with spectra computed for armchair and zigzag nanotubes. We also demonstrate the approach by computing the Density of States. In addition to the computational efficiency afforded by Objective Structures in providing the transforma- tions to almost-diagonalize the Hessian, the framework provides an important conceptual simplification to interpret the phonon curves. Our findings include that, first, not all non-optic long-wavelength modes are zero energy and conversely not all zero energy modes are long-wavelength; second, the phonon curves accurately predict both the onset as well as the soft modes for instabilities such as torsional buckling; and third, unlike crystals where phonon stability does not provide information on stability with respect to non-rank-one deformation modes, phonon stability in nanotubes is sufficient to guarantee stability with respect to all perturbations that do not involve structural modes. Our finding of characteristic oscillations in the phonon curves motivates a simple one-dimensional geometric nonlocal model of energy transport in generic Objective Structures. The model shows the interesting interplay between energy transport along axial and helical directions.

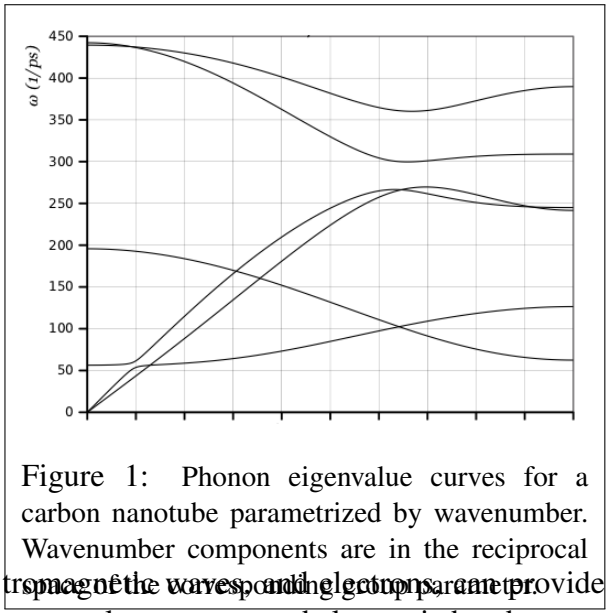

Figure 1: Phonon eigenvalue curves for a carbon nanotube parametrized by wavenumber. Wavenumber components are in the reciprocal space of the corresponding group parameter.

Fig. 1 shows the eigenvalues obtained from such a procedure for a deformed nanotube, and Fig. 8 some of the corresponding normal modes. Many structural transformations, both in crystals and in OS, can be detected and predicted using the phonon spectrum. In particular, a zero eigenvalue indicates a "soft mode" or a deformation mode that costs no energy. Hence, these provide an indicator of the structural transformation.

In addition to the insight into structural transformations, the similarity transformation above enables analogies of other wave-nanostructure/crystal interactions. For example, interactions between OS and light waves, electromagnetic waves, and electrons, can provide new analogs of photonics, X-ray diffraction and nanoscale antennas, and electronic bandstructures respectively.

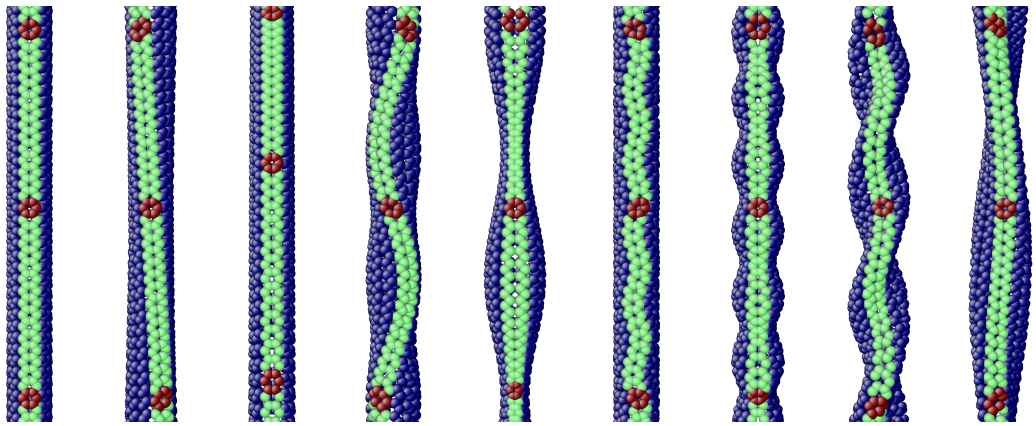

Figure 2: Selected phonon deformation modes of a carbon nanotube. First figure is the reference state. The colors of the atoms have no significance and are only to enable easy visualization.

Relevant Publication: Symmetry-Adapted Phonon Analysis of Nanotubes. Amin Aghaei, Kaushik Dayal, and Ryan Elliott. J. Mech. Phys. Solids, 61:557, 2013.

2.1.1 Dependence of Sounds Speeds on Pre-Stretch

External loads typically have an indirect influence on phonon curves, i.e., they influence the phonon curves by changing the state about which linearization is performed. We show that in nanotubes, the axial load has a direct first-order influence on the long-wavelength behavior of the transverse acoustic (TA) mode. In particular, when the tube is force-free, the TA mode frequencies vary quadratically with wave number and have curvature (second derivative) proportional to the square-root of the nanotube's bending stiffness. When the tube has non-zero external force, the TA mode frequencies vary linearly with wave number and have slope proportional to the square-root of the axial force. Therefore, the TA phonon curves – and associated transport properties – are not material properties but rather can be directly tuned by external loads. In addition, we show that the out-of-plane shear deformation does not contribute to this mode and the unusual properties of the TA mode are exclusively due to bending. Our calculations consist of 3 parts: First, we use a linear chain of atoms as an illustrative example that can be solved in close-form; second, we use our recently developed symmetry-adapted phonon analysis method to present direct numerical evidence; and finally, we present a simple mechanical model that captures the essential physics of the geometric nonlinearity in slender nanotubes that couples the axial load directly to the phonon curves. We also compute the density of states and show the significant effect of the external load.

Relevant Publication: Anomalous Phonon Behavior of Carbon Nanotubes: First-Order Influence of External Load. Amin Aghaei, Kaushik Dayal, and Ryan Elliott. J. Appl. Phys., 113:023503, 2013.

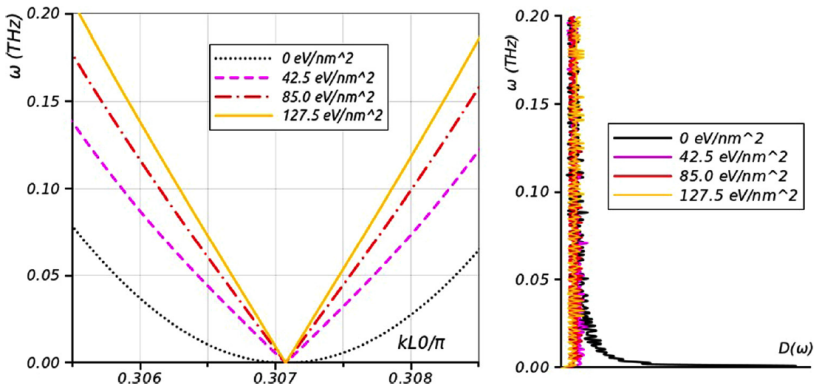

FIG. 3. The effect of axial stress on (left) the dispersion relation of the TA phonon modes and (right) the DOS of a (7, 6) SWNT.

Figure 3: The leading-order dependence of the long-wavelength frequency of the phonon modes for different levels of axial stress.

2.2 Multiscale Methods for Electron Scattering at Defects

We consider the scattering of incident plane-wave electrons from a defect in a crystal modeled by the time-harmonic Schrodinger equation. While the defect potential is localized, the far-field po- tential is periodic, unlike standard free-space scattering problems. Previous work on the Schrodinger equation has been almost entirely in free-space conditions; a few works on crystals have been in one- dimension. We construct absorbing boundary conditions for this problem using perfectly matched layers in a tight-binding formulation. Using the example of a point defect in graphene, we examine the efficiency and convergence of the proposed absorbing boundary condition.

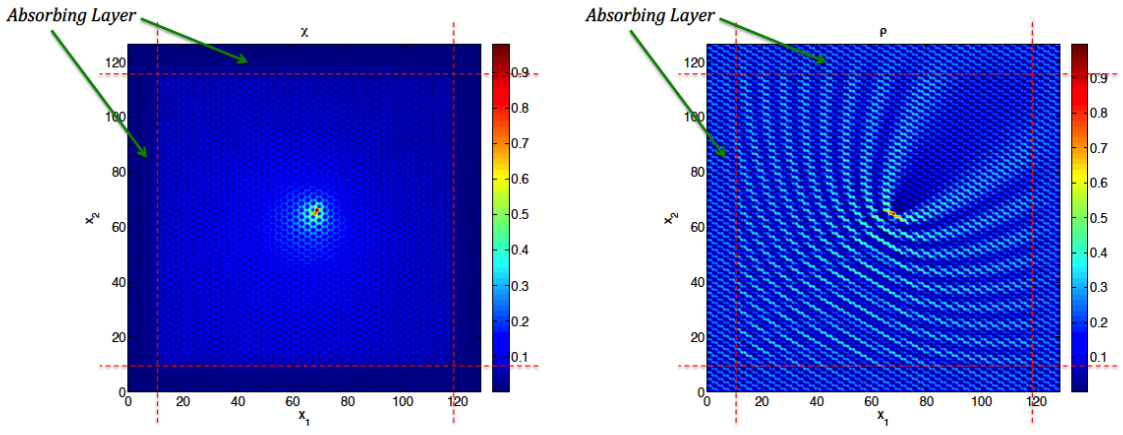

Figure 4: Perfectly matched layers (PML) to compute electron scattering at defects in extended crystalline systems (2D graphene). Left: the scattered wave; right: the incident and scattered wave superposed. It can be noticed that there is minimal spurious reflection into the computational domain.

While current work has demonstrated it for flat graphene sheets, ongoing work is extending it to

graphene and other 2D materials undergoing complex bending deformations.

Relevant Publications: Computational Multiscale Methods for Defects: 1. Line Defects in Liquid Crystals; 2. Electron Scattering in Defected Crystals Hossein Pourmatin Ph.D. Thesis in Computational Mechanics, Carnegie Mellon University, 2014; Multiscale Real-Space Quantum-Mechanical Tight-Binding Calculations of Electronic Structure in Crystals with Defects using Perfectly Matched Layers. Hossein Pourmatin and Kaushik Dayal. Submitted.

2.3 Quasi Objective Structures to Model Complex Bending Deformations in 2D Nanostructures

We develop a multiscale method for defects in low-dimensional atomic and molecular systems that undergo complex bending deformations with non-zero Gaussian curvature. Standard multiscale atomistic methods for defects are largely in the context of crystals, including flat atomic layers. Far from the defect, these methods exploit the close-to-crystalline aspect of the deformation, and approximate the structure locally by a perfect crystal to enable efficient computation. Recent multiscale methods that extend these approaches to curved nanostructures are restricted to deformations with vanishing Gaussian curvature. Therefore, they cannot see the leading order membrane or stretching energy, though this energy can greatly dominate the bending energy when deformations have non-zero Gaussian curvature.

We therefore introduce a multiscale atomistic framework for two-dimensional materials that can capture the energetics of deformations with Gaussian curvature. Our technical strategy is based on a generalization of Objective Structures (OS) introduced by James; OS are a large class of nanostructures with symmetry properties that are rooted in frame-indifference. OS have many attractive features, e.g., a connection to group theory, potentially a fundamental basis in the structure of materials analogous to crystals, and so on. While OS have these attractive properties that make them valuable as a tool for multiscale modeling, they do not include extended nanostructures with Gaussian curvatures. Therefore, our technical strategy introduces a generalization of OS, that we term quasi-OS (qOS). qOS have the property that they can have Gaussian curvature, but recover the attractive properties of OS in certain key limits such as vanishing Gaussian curvature. We use qOS as a means to efficiently estimate energies and forces in large portions of the naostructure away from the defect, thereby enabling multiscale calculations for large systems.

We apply the multiscale method to two key problems relating to defects and their interaction with imposed deformations. First, we examine the behavior of a dislocation in a graphene sheet. We find that the reduction in the bending rigidity in graphene due to a single dislocation is about 40in the configuration that we consider. Second, we examine the behavior of foreign particles on the surface of a gel-phase lipid bilayer. Treating the region of lipid bilayer in the vicinity of the particles as defected enables us to examine a setting of relevance to endocytosis. We find that the interplay between the natural curvature of the membrane and the local curvature induced by the nanoparticles plays an important role in the self-assembly of the nanoparticles on the surface. In addition to these examples, we compare our method in certain settings with full molecular statics to examine the error induced by our approximations.

Relevant publication: Symmetry-Adapted Molecular Modeling of Nanostructures and Biomem-

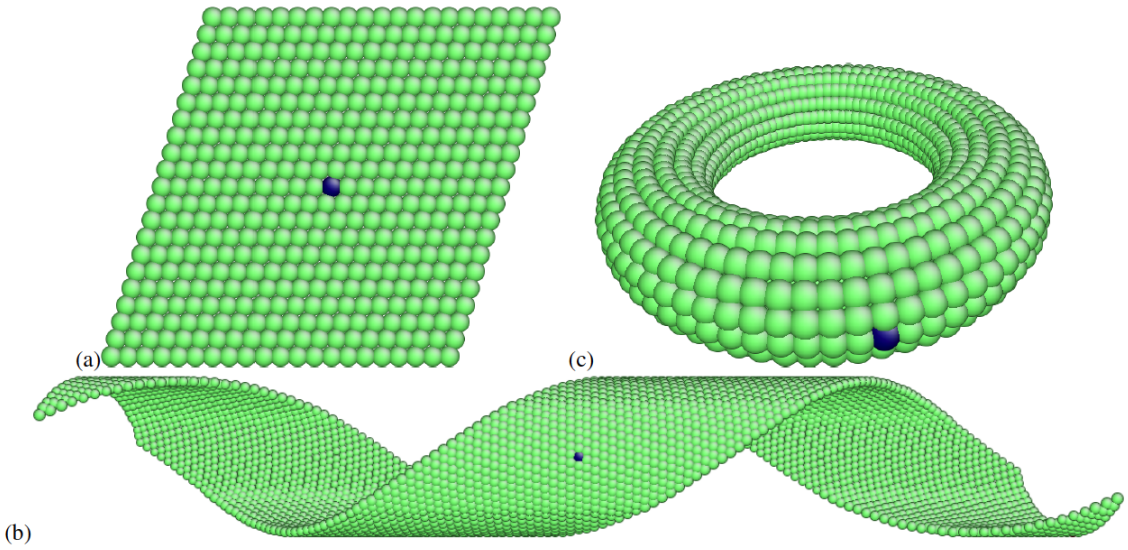

Figure 5: (a) and (b) are examples of perfect Objective Structures; atoms away from the boundary all feel the same environment. (c) is a torus in which different atoms see different environments. This is closely related to a sheet with non-zero Gaussian curvature which is not an OS, even locally. The multiscale strategy is to approximate different parts of the sheet by patches taken from different tori.

branes Amin Aghaei Ph.D. Thesis in Computational Mechanics, Carnegie Mellon University, 2013

2.4 Strain Gradients in Nanostructures, Liquid Crystal Defects, Statistical Mechanics of Electromechanical Materials

While not possible to apply in bulk crystals easily, in nanostructures it is possible to apply large strain gradients even with relatively small strains. Flexoelectricity is a continuum model for the coupling between strain gradients and induced polarizations at these scales. OS provides a natural framework to understand strain gradients in nanostructures. Most technologically relevant ferroelectrics typically lose piezoelectricity above the Curie temperature. This limits their use to relatively low temperatures. Exploiting a combination of flexoelectricity and simple functional grading, we propose a strategy for high-temperature electromechanical coupling in a standard thin film configuration. We use continuum modeling to quantitatively demonstrate the possibility of achieving apparent piezoelectric materials with large and temperature-stable electromechanical coupling across a wide temperature range that extends significantly above the Curie temperature. With Barium and Strontium Titanate, as example materials, a significant electromechanical coupling that is potentially temperature-stable up to 900 C is possible.

Relevant publication: Piezoelectricity above the Curie temperature? Combining flexoelectricity and functional grading to enable high-temperature electromechanical coupling. Raouf Mbarki, Nadia Baccam, Kaushik Dayal, and Pradeep Sharma. Appl. Phys. Lett., 104:122904, 2014.

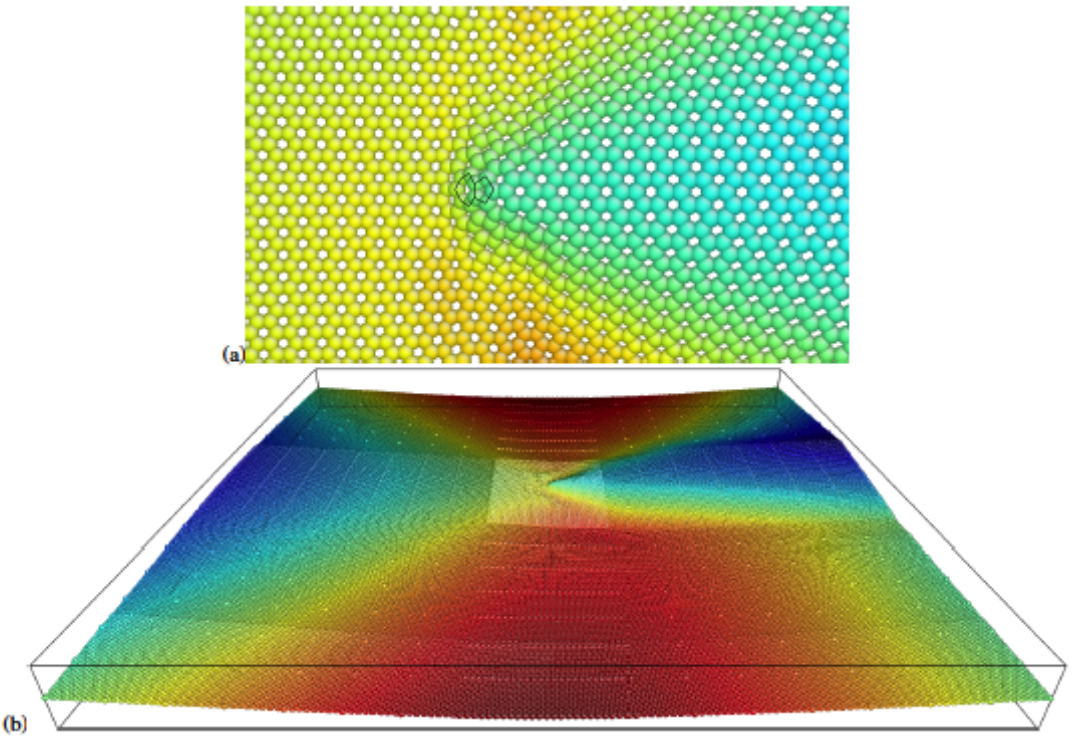

Figure 6: Example of dislocation in a graphene sheet. Top: the atomic configuration of the unrelaxed dislocation; bottom: the relaxed configuration showing complex bending that is not localized at the defect core.

Nematic liquid crystals composed of rod-like molecules have an orientational elasticity that accounts for the energetics of the molecular orientation. This elasticity can be described by a unit vector field; the unit vector constraint interacts with even fairly simple boundary conditions to cause discli- nation defects. Disclinations are entirely a topological consequence of the kinematic constraint, and occur irrespective of the particular energetic model. Because disclinations are topological defects, they cannot be regularized by adding higher gradients, as in phase-field models of interface defects. On the contrary, the higher gradient terms would cause even greater singularities in the energy. In this paper, we formulate an integral-based nonlocal regularized energy for nematic liquid crystals. Our model penalizes disclination cores and thereby enforces a finite width, while the integral regularization ensures that the defect core energy is bounded and finite. The regularization at the same time tends to the standard gradient-based energies away from the disclination, as well as building in the head-tail symmetry. We characterize the formulation in its ability to describe disclinations of various strengths, and then apply it to examine: (1) the stability and decomposition of various disclinations, and the competition between bend and splay energies in determining the relative stability of integer and half-integer disclinations (2) the coalescence of a plus-half and minus-half disclination pair; we find the disclinations do not move at the same velocities towards each other, suggesting that the asymmetry of the director field plays a dominant role despite the equal-and-opposite topological strengths of the disclinations.

Relevant publications: Disclinations without Gradients: A Nonlocal Model for Topological De-

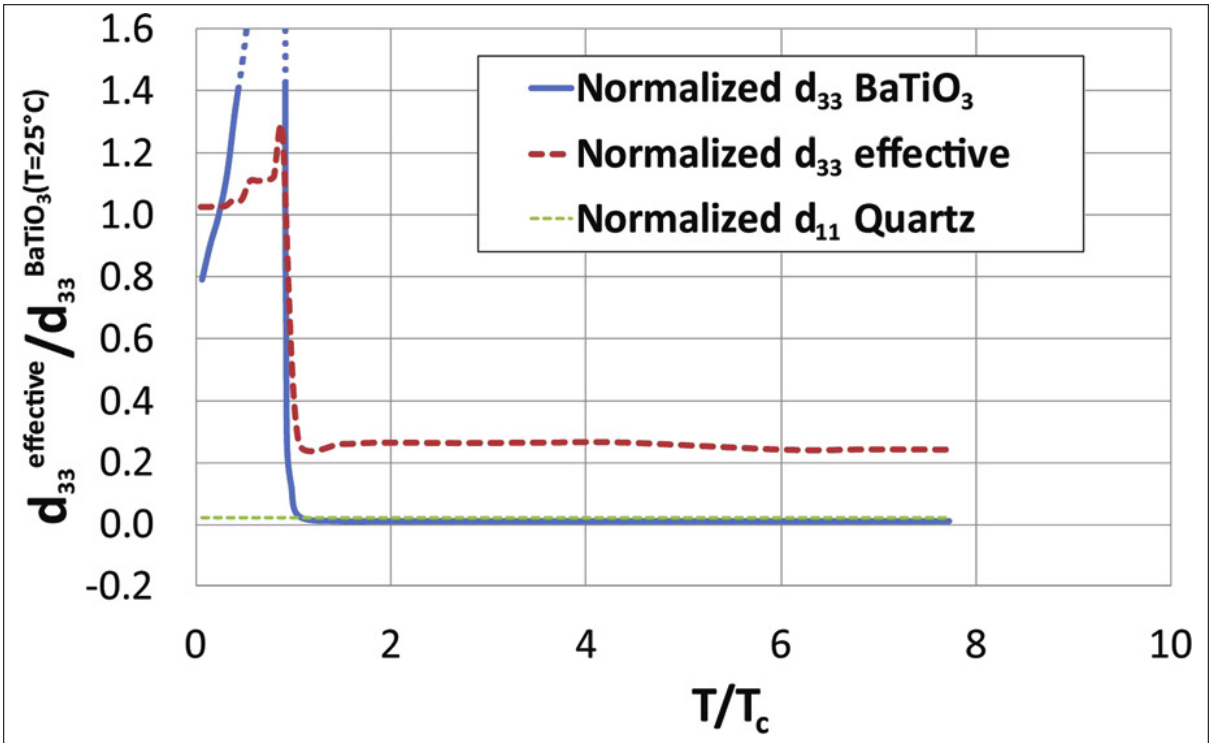

Figure 7: A combination of strain gradients and compositional gradients provides a prediction that flexoelectric deformation-polarization coupling (dashed thick curve) will be observed well above the Curie temperature of the individual component ferroelectrics. Quartz and barium titanate are shown for comparison as benchmark piezoelectric and ferroelectric materials.

fects in Liquid Crystals. Robert Macedo, Hossein Pourmatin, and Kaushik Dayal. Submitted.

A multiscale analysis of the electromechanical coupling in elastic dielectric is conducted, starting from the discrete monomer level through the polymer chain and up to the macroscopic level. Three models for the local relations between the molecular dipoles and the electric field that can fit a variety of dipolar monomers are considered. The entropy of the network is accounted for within the framework of statistical mechanics with appro- priate kinematic and energetic constraints. At the macroscopic level closed form explicit expressions for the behaviors of amorphous dielectrics and isotropic polymer networks are determined. None of which admits the commonly assumed linear relation between the polarization and the electric field. The analysis reveals the dependence of the mac- roscopic coupled behavior on three primary microscopic parameters: the model assumed for the local behavior, the intensity of the local dipole, and the length of the chain. We show how these parameters influence the directional distributions of the monomers and the hence the resulting overall response of the network. In particular, the dependences of the polarization and the polarization induced stress on the deformation of the dielectric are illustrated. More surprisingly, we also reveal a dependence of the stress on the electric field which stems from the kinematic constraint imposed on the chains.

The above analysis makes important simplifying assumptions, namely that the interactions between charges within the system are negligible compared to the interaction with the external field. Ongoing work aims to relax this assumption.

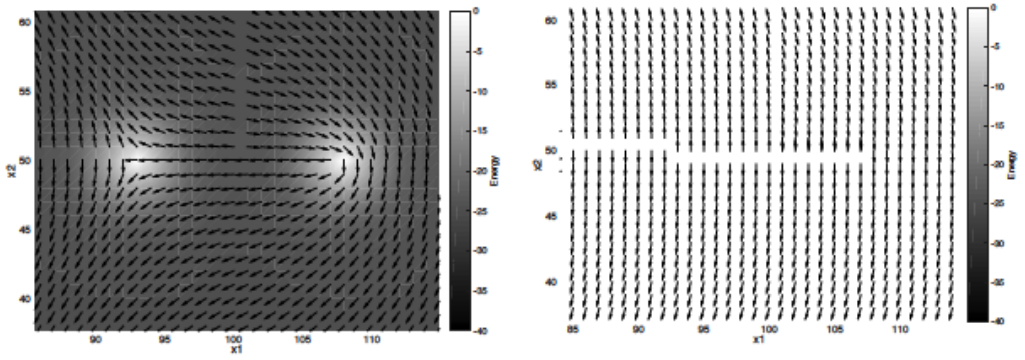

Figure 7: Initial configuration (left) with two $\pm\frac{1}{2}$ defects, and the final defect-free configuration (right).

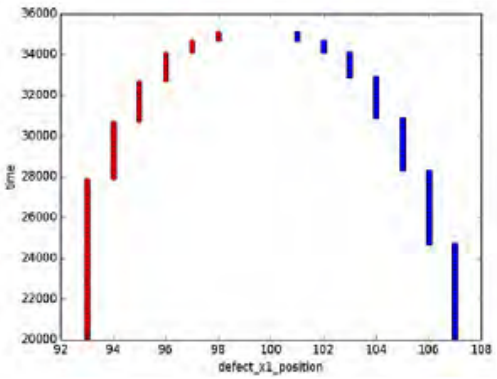

Figure 8: Disclination core positions as a function of time. Red circles are $-\frac{1}{2}$ and blue squares are $+\frac{1}{2}$. The disclination cores are located by finding the mesh point with the highest energy density. The motion appears discontinuous because we only sample over a discrete mesh. The higher velocity of the $+\frac{1}{2}$ disclination is clear from the plot. The velocity increases as the disclinations approach, as is expected.

Figure 8: Coalescence of a +1/2 and -1/2 defect pair showing asymmetry in the approach velocities of the defects.

3 Papers and PhD Theses

- Computational Multiscale Methods for Defects: 1. Line Defects in Liquid Crystals; 2. Electron Scattering in Defected Crystals Hossein Pourmatin Ph.D. Thesis in Computational Mechanics, Carnegie Mellon University, 2014
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- Electroelasticity of polymer networks. Noy Cohen, Kaushik Dayal, and Gal deBotton. To appear in J. Mech. Phys. Solids.
- Multiscale Real-Space Quantum-Mechanical Tight-Binding Calculations of Electronic Structure in Crystals with Defects using Perfectly Matched Layers. Hossein Pourmatin and Kaushik Dayal. Submitted.
- Disclinations without Gradients: A Nonlocal Model for Topological Defects in Liquid Crystals. Robert Macedo, Hossein Pourmatin, and Kaushik Dayal. Submitted.
- Fractional Hereditariness of Lipid Membranes: Instabilities and Linearized Evolution. Luca Deseri, Pietro Pollaci, Massimiliano Zingales, and Kaushik Dayal. To appear in J. Mech. Behav. Biomed. Mater.
- Piezoelectricity above the Curie temperature? Combining flexoelectricity and functional grading to enable high-temperature electromechanical coupling. Raouf Mbarki, Nadia Baccam, Kaushik Dayal, and Pradeep Sharma. Appl. Phys. Lett., 104:122904, 2014.
- Atomistic-to-Continuum Multiscale Modeling with Long-Range Electrostatic Interactions in Ionic Solids. Jason Marshall and Kaushik Dayal. J. Mech. Phys. Solids, 62:137, 2014. Invited Article for the Rodney Hill Anniversary Issue.
- Anomalous Phonon Behavior of Carbon Nanotubes: First-Order Influence of External Load. Amin Aghaei, Kaushik Dayal, and Ryan Elliott. J. Appl. Phys., 113:023503, 2013.
- Symmetry-Adapted Phonon Analysis of Nanotubes. Amin Aghaei, Kaushik Dayal, and Ryan Elliott. J. Mech. Phys. Solids, 61:557, 2013.
- Tension-and-Twist of Chiral Nanotubes: Torsional Buckling, Mechanical Response, and Indicators of Failure. Amin Aghaei and Kaushik Dayal. Modelling Simul. Mater. Sci. Eng., 20:085001, 2012.

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Abstract

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4) new strategies using strain gradient effects at the nanoscale ("flexoelectricity") to achieve temperature-

stable electromechanical coupling for high temperatures
5) development of new models for defect dynamics in liquid crystals
6) the statistical mechanics of non-crystalline materials.

The methods will be relevant to many other nanostructures and materials of interest to the Air Force, particularly electronic materials and energy-storage materials.

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None.

Change in AFOSR Program Manager, if any:

Dr. Fariba Fahroo was replaced by Dr. Jean-Luc Cambier.

Extensions granted or milestones slipped, if any:

NCE from Jun 31 2015 to Dec 31 2015.

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

Report Document - Text Analysis

Appendix Documents

2. Thank You

E-mail user

Mar 31, 2016 23:00:41 Success: Email Sent to: kaushik.dayal@cmu.edu