# 13w5004/Mathematics and Mechanics in the search for new Materials

## ABSTRACT

| | Name | Speaker? | Constraint | Title | Abstract |
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| | Abeyaratne, Rohan | No | | | |
| | Ball, John | No | | | |
| | Banerjee, Amartya | Tue | No Friday | A Novel Spectral Scheme for Abinitio Simulations of Objective Structures | Objective structures are atomic/molecular configurations which generalize the notion of crystals and are such that all the constituent atoms/molecules of the structure "see" the same environment up to orthogonal transformations and translations. These structures are ubiquitously present in all of materials science, biology and nanotechnology, and due to their association with large degrees of symmetry, they are likely to be a fertile source of materials with remarkable material properties. In this work, drawing analogies from the classical plane-wave density functional theory method of solid state physics, we present a novel spectral scheme for studying objective structures using Kohn-Sham Density Functional Theory. This opens up the possibility of carrying out efficient and accurate abinitio simulations of a large class of nano-materials and structures. First, we demonstrate how the equations of Kohn-Sham Density Functional Theory for objective structures admit interpretation in terms of symmetry adapted cell problems. Next, we propose a complete orthonormal basis set for discretizing these cell problems. We then discuss the significant algorithmic challenges associated with the the efficient solution of the discretized cell problems. We describe our progress in addressing these challenges through transform methods of evaluation of certain nonlinearities, the use of radial multipole expansions and the use of a matrix-free block-preconditioned iterative diagonalization procedure. We also mention how our implementation benefits from two-level parallelism present in our scheme and the ability of the scheme to seamlessly make use of arbitrary point group symmetries. Finally, we present applications of our spectral scheme to the study of some problems in nano-mechanics, including the study of properties of nano-clusters and simulations of the bending of nano-beams. |
| | Bhattacharya, Kaushik | No | | | |
| | Chen, Xian | Thu | | Enhanced reversibility and unusual microstructure of a phase-transformating material satisfying the cofactor conditions | The cofactor conditions, as the conditions of compatibility between phases consist of two main subconditions: (CC1) \lambda_2 = 1, which means the middle principle stretch of the transformation is unity, (CC2) (a.v2)(n.v2)=0 where the vector n is the normal of twinning plane, the vector a corresponds to the twinning shear and the vector v2 is the undistorted direction associated with the middle principle stretch, and a mild inequality condition (CC3) that is always true for Type I and Type II twin system of martensite. The microstructure of a material undergoing martensitic transformation has strongly dependence on the conditions of compatibility, and further influences the macroscopic properties of the material. Here we report an example of a phase-changing material Zn45Au30Cu25 with the satisfaction of the cofactor conditions for both Type I and Type II twins. Theoretically, as a result of the satisfaction of both Type I and Type II cofactor conditions, two martensite variants can form a triple junction with austenite with perfect fit at each of the interfaces , while they can also form a quad-junction with the other two variants through Type II twinning interfaces without paying additional elastic energy.<br><br>Macroscopically, many compatible triple and quad junction with different volume fraction become building blocks for the microstructure of the material undergoing phase transformation. Experimentally, we have observed the riverine strip microstructures as well as zig-zag interfaces in this material by the optical microscopy, which is completely unreproducible for the consecutive transformation cycles while the hysteresis and the latent heat are stable for each of the cycles. To further quantify the orientation correspondences between the real microstructure observed under the optical microscopy and the calculated morphology by the theory, we use the electron backscatter diffraction technique to measure the orientation for each martensite variant, then verify the cofactor conditions by calculating the rotation matrix connecting the adjacent variants. |
| 1 | Clifton, Rod | Thu | | Mechanical properties of the elastomer polyurea | |
| | Dabade, Vivekanand | No | | | |
| 2 | Daly, Samantha | Tue | | Multi-Scale Experimental Studies of Phase Transformations | This talk will discuss two experimental studies into a solid-to-solid state phase transformation in Nickel-Titanium that underlies its unique properties, including its ability to remember a previously defined shape and its superelasticity. The first, performed at the meso- and macro- scale, examines phase transformation as a function of crystallographic texture and mechanical cycling. This includes the discovery of a remarkable cyclic strain similarity in the formation of one of the phases at the microscopic length scale, and a discussion of the impact of crystallographic texture on this similarity. The second investigation utilizes a novel methodology to quantitatively examine full-field deformations (indicative of transformation) at the grain level. This is achieved by combining an optical technique known as digital image correlation with scanning electron microscopy, an approach termed here as SEM-DIC. The development of the methodology will be briefly discussed, including new self-assembled nanoparticle patterning techniques for unprecedented spatial resolution, and approaches to correct micrographs for the complex distortions inherent in SEM imaging. Using the DIC-calculated displacements, the progression of phase transformation and its relation to the underlying crystallography is examined at the grain level in mechanically loaded tensile samples. Large data mining approaches are adopted for statistical examination of this unique full-field data across fields of view ranging from 20μm - 500μm horizontal field width. |
| 3 | Dayal, Kaushik | Tue | | Multiscale Atomistic-to-Continuum Method for Atomic Monolayers Undergoing Bending | The framework of Objective Structures introduced by Richard D. James provides a method to systematically examine the behavior of various geometrically complex nanostructures. These nanostructures include rod-like objects as well as flat sheets. In this talk, we describe an extension of this framework to sheets that undergo bending in complex ways. We then apply the extended framework to develop a computational atomic multiscale method to understand the atomic structure of defects in these systems. |
| | DeSimone, Antonio | No | | | |
| 4 | Dolzmann, Georg | Thu | | Analytical and numerical aspects of relaxation in the calculus of variations | |
| 5 | Eliot, Ryan | Fri | | A New Framework for the Interpretation of Modulated Martensites in Shape Memory Alloys | Shape memory alloys (SMAs) are a class of materials with unusual properties that have been attributed to the material undergoing a Martensitic Phase Transformation (MPT). An MPT consists of the material's crystal structure evolving in a coordinated fashion from a high symmetry austenite phase to a low symmetry martensite phase. Often in SMAs,<br>the austenite is a B2 cubic configuration that transforms a Modulated Martensite (MM) phase. MMs are long-period stacking order structures consisting of [110]cubic basal planes. First-principles computational results have shown that the minimum energy phase for these materials is not a MM, but a short-period structure called the Ground State Martensite.<br>It is commonly argued that energy contributions associated with kinematic compatibility constraints at the austenite-martensite interface explain the experimental observation of meta-stable MMs, as opposed to the expected Ground State Martensite phase. To date, a general approach for predicting the properties of the MM structure that will be observed for a particular material has not been available.<br><br>In this work, we develop a new framework for the interpretation of MMs as natural features of the material's energy landscape (expressed as a function of the lattice parameters and individual atomic positions within a perfect infinite crystal). From this energy-based framework, a new understanding of MMs as a mixture of two short-period Base Martensite phases is developed. Using only a small set of input data associated with the two Base Martensites, this MM Mixture Model (M4) is capable of accurately predicting the energy, lattice constants, and structural details of an arbitrary Modulated Martensite phase. This is demonstrated by comparing the M4 predictions to computational results from a particular<br>empirical atomistic model. |

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| 6 | Fonseca, Irene | Fri | | Variational Methods for Crystal Surface Instability | Using the calculus of variations it is shown that important qualitative features of the equilibrium shape of a material void in a linearly elastic solid may be deduced from smoothness and convexity properties of the interfacial energy.<br><br>In addition, short time existence, uniqueness, and regularity for an anisotropic surface diffusion evolution equation with curvature regularization are proved in the context of epitaxially strained two-dimensional films. This is achieved by using the $H^{-1}$-gradient flow structure of the evolution law, via De Giorgi's minimizing movements. This seems to be the first short time existence result for a surface diffusion type geometric evolution equation in the presence of elasticity. |
| 7 | Friesecke, Gero | Tue | Mon-Wed | Ab initio versus empirical parametrization of potential energy surfaces in molecular simulations | Currently, in molecular simulation there is no accepted consensus on empiricism.<br><br>At one end of the spectrum, we have the ab-initio philosophy. Start from the universal, ''gold standard'' but hard to compute, ab-initio Born-Oppenheimer potential energy surface (PES) of quantum mechanics; then approximate to achieve computational feasibility. At the opposite end lies the fully empirical strategy, exemplified by packages such as CHARMM. Start from a simple functional form of the PES (or ''force field'', as a PES is customarily called in biochemistry); now parameterize via molecule-specific experimental data such as vibrational spectra, binding energies, torsion barriers.<br><br>I will discuss strengths and shortcomings of both approaches, as well as of intermediate ones, and make some remarks on the intrinsic difficulties that arise when trying to integrate information from both camps so as to maximise predictive power. |
| 8 | Gavini, Vikram | Tue | | Electronic Structure Studies on Defects in Crystalline Materials | Defects play a crucial role in influencing the macroscopic properties of solids—examples include the role of dislocations in plastic deformation, dopants in semiconductor properties, and domain walls in ferroelectric properties. These defects are present in very small concentrations (few parts per million), yet, produce a significant macroscopic effect on the materials behavior through the long-ranged elastic and electrostatic fields they generate. The strength and nature of these fields, as well as other critical aspects of the defect-core are all determined by the electronic structure of the material at the quantum-mechanical length-scale. Hence, there is a wide range of interacting length-scales, from electronic structure to continuum, that need to be resolved to accurately describe defects in materials and their influence on the macroscopic properties of materials. This has remained a significant challenge in multi-scale modeling, and a solution to this problem holds the key for predictive modeling of complex materials systems.<br><br>In an attempt to address the aforementioned challenge, this talk presents the development of a seamless multi-scale scheme to perform electronic structure calculations at macroscopic scales. The key ideas involved in its development are (i) a real-space variational formulation of electronic structure theories, (ii) a nested finite-element discretization of the formulation, and (iii) a systematic means of adaptive coarse-graining retaining full resolution where necessary, and coarsening elsewhere with no patches, assumptions or structure. This multi-scale scheme has enabled, for the first time, calculations of the electronic structure of multi-million atom systems using orbital-free density-functional theory, thus, paving the way for an accurate electronic structure study of defects in materials. The accuracy of the method and the physical insights it offers into the behavior of defects in materials is highlighted through studies on vacancies and dislocations. Current efforts towards extending this multi-scale method to Kohn-Sham density functional theory will also be presented, which include: (i) the development of higher-order adaptive finite-element formulation for efficient real-space Kohn-Sham DFT calculations; (ii) the development of a linear-scaling approach that is applicable to both insulating and metallic systems. |
| 9 | Giovanna Mora, Maria | Mon | | A quasistatic evolution model for perfectly plastic plates derived by Gamma-convergence | In this talk we shall discuss the rigorous derivation of a quasistatic evolution model for a linearly elastic - perfectly plastic thin plate. As the thickness of the plate tends to zero, we shall prove via Gamma-convergence techniques that solutions to the three-dimensional quasistatic evolution problem of Prandtl-Reuss elastoplasticity converge to a quasistatic evolution of a suitable limiting model. Such a model has a genuinely three-dimensional nature, unless specific data are prescribed. In particular, the stretching and bending components of the stress decouple only in the equilibrium condition, while the whole stress is involved in the stress constraint and in the flow rule.<br>This is based on a joint work with Elisa Davoli (Carnegie Mellon University). |
| 10 | Healey, Tim | Wed | | Existence of global O(3)-symmetry-breaking solutions in a model for two-phase lipid bilayer vesicles | We consider the analysis of a well known phase-field/elastic-shell model for 2-phase (fluid-fluid) equilibria of certain lipid bilayer vesicles. While the in-plane fluidity suggests a spatial formulation, the deformable elastic surface demands a material description. However the latter is invariant under all smooth isomorphisms of the reference configuration (the unit sphere) into itself, which leads to difficulties in the analysis and in numerical approaches. Instead we employ a certain radial graph description (well known in the differential geometry literature), which effectively "mods out" the in-plane fluidity. The formulation fulfills all necessary hypotheses for the use of a nonlinear Fredholm degree. With this in hand, we use symmetry-breaking methods and global bifurcation theory to obtain the existence of an enormous set of global, symmetry-breaking solution branches. To the best of our knowledge, these are the first existence results (axisymmetric solutions aside) for this class of problems. |
| | James, Richard D. | No | | | |
| 11 | Kim, K.-S. | Thu | No Friday | Search for new materials with ruga mechanics | |
| 12 | Kinderlehrer, David | Mon | | A theory and challenges for coarsening in microstructure | Cellular networks are ubiquitous in nature. Most technologically useful materials arise as polycrystalline microstructures, composed of a myriad of small crystallites, the grains, separated by interfaces, the grain boundaries. The energetics and connectivity of the network of boundaries are implicated in many properties across all scales of use. Coarsening is governed primarily by the attempt of the system to decrease the interfacial energy subject to spatial constraints. The recently discovered grain boundary character distribution (GBCD) shows that the boundary , and, more generally, material texture has order. We discuss a theory for the evolution of this statistic which gives rise to many interesting questions and challenges. We still have much to learn about these very ancient questions. |
| 13 | Kohn, Robert | Fri | | A variational perspective on wrinkling patterns in thin elastic sheets | Thin sheets exhibit a daunting array of patterns. A key difficulty in their analysis is that while we have many examples, we have no classification of the possible "patterns." I have explored an alternative viewpoint in a series of recent projects with Peter Bella, Hoai-Minh Nguyen, Jeremy Brandman, and Jacob Bedrossian. Our goal is to identify the *scaling law* of the minimum elastic energy (with respect to the sheet thickness, and the other parameters of the problem). Success requires proving upper bounds and lower bounds that scale the same way. The upper bounds are usually easier, since nature gives us a hint. The lower bounds are more subtle, since they must be ansatz-independent. In many cases, the arguments used to prove the lower bounds help explain "why" we see particular patterns. My talk will give an overview of this activity, and details of some examples. |
| 14 | Liu, Liping | Mon | | An energy formulation of continuum magneto-electro-elastics with applications | We present an energy formulation of continuum electro-elastic and magneto-electro-elastic materials. Based on the principle of minimum free energy, we propose a form of total free energy of the system in three dimensions, and then systematically derive the theories for a hierarchy of materials including dielectric elastomers, piezoelectric ceramics, ferroelectrics, flexoelectric materials, magnetic elastomers, magneto-electric materials, piezo-electric-magnetic materials among others. The effects of mechanical, electrical and magnetic boundary devices, external charges, polarizations and magnetization are taken into account in formulating the free energy. The linear and nonlinear boundary value problems governing these materials are explicitly derived as the Euler-Lagrange equations of the principle of minimum free energy. Finally, we illustrate the applications of the formulations by presenting solutions to a few simple problems and give an outlook of potential applications. |

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| 15 | Luskin, Mitchell | Thu | | Theory-Based Development and Benchmarking of Atomistic-to-Continuum Coupling Methods | The building blocks of micromechanics are the nucleation and movement of point, line, and surface defects and their long-range elastic interactions. Computational micromechanics has begun to extend the predictive scope of theoretical micromechanics, but mathematical theory able to assess the accuracy and efficiency of multiscale methods is needed for computational micromechanics to reach its full potential.<br><br>Many materials problems require the accuracy of atomistic modeling in small regions, such as the neighborhood of a crack tip. However, these localized defects typically interact through long range elastic fields with a much larger region that cannot be computed atomistically. Materials scientists have proposed many methods to compute solutions to these multiscale problems by coupling atomistic models near a localized defect with continuum models where the deformation is nearly uniform on the atomistic scale.<br><br>During the past several years, a theoretical structure has been given to the description and formulation of atomistic-to-continuum coupling methods, and corresponding numerical analysis and benchmark computational experiments have clarified the relation between the various methods and their sources of error. Our theoretical foundation has enabled the development of more accurate and efficient coupling methods. |
| 16 | Milton, Graeme | Tue | | Nonlinear mechanical metamaterials constructed from rigid bars and pivots | A basic question is what non-linear mechanical behaviors can one get in periodic materials constructed from rigid bars and pivots? It turns out that the range is enormous. Materials for which the only easy mode of macroscopic deformation is an affine deformation, can be classed as unimode, bimode, trimode,...hexamode, acccording to the number of easy modes of deformation. We give a complete chacterization of possible behaviors of nonlinear unimode materials, and an example of a bimode material. |
| 17 | Otto, Felix | Thu | | Cubic-to-tetragonal martensitic phase transition:<br>Scaling laws for energy in geometrically linear description with surface tension | |
| 18 | Rizzoni, Raffaella | Tue | No Friday | Bending and shape recovery of NiTi strips in free and partially constrained conditions | Motivated by the development of smart structures obtained by integrating SMA strips into polymeric plates, we have recently theoretically, numerically and experimentally investigated the bending and recovery behavior of thermally trained NiTi strips.<br><br>This talk presents a quasi-closed form solution for the curvature evolution of a SMA beam subject to uniform bending and free recovery, based on a one dimensional phenomenological constitutive model for SMAs. A comparison with numerical results extending the previous analysis and with experimental data obtained by heating NiTi strips in an Ethylene Glycol based water solution is discussed.<br><br>Recent experimental results of recovery tests in partially constrained conditions are also shown, performed on a dedicated functional structure activated via fluid circulation.<br><br>Joint work with M. Merlin, D. Casari, A. Fortini (University of Ferrara), and S. Marfia (University of Cassino). |
| 19 | Romo, Celia Reina | Mon | | F=FeFp? A kinematic analysis of finite crystal plasticity | |
| | Safranak, Lee | No | | | |
| 20 | Salje, Ekhard | Tue | | Domain boundary engineering: a new type of functional materials | Surfaces and interfaces may show useful functionalities which do not exist in the bulk. Twin boundaries are currently the dominant topic of research on 'Functional Interfaces'. They were found to be (super-)conducting, ferroelectric and ferromagnetic while none of these properties exist in the bulk. They also lead to fast ionic diffusion which makes them useful for medical applications. I will give examples for these functional materials. Their theoretical description is based on coupling theory where the disappearance of the structural order parameter in the twin boundary allows secondary order parameters to emerge. An additional degree of freedom is the mobility of the twin boundaries so that many of the functional properties can be enhanced by resonance in a high frequency conjugated field. |
| 21 | Schloemerkemper, Anja | Tue | | About zero-energy states of monoclinic-I martensite and bounds on its free energy | Within the framework of the geometrically linear theory of elasticity we study the zero-energy states of monoclinic-I martensite as well as upper and lower bounds on the free multi-well energy landscapes.<br>I will in particular discuss special relations between material parameters that occur in our mathematical analysis and might motivate the search for new shape memory materials. |
| 22 | Schryvers, Dominique ( | Mon | | Electron Microscopy in the search for new materials | The lecture will review some recent applications of conventional and advanced transmission and scanning electron microscopy in the search for new functional materials. The focus will be on materials exhibiting phase transformations such as shape memory systems, but also nanostructured materials and small particles will be addressed. |
| 23 | Sittner, Petr | Wed | | Special issues in mechanics of superelastic NiTi: elastic moduli, cyclic stability and corrosion fatigue | In my talk, I will present and discuss selected results of experimental investigations we performed on thin superelastic NiTi wires in view of their safe applications in medical devices and NiTi textiles. First is the longstanding issue of Young's moduli of the superelastic NiTi wire in austenite and martensite states which has not been successfully solved yet in spite of its crucial importance for the design of superelastic medical devices. Questions why the Young's modulus of NiTi wires in tension is always reported to be lower in the martensite state than in the austenite state while theoretical predictions suggest exact opposite, why unacceptably wide ranges of their values appear in material property tables and how the macroscopic Young's modulus of the NiTi wire evolves with temperature, stress and strain will be addressed. Second, I will try to show that the cyclic stability of superelastic tensile stress-strain response of NiTi wire is mainly related to the marginal plastic slip accompanying stress induced martensitic transformation which leads to the build up of internal stresses in the cycled polycrystalline microstructure. Finally, based on the results of recent systematic investigation of cyclic deformation of NiTi wire structures in biological fluids, I will propose a plausible mechanism for premature fatigue failure of NiTi medical devices cyclically deformed in corrosive liquid environments. |
| | Song, Yintao | Wed | | Multiferroic energy conversion and thermodynamics | A material that changes the ferroelectric or ferromagnetic property during a martensitic phase transformation is considered to be a multiferroic material. Such changes in ferroic properties during martensitic phase transformation can be utilized to convert heat directly into electricity. In this short talk, the demonstration of the ideal will be reviewed and the thermodynamics of the method will be briefly discussed. |
| 24 | Takeuchi, Ichiro | Thu | Thu-Fri | Thermoelastic cooling and latest development in combinatorial mapping of alloy phase diagrams | Our earlier work on combinatorial search of shape memory alloys which satisfy James and Ball's compatibility conditions has led to identification of quaternary alloys with unprecedented functional fatigue behaviors in bulk alloys. Investigation of shape memory alloys with long fatigue life has then led to a new application of such alloys: thermoelastic cooling. Sometimes also known as elastocaloric cooling, this solid state cooing technology is found to be very efficient and has relatively high temperature lift. I will also discuss the latest development in combinatorial mapping of structural phase diagrams of ternary systems. |
| 25 | Twarock, Reidun | Wed | | Biomaterials Science: Structural Transitions in Viral Capsids | A large number of human, animal and plant viruses have protein containers that provide protection for their genomes. In many cases the organisation of these containers can be described via surface lattices with icosahedral symmetry. In this talk, mathematical tools for the modelling of such capsid structures will be introduced and used to model the structural transitions these containers must undergo in order to become infective. These transitions result in expansions of the capsid with simultaneous rearrangements of the protein lattice and such containers and lattice transitions could provide inspiration for the design of new protein containers in bionanotechnology. |
| 26 | Wuttig, Manfred | Mon | | TBA | |