

CMS Summer school on 'Microstructure: evolution and dynamics'
Aug 25-29, 2013

Schedule

	SUN	MON	TUE	WED	THU
9:00-10:00		Carlen	Zimmer	Voorhees	Wetton
10:00-11:00	Promislow	Wetton	Voorhees	Zimmer	Promislow
11:00-12:00	Zimmer	Tsori	Sternberg	Golovaty	Rabkin
	Talmon		Lunch		
12:00-14:00			Lunch	Excursion	
14:00-15:00		Zimmer	Wetton		Voorhees
15:00-16:00	Carlen				
16:00-17:00	Wetton	Promislow	Carlen		
		Bus stops at Beach	Bus stops at the German colony	Excursion	Bus stops at Beach

There will be 5 lecture mini-series, given by our main speakers. Each mini-lecture series will consist of four one hour lectures. In addition, there will be several outreach lectures (marked in green) in which potential applications are emphasized.

The first workshop lecture will begin on Sunday at 9:30, and the final workshop lecture will end on Thursday evening. Note that the schedule on Sunday is delayed at half an hour during the whole day (14:00 lecture starts at 14:30, etc).

On Tuesday we will have lunch for all participants in Amado 8th floor lounge between 12:00-14:00. An excursion to Akko will leave Wednesday at 12:00, we will eat lunch at Hummus Said in Akko. On other days, lunch (participants on their own) & discussion time is set between 12:00-14:00.

Accommodation for participants is provided at a hotel outside the campus. We will provide transportation to and from the hotel. The bus will make optional stops at places of interest, e.g., the beach or the German colony.



Program

Mini-courses series program

Eric Carlen (Rutgers University)
[Kinetic theory methods in phase kinetics](#)

Keith Promislow (Michigan State University)
[Structure formation in multi-component polymer materials](#)

Peter Voorhees (Northwestern University)
[Interfacial Evolution in Materials](#)

Brian Wetton (University of British Columbia)
[Numerical methods for energy gradient flows from materials science models](#)

Jonathan Zimmer (University of Bath)
[Upscaling from particles to PDEs](#)

Outreach lectures

Dmitry Golovaty, The University of Akron
[Connecting the discrete and continuum theories for carbon nanotubes – a simple example](#)

Yoav Tsori, BGU
[Statics and dynamics of phase transitions in electric fields](#)

Ishi Talmon, Technion
[Cryo-TEM and Cryo-SEM of Nanostructured Liquid Systems](#)

Eugen Rabkin, Technion
[Capillary-driven topography and microstructure evolution in metals: matching experiment with theory](#)

Peter Sternberg, Indiana University
[Identifying Global Minimizers to a Nonlocal Isoperimetric Problem](#)

Minicourse abstracts

[Kinetic theory methods in phase kinetics](#)

Eric Carlen (Rutgers University)

The phenomena of interest in phase kinetics can be viewed on many different space and time scales. On a very large scale, observed over long times, phase interfaces appear very sharp, and the evolution is specified in terms of equations for the motion of the sharp interface. On shorter “mesoscopic” length scales over which the the interface between the phases is not sharp, one has different equations, typically of Cahn-Hilliard type, for the phase densities. It is of interest to relate the solutions of the equations of motion for the sharp interface to solutions of the mesoscopic equations. A typical way to approach such a problem is to use matched asymptotic expansions.

A similar problem arises in the kinetic theory of dilute gasses in which one seek to relate solutions of the Euler equation to solutions of the Boltzmann equation. A different set of methods developed by Caflisch has been successful *this context, which is based on a controlled Chapman-Enskog expansion. Recent joint work with Carvalho and Orlandi has developed this approach in the phase kinetics setting. In these lectures, we shall explain this approach, and develop some of tools need to apply it, with special emphasis on potential applications involving surface diffusion.*

[Structure formation in multi-component polymer materials](#)

Keith Promislow (Michigan State University)

The Cahn-Hilliard free energy has a rich history as a model of coarsening in binary mixtures of incompatible materials. However many of the polymeric materials of interest for energy conversion applications do not coarsen, that is phase separate into larger and larger domains, rather they self-assemble nanoscale networks that serve the charge-selective networks that drive fuel cells, bulk heterojunction solar cells, and membrane separators in Lithium ion batteries. Self assembly in polymeric materials is mediated by functionalization of polymers, that is the attachment of ionic sidechains which modify their solubility, rendering them amphiphilic. The free energy of functionalized polymers rewards the formation of interface and has complicated relations between local density of the constituent phases and the material pressure.

We present the functionalized Cahn-Hilliard free energy, a higher-order reformulation of the Cahn-Hilliard free energy, which remaps the critical points, in particular it rewards critical points with high interfacial surface area and low mixture pressure. The analysis of the FCH and its gradient flows requires new techniques, in particular dynamical systems plays a much larger role in identifying interfacial structures, while differential geometry and extensions of Ricci flows determine morphological evolution. On the other hand, the usual framework of Γ -convergence is up-ended.

We will present an overview of the Cahn-Hilliard free energy, provide sufficient chemical background to motivate the FCH free energy. Explain the role of dynamical systems in interface selection, present the underpinnings of the differential geometric reductions, and derive some simple examples of morphological competition.

[Interfacial Evolution in Materials](#)

Peter Voorhees (Northwestern University)

Central to predicting a broad array of materials properties is the need to know the morphology and spatial distribution of interfaces in a material. These interfaces could be between grains, crystallographic variants of a given phase, or between two phases. A promising approach to predicting the morphology of interfaces for a given processing pathway is the phase field method. In this approach interfaces are modeled as continuous transition regions and thus the boundary conditions that are normally placed at the interfaces in the traditional approach are embedded in the defining partial differential equation. Thus, phase field equations hold throughout the entire domain, thus obviating the need to explicitly track the location of the boundary. A further advantage of phase field methods is the ability to include a very wide range of driving forces for interface motion, from magnetic to electrical and chemical and that they allow for topological transitions. Finally, the flexibility of the method enables experimentally measured complex three-dimensional structures to be used as initial conditions in a phase field code. If the morphology of the interfaces is measured using a non-destructive technique, such as X-ray tomography, then it is possible to compare the detailed morphology predicted by simulation and that measured experimentally at a later time. The phase field equations will be developed, and the connection with experiment will be emphasized. Finally, a discussion of the phase field crystal method, a phase field method that models the atomic evolution of materials on diffusive time scales, will be given.

[Numerical methods for energy gradient flows from materials science models](#)

Brian Wetton (University of British Columbia)

Numerical methods are considered for partial differential equations describing structural evolution in some materials science models. The models are characterized by an energy gradient flow. Examples considered are the Allen-Cahn, Cahn-Hilliard and Functionalized Cahn-Hilliard equations. Basic ideas in spatial and temporal discretization are described, with application to these problems. Sample MATLAB codes for benchmark problems and references to more advanced material will be given. In certain limits of these equations, interfaces moving with certain geometric motions are found. As a final topic, numerical methods for computing these interface motions directly are discussed. Topics by lecture:

1. Introduction and spatial discretization (Finite Difference/Volume, Finite Element, Spectral)
2. Time stepping and the solution of the systems arising from implicit schemes
3. Adaptive strategies
4. Methods for geometric motion of interfaces

[Upscaling from particles to PDEs](#)

Jonathan Zimmer (University of Bath)

One prominent example of microstructures occurs in so-called martensitic materials. These are phase transitions in metals where at low temperatures several stable configurations ("variants") can coexist. To understand the time evolution of such materials, we need to understand the evolution of the underlying microstructure. Our present understanding of this phenomenon is quite limited, and we will focus on the simplest possible case of a single moving interface separating two stable states. As will be discussed in the lectures, the straightforward application of the elastodynamic setting (PDEs) leads to ill-posed equations. Therefore, we start with a microscopic ("atomistic") model, namely a nonlocal Hamiltonian equation of motion. We discuss the rigorous existence theory of travelling interfaces under suitable assumptions. In a second part, a theory going back to Abeyaratne and Knowles and others will be described which allows us to single out special solutions of the equations of elastodynamics, thus rendering the equations of elastodynamics in this setting well-posed by providing a selection criterion. We will describe the current understanding how this selection criterion can be related to the microscopic theory described above, and sketch related open problems.

Outreach lecture abstracts

[Connecting the discrete and continuum theories for carbon nanotubes – a simple example.](#)

Dmitry Golovaty (University of Akron)

A multi-walled carbon nanotube can be visualized as a set of one or more concentric cylindrical graphene sheets. Each graphene sheet is one-atom thick and contains carbon atoms arranged in a hexagonal lattice. Neighboring atoms within a sheet interact via strong covalent bonds, making graphene essentially inextensible, but amenable to large elastic bending deformation. The interaction between the shells is of a weak Van-der-Waals-type and allows for an easy relative sliding between the shells. At the microscopic level, the energy of a multiwalled carbon nanotube consists of the energies of the weak and strong interactions. When upscaled to the macroscopic level, the nanotube can typically be represented by an elastic shell and the strong interactions energy reduces to an elastic energy. The macroscopic analog of weak interactions can be thought of as a pressure-type term that depends only on the local distance between the tubes.

In my talk, I will demonstrate that this reduction is not always correct as the weak interactions also depend on relative arrangements of atoms of the neighboring shells. I will discuss how one can borrow from the idea of a Gamma-development from calculus of variations to obtain a macroscopic Ginzburg-Landau-type model of a multiwalled nanotube. I will also connect the predictions of the model to experimental observations.

Capillary-driven topography and microstructure evolution in metals: matching experiment with theory

Eugen Rabkin (Department of Materials Science and Engineering, Technion)

Development of atomic force microscopy (AFM) allowed measurements of surface topography of solids with unprecedented accuracy. We will show that fine features of the grain boundary grooves observed in AFM cannot be described in the framework of classical Mullins model with isotropic surfaces and immobile grain boundaries. We introduce the model of strong surface anisotropy and demonstrate how facets (i.e. atomically flat surface regions of particularly low energy) nucleate and grow in the grain boundary groove regions [1]. Furthermore, we demonstrate how quantitative analysis of surface features in the wake of migrating grain boundaries allows determining the dynamics of grain boundary movement in the post-mortem studies [2].

Further examples will demonstrate the applications of AFM to the study of thermal stability of thin films. We show how surface anisotropy affects the morphologies obtained in the course of solid state dewetting of thin films [3-5]. Slow diffusivity along the singular surfaces of textured films changes the dewetting mechanism from the surface- to grain- or interphase boundary diffusion controlled one. The models allowing extracting the relevant diffusion parameters from experimentally measured surface topographies will be introduced [4-6].

1. L. Klinger, E. Rabkin Effects of surface anisotropy on grain boundary grooving *Interface Sci.* 9 (2001) 55-63
2. E. Rabkin, Y. Amoyal, L. Klinger Scanning probe microscopy study of grain boundary migration in NiAl *Acta mater.* 52 (2004) 4953-4959
3. O. Malyi, L. Klinger, D.J. Srolovitz, E. Rabkin Size and shape evolution of faceted bicrystal nanoparticles of gold on sapphire *Acta mater.* 59 (2011) 2872-2881
4. O. Malyi, E. Rabkin The effect of evaporation on size and shape evolution of faceted gold nanoparticles on sapphire *Acta mater.* 60 (2012) 261-268
5. D. Amram, L. Klinger, E. Rabkin Anisotropic hole growth during solid-state dewetting of single crystal Au-Fe thin films on sapphire *Acta mater.* 60 (2012) 3047-3056
6. O. Kovalenko, J.R. Greer, E. Rabkin Solid state dewetting of thin iron films on sapphire substrates controlled by grain boundary diffusion *Acta mater.* 61 (2013) 3148-3156

Identifying Global Minimizers to a Nonlocal Isoperimetric Problem

Peter Stenberg (Indiana University)

The nonlocal isoperimetric problem is a variational problem related to the so-called Ohta-Kawasaki energy modeling micro-phase separation in diblock copolymers. The O-K energy is itself a nonlocal perturbation of the classical Cahn-Hilliard energy. In this problem, there are two competing mechanisms—the local one favors low surface area while the nonlocal one favors high surface area. This makes for a rich and complicated energy landscape. After introducing the problem and its main features, I will discuss some work I've done with Ihsan Topaloglu on identifying the global minimizer of this problem in a few settings.

Cryo-TEM and Cryo-SEM of Nanostructured Liquid Systems

Yeshayahu (Ishi) Talmon

Department of Chemical Engineering and The Russell Berrie Nanotechnology Institute (RBNI)

For complete nanostructural characterization of nanostructured liquids ("complex liquids"), i.e., liquid systems with aggregates or building blocks on the nanometric scale, one needs reliable direct-imaging methods. Cryogenic-temperature transmission electron microscopy (cryo-TEM) is now accepted as an essential tool in the study of complex liquids. Methodologies have been developed to capture the nanostructure of liquid systems, while preserving their original state at a given concentration and temperature. Cryo-TEM is now widely used to study synthetic, biological, and medical systems. Originally developed for aqueous systems, it has been also applied successfully in the study of non-aqueous systems. However, this methodology cannot be used to study highly viscous systems, or those containing objects larger than several hundreds of nanometers. For those we need scanning electron microscopy (SEM).

Liquid nanostructured systems can now be studied by cryo-SEM, using much-improved cryogenic specimen holders and transfer systems. That and recent developments in high-resolution scanning electron microscopy (HR-SEM) have made it an ideal tool for the study of nanoparticles and colloids in viscous systems, or in systems containing large objects, hundreds of nanometers and larger, in which small (nanometric) features are to be imaged. Improved field-emission electron guns, electron optics

and detectors have made it possible to image features down to a few nanometers. In recent years we have developed a novel cryo-SEM methodology that preserves the original nanostructure of labile complex liquids at specified composition and temperature, quite similarly to what had been done in cryo-TEM. It can be used to directly image aqueous and nonaqueous systems alike.

In my talk I will describe briefly the continuously evolving state-of-the-technology of cryo-TEM and cryo-SEM, and demonstrate the application of these complementary methodologies in the study of nanostructured liquids, showing examples how it has helped support theoretical models. I will present recent data on polyelectrolyte complexes, including lipoplexes of DNA and cationic lipids, and high-resolution direct imaging of microemulsions and of carbon nanotubes in solution and in a nematic phase in chlorosulfonic acid.

[Statics and dynamics of phase transitions in electric fields](#)

Yoav Tsori (Ben Gurion University of the Negev)

Phase transitions can be provoked by a change of the temperature, concentration, pressure, etc. Electric fields are interesting because they are switchable and become more effective as the system size decreases. We will review the recent fundamentals understanding gained in phase transitions in field gradients. This demixing has consequences in microfluidic flows, in electrolubrication, in chemical reactions, and in colloidal stabilization. If time permits we will describe a mathematical model for the demixing dynamics and a new type of interfacial instability.