Princeton Center for Theoretical Science

The Princeton Center for Theoretical Science is dedicated to exploring the frontiers of theory in the natural sciences. Its purpose is to promote interaction among theorists and seed new directions in research, especially in areas cutting across traditional disciplinary boundaries.

The Center is home to a corps of Center Postdoctoral Fellows, chosen from nominations made by senior theoretical scientists around the world. A group of senior Faculty Fellows, chosen from science and engineering departments across the campus, are responsible for guiding the Center. Center activities include focused topical programs chosen from proposals by Princeton faculty across the natural sciences. The Center is located on the fourth floor of Jadwin Hall, in the heart of the campus "science neighborhood". The Center hopes to become the focus for innovation and cross-fertilization in theoretical natural science at Princeton.

Faculty Fellows
Paul Steinhardt, Director (on leave 2012-2013)
Igor Klebanov, Acting Director
Adam Burrows, Acting Associate Director
Curtis Callan
Roberto Car
Garnet Chan
David Huse
Jeroen Tromp
Herman Verlinde

Center Postdoctoral Fellows
Daniel Harlow 2012-2015
Yoav Kallus 2011-2014
Samuel Lee 2012-2015
Mariangela Lisanti 2010-2013
Joseph Maciejko 2011-2014
Elisabetta Matsumoto 2011-2014
Timothy Merlis 2011-2014
Rahul Nandkishore 2012-2015
Marco Schiro′ 2010-2013
Alexander Tchekhovskoy 2010-2013
Mosahito Yamazaki 2010-2013

To find out more about Center Postdoctoral Fellowships and Programs see:
http://pcts.princeton.edu/pcts

PRINCETON CENTER FOR THEORETICAL SCIENCE

Through the Looking Glass: A Glimpse into the Geometry and Topology of Materials

POSTER SESSION
3 December 2012
Jadwin Hall, Room 407
5:00 – 7:00 pm

Program Organizers

Elisabetta Matsumoto, PCTS, Princeton University
Christian Santangelo, University of Massachusetts, Amherst

Through the Looking Glass: A Glimpse into the Geometry and Topology of Materials

3-5 December 2012

POSTER SESSION

Title: "Characterizing the building blocks of polycrystals"

Contributor: Emanuel Lazar, Columbia University

Abstract: The underlying structure of materials such as polycrystalline metals and ceramics can be viewed as cell decompositions of real 3-dimensional space. A first step in characterizing these structures involves characterizing the topology of its constituent 3-cells. In a recent paper, the authors introduced a method to completely describe the topology of individual grains, bubbles, and cells in three-dimensional polycrystals, foams, and other multicellular microstructures. After briefly describing this method, we present some data collected from grain-growth and Poisson-Voronoi tessellations. We describe some of the key topological features which distinguish these structures from one another and suggest further lines of research building on this work.

Title: Coarsening Dynamics of Curved Hexagonal Phases

Contributor: Nicolás. A García, Leopoldo R. Gómez, Daniel A. Vega
Universidad Nacional del Sur-CONICET
Bahía Blanca, Argentina.

Abstract: The coarsening dynamics of two dimensional hexagonal phases deposited on curved backgrounds is studied for the first time by using numerical simulations. An initial liquidlike disordered system is quenched into the hexagonal phase and the ordering process is followed as a function of time for different curvatures of the underlying substrate. Early hexagonal seeds preferentially form in regions of low curvature, where the geometrical frustration in the lattice is reduced. The growth of these seeds creates a polycrystalline phase containing out of equilibrium defect configurations. Further relaxation towards equilibrium involves mechanisms of grain growth and defect annihilation, where the strain field introduced by the geometry is partially screened out by topological defects.

Title: "Computational Characterization of Microporous Networks and Discovery of Shape-selective Materials for Separations and Catalysis"

Contributors: E. L. First, C. E. Gounaris, J. Wei, and C. A. Floudas

Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, USA

Abstract: Crystalline microporous materials, such as zeolites and metal-organic frameworks (MOFs), are commonly used for shape-selective separations and catalysis, in which molecules are discriminated based on their shape and size. With the large number of structures available, computational techniques are needed to select from databases the most promising structures for an application. We have developed a computational approach based on mathematical optimization, computational geometry, and graph theory to study the three-dimensional pore structure of microporous materials. The method describes and classifies all void spaces by identifying portals, channels, cages, and their connectivity. The pore characterizations are used to calculate important quantities such as pore-size distribution, accessible volume, surface area, largest-cavity and pore-limiting diameters, and probability of pore occupancy.

Our method has been applied to several databases of materials including zeolites, hypothetical zeolites, zeolite-like structures, MOFs (including zeolitic imidazolate frameworks, ZIFs), and hypothetical MOFs. By aggregating data from a variety of structures, we gain insights about the size selectivity of microporous materials. Additionally, we have developed methods to compute the activation energy required for guest molecules to pass through portals and the possible pathways that molecules can take. This enables us to calculate the shape selectivity between two molecules in a given microporous structure, and by screening databases of materials, we identify the best materials for a given application.

We have created the freely-available web tools ZEOMICS (http://helios.princeton.edu/zeomics/) and MOFomics (http://helios.princeton.edu/mofomics/) that implement our algorithms. and feature online databases of pore structure characterizations. They offer user-friendly interfaces that enable users to submit structures of interest to be automatically processed on our servers. A three-dimensional display provides colorful visualizations of the pore structures.

References:

1. First, E. L., Floudas, C. A. MOFomics: Computational pore characterization of metal-organic frameworks. *Microporous and Mesoporous Materials*, 165:32–39, 2013.
2. First, E. L., Gounaris, C. E., Wei, J., and Floudas, C. A. Computational characterization of zeolite porous networks: an automated approach. *Physical Chemistry Chemical Physics*, 13(38):17339–17358, 2011.
3. Gounaris, C. E., Wei, J., Floudas, C. A., Ranjan, R., and Tsapatsis, M. Rational design of shape selective separations and catalysis: Lattice relaxation and effective aperture size. *AIChE Journal*, 56(3):611–632, 2009.
4. Gounaris, C. E., Wei, J., and Floudas, C. A. Rational design of shape selective separation and catalysis–II: Mathematical model and computational studies. *Chemical Engineering Science*, 61(24):7949–7962, 2006.
5. Gounaris, C. E., Floudas, C. A., and Wei, J. Rational design of shape selective separation and catalysis–I: Concepts and analysis. *Chemical Engineering Science*, 61(24):7933–7948, 2006.

Title: Creating Controlled Thickness Gradients in Polymer Thin Films via Flowcoating

Contributor: RALEIGH DAVIS, SAHANA JAYARAMAN, RICHARD REGISTER, PAUL CHAIKIN

Abstract: Flow coating is a technique which has a unique capacity to create polymer thin (10-1000 nm) films which possess a thickness gradient. This has greatly enhanced the throughput of many experiments which seek to investigate the effect of film thickness on polymer structure or properties by enabling one to study a wide range of film thicknesses using only a single

flowcoated sample. Until recently, there was limited understanding of how to predict or control the film thickness profiles generated with this device. A recently published first-principles approach uses Landau-Levich theory to derive an equation which identifies the experimental variables which are thought to govern film thickness. These parameters are the capillary number (a function of the solution viscosity, surface tension, and coating blade velocity) as well as the gap height between the blade and the substrate. In this work, many of these experimental variables, as well as some others, were varied and the resulting film thickness values showed excellent quantitative agreement with the model. These results, coupled with the first principles model, provide a design method which allows a user to produce polymer thin films of virtually any desired thickness profile.

Title: Defect Induced Shape Instabilities in Hexagonally Textured Free-Standing Membranes

Contributor: Aldo D. Pezzutti, Marcelo A. Villar, and Daniel A. Vega
Universidad Nacional del Sur-CONICET
Bahía Blanca, Argentina.

Abstract: We study the coupling between geometry and defects in flexible membranes suffering a symmetry breaking phase transition. The system is described through a simple model that includes a Brazovskii contribution for the crystalline phase and a Helfrich-Canham free energy penalization for the membrane shape. At the early stage of the phase separation process there is a poor coupling between the membrane shape and the order parameter describing liquid-to- crystal transition. Then, the membrane geometry is determined by the bending stiffness and surface tension. During the nucleation and growth process, defects appear naturally. The overall dynamics is governed by the interplay between the geometry of the host membrane and the defects of the hexagonal texture.

Title: “Defect mechanics in crystalline packings of spherical caps”

Contributor: Amir Azadi, Hasbrouck Laboratory, University of Massachusetts, Amherst

Abstract: Topological defects are ubiquitous in 2D curved crystals. We study the structural features and underlying principals of dislocation mechanics in a crystalline spherical cap. Using nonlinear elasticity, we show that frustration arising from the curvature drives the stability of finite length radial grain boundaries in the ground-state packing. For sufficiently large caps at intermediate Gaussian curvature, linear arrays of dislocations relieve the geometric stresses. The number and length of grain boundaries grows with both the curvature and the size of crystalline patch. We also determine the elastic response of the system subject to radial tension. The interplay between the geometrically induced stresses and the tension leads to inhomogeneous stresses that determines the stability of the grain boundaries. The imposed tension stretching the curved crystal radially destabilizes the curvature-induced compressive zone and decrease the length of the grain boundaries. We characterize the transition from a polycrystalline structure to the perfect packing where all dislocations will be expelled at a critical tension that depends on the system size and the curvature. We find scaling laws for the number and length of minimal configurations of grain boundaries.

Title: Distorted tetrahedral shapes of nematic vesicles

Contributor: Nguyen Thanh Son and Jonathan V. Selinger

Abstract: In all membranes with internal orientational or crystalline order, there is a geometric coupling between the 2D internal order and the 3D shape. Nonuniformity in the internal order tends to induce curvature, and curvature provides an effective potential acting on the internal order. For a closed vesicle with nematic liquid-crystalline order, there must be a total topological charge of +2, which will normally occur as four defects of charge +1/2 each. Previous research has suggested that these four defects will form a regular tetrahedron, leading to a tetrahedral shape of the vesicle [1], which may be useful in designing colloidal particles for photonic applications [2]. Here, we develop an explicit model to calculate the energies of defect structures in nematic vesicles. When the liquid-crystal interaction energy is a purely 2D intrinsic interaction, we find that the perfect tetrahedral shape is stable only up to a maximum interaction strength (Frank constant), at which point it changes to an elongated rectangular configuration. When the liquid-crystal interaction energy is 3D intrinsic and extrinsic interaction, the perfect tetrahedral shape is never stable; the vesicle is a distorted tetrahedron for small Frank constant and a highly elongated rectangle for larger Frank constant. These results show the difficulty in designing tetrahedral structures for photonic crystals.

[1] J. Park, T. C. Lubensky, and F. C. MacKintosh, Europhys. Lett. 20, 279 (1992).

[2] D. R. Nelson, Nano Lett. 2, 1125 (2002).

Title: Dynamics of flexible bodies

Contributor: James Hanna, University of Massachusetts

Abstract: We present two examples of flexible body dynamics: 1) standing waves on a rotating conical sheet, 2) reflection of a wave from the free end of a towed string.

Title: "Sound is shape: Infinitesimal inverse spectral geometry of graphs"

Contributor:Tejal Bhamre

Abstract: In 1966, Kac posed the famous question 'Can one hear the shape of a drum', that is, is there a relationship between the shape of flat membranes and their acoustic oscillation spectrum.

The general field of inverse spectral geometry also studies how to deduce the geometric shape of a curved manifold from the spectra of operators on it. This could have basic applications in physics, because it relates differential geometry, the language of general relativity, to the language of quantum theory, functional analysis. For example, using spectral geometry, it has been proposed that spacetime can be both continuous and discrete simultaneously, mathematically in the same way that information can.

Here, we study spectral geometry by looking at a discrete, finite dimensional version of the problem of inverse spectral geometry. To this end, we sample the manifold at discrete points. We developed an algorithm to constructively build up the shape of our manifold up to the scale of the spacing of our samples. Our results yield a discrete 'Fourier transform' between sound and shape.