Mathematics and Mechanics in the Search for New Materials

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1 Overview of the Field

The workshop brought together mathematicians and physical scientists to discuss mathematical problems that arise from materials science. Materials science is undergoing rapid development. A number of new techniques for synthesis have recently been introduced, and it is possible today to synthesize compounds today that were impossible a decade ago. New techniques of characterization, including scanning probe microscopy, are now available and they have provided a new view on material microstructure. Finally, the availability of computational power has made it possible to study a number of previously inaccessible problems. Yet, most materials are still discovered through inspired accident and improved through expert empiricism. The essential reason for this is the complexity and the range of interactions between the electronic, atomistic, microstructural and macroscopic scales that determine the properties of materials. Mathematics can, and has, contributed to understanding this complexity.

2 Recent Developments and Open Problems

A longstanding challenge in Materials Science is finding predictive methods of developing new materials in light of the complexity of the interactions between electronic, atomistic, microstructural and macroscopic scales that determine the properties of materials. This complexity and range make it very hard to develop a systematic and predictive theory of behavior. Indeed, quantum mechanics (Schrödinger's equation) is used at the electronic scale, molecular dynamics at the atomistic scales, phase-field or similar theories at the microstructural scales and phenomenological constitutive laws at the macroscopic scales. These theories involve fundamentally different variables and different concepts, and how one is subsumed by the other is not completely clear. A further difficulty is that interesting behavior often occurs at isolated compositions or microstructures.

Mathematics can, and has, contributed to understanding this complexity. Homogenization theory has provided insights into composite materials, meta-materials and in understanding discrete (atomistic) to continuum limits. Regularity of the solutions of partial differential equations has enabled an understanding of thin films (especially what is now called rigidity) and failure through cavitation and fracture. The calculus of variations has provided a clear understanding of why microstructure arises in phase transitions, and tools like Young measures have led to methods which give an implicit understanding of microstructure. Bifurcation theory is leading to new understanding of pattern formation during microstructure evolution. In each of these examples, essential questions of materials science modeled in a rigorous manner have led to fundamental and deep questions of mathematics, and progress in mathematics has led to non-trivial insights into

material behavior. Further, mathematical insights have led to new computational approaches. Indeed, we are now beginning to see examples where this interactive advance is leading to the development of entirely new materials and structures.

3 Presentation Highlights

3.1 Linking electronic, atomistic and continuum methods

A Novel Spectral Scheme for Ab Initio Simulations of Objective Structures, Amartya Bannerjee 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 ab initio 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.

Multiscale Atomistic-to-Continuum Method for Atomic Monolayers Undergoing Bending, Kaushik Dayal 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.

Ab initio versus empirical parametrization of potential energy surfaces in molecular simulations, Gero Friesecke Currently, in molecular simulation there is no accepted consensus on empiricism. 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.

I 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.

Electronic Structure Studies on Defects in Crystalline Materials, Vikram Gavini 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 material's 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.

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.

Theory-Based Development and Benchmarking of Atomistic-to-Continuum Coupling Methods, Mitchell Luskin 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.

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.

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.

3.2 Microstructure and its evolution

Analytical and numerical aspects of relaxation in the calculus of variations, Georg Dolzmann In this lecture we discuss mathematical concepts that are related to the prediction of soft behaviour of materials in the framework of a variational formulation in nonlinear elasticity. In particular, we discuss the set of affine boundary conditions, for which minimizing sequences exist for which the energy of the system tends to zero. In the mathematical language, this set of boundary conditions is called the quasiconvex hull of the zero set of the nonnegative energy density W. We review some classical results starting with the work of Ball and James and present ongoing work on the relaxation of a frame invariant energy density related to a two-dimenisonal model of the cubic to tetragonal phase transformation.

Variational Methods for Crystal Surface Instability, Irene Fonseca 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.

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.

A theory and challenges for coarsening in microstructure, David Kinderlehrer 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.

Nonlinear mechanical metamaterials constructed from rigid bars and pivots, Graeme Milton 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, according 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.

Cubic-to-tetragonal martensitic phase transition: Scaling laws for energy in geometrically linear description with surface tension, Felix Otto The talk discussed scaling of the energy in models of martensitic inclusions incorporating interfacial energy.

F=FeFp? A kinematic analysis of finite crystal plasticity, Celia Reina Romo The kinematic description of finite elastoplasticity based on the decomposition F=FeFp is currently standard in the continuum mechanics community. Besides its acceptance, many issues have remained unresolved, such as the uniqueness of the decomposition, the characterization of the plastic deformation without reference to the intermediate configuration or its micromechanical understanding. In this talk, we will unveil some of these issues via a careful kinematic analysis of elastoplastic deformations at the microscale.

About zero-energy states of monoclinic-I martensite and bounds on its free energy, Anja Schlömerkemper 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. 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.

3.3 Symmetry and bifurcation

A New Framework for the Interpretation of Modulated Martensites in Shape Memory Alloys, Ryan Elliott 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). A 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, 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. 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.

In this work, we develop a new framework for the interpretation of MMs as natural features of the materials 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 empirical atomistic model.

Existence of global $O(3)$-symmetry-breaking solutions in a model for two-phase lipid bilayer vesicles, Tim Healey 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.

Search for New Multi-functional Materials with Ruga Mechanics, Kyung-Suk Kim In recent years nano science and technology has enabled us to explore new functional properties of hierarchical ruga structured materials through folding or wrapping thin surface layer structures with nanometer scale features. The Latin word ruga means a state of a large-amplitude wrinkle, crease, fold or ridge to form various 1-D or 2-D patterns. As multi-scale surface morphologies of rugae determine effective properties such as wetting, adhesion, friction and optoelectronic properties, ruga state control is considered as a viable method for real-time regulation of effective surface properties. It is found that graded or layered elastic properties of the substrate can provide diverse bifurcation paths of surface deformation under lateral compression, producing various surface ruga states. Here we introduce mathematical analysis of sequential bifurcation processes in surface deformation of a neo-Hookean substrate with its elastic modulus exponentially decaying along the depth from its free surface. In turn, iso-periodic-compression Ruga Phase Diagram of neo-Hookean solids with their moduli exponentially decaying with depth has been constructed, and its implications on engineering multi-scale ruga structures are presented.

A variational perspective on wrinkling patterns in thin elastic sheets, Bob Kohn 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.

Biomaterials Science: Structural Transitions in Viral Capsids, Reidun Twarock 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.

3.4 The search for new multiferroic materials and applications

Enhanced reversibility and unusual microstructure of a phase-transforming material satisfying the cofactor conditions, Xian Chen The cofactor conditions, as the conditions of compatibility between phases consist of two main subconditions: (CC1) $\lambda_2 = 1$, which means the middle principal stretch of the transformation is unity, (CC2) $(a.v_2)(n.v_2) = 0$ where the vector n is the normal of twinning plane, the vector a

corresponds to the twinning shear and the vector v_2 is the undistorted direction associated with the middle principal 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 strong 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.

Macroscopically, many compatible triple and quad junctions 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 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.

An energy formulation of continuum magneto-electro-elastics with applications, Liping Liu 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.

Domain boundary engineering: a new type of functional materials, Ekhard Salje 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.

Thermoelastic cooling and latest development in combinatorial mapping of alloy phase diagrams, Ichiro Takeuchi 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.

Nano-Magnetism of Magnetostriction, Manfred Wuttig The nature of the large magnetostriction in body-centered Fe-based solid solutions has been widely discussed in the literature. Here, we use a combination of magnetostriction, magnetization, torque, and TEM measurements of specially annealed Co65Fe35 to show that the magnetostriction is caused by coherent uniaxial nano-precipitates. We show further that

these nano-precipitates lower the magnetocrystalline anisotropy in Fe-Ga alloys and are responsible for the lowering of the elastic constant. In addition, we demonstrate that the precipitates create the sig-nature linear susceptibility of FeCo alloys, known technologically as Permendur. Since all bcc Fe-Co, Fe-Ga, Fe-Al, and Fe-Ge solid solutions investigated in this study are Permendurs, i.e. display a linear and reversible susceptibility as well as a small magnetocrystalline anisotropy as well as significant magnetostriction, we propose that nano-precipitates are responsible for the unique combination of magnetic properties of the family of bcc Fe-Co, Fe-Ga, Fe-Al, and Fe-Ge solid solutions.

Multiferroic energy conversion and thermodynamics, Yintao Song 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.

3.5 Shape-memory alloys and its applications

Multi-Scale Experimental Studies of Phase Transformations, Samantha Daly 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.

Bending and shape recovery of NiTi strips in free and partially constrained conditions, Rafaella Rizzoni 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.

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.

Recent experimental results of recovery tests in partially constrained conditions are also shown, performed on a dedicated functional structure activated via fluid circulation.

Joint work with M. Merlin, D. Casari, A. Fortini (University of Ferrara), and S. Marfia (University of Cassino).

Special issues in mechanics of superelastic NiTi: elastic moduli, cyclic stability and corrosion fatigue, Petr Sittner 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 the 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.

3.6 New materials at high pressures

Mechanical properties of the elastomer polyurea, Rod Clifton This talk described the unusual viscoelastic properties of polyurea when subjected to combined shear and pressure.

4 Outcome of the Meeting

4.1 Scientific outcomes

A major outcome of the meeting was the connections between mathematicians and physical scientists. We list below the comments of various participants.

James An interesting link was discovered at the workshop during the discussion following the talk of Reidun Twarock. During her lecture she explained that the structures of the capsids of numerous animal viruses, including not only the overall icosahedral structure but also the detailed structure of the subunits, could be understood by by applying a finite set of powers of two generators of an isometry group to a point in $\mathbb{R}^3$.

This provides an interesting link to the theory of "objective structures" of James, which can be viewed essentially as the union of orbits of a discrete group of isometries on a finite set of points in $\mathbb{R}^3$. The distinction is that the generators used by Twarock do not generate a discrete group. There are a great many nondiscrete groups of isometries and the subfamily used by Twarock enjoys a certain uniformity property. As explained by Twarock, there are links between these ideas and the "method of projection" from higher dimensions used to construct quasicrystals.

The possible implications of this circle of ideas is that potentially a large class of non-periodic (and non-objective) structures seen in Nature, including possibly quasicrystals, polymers, glasses, can be viewed as the action of a nondiscrete group of isometries on a set of simple structures.

Kohn (1) Prior to the meeting I did not know that K-S Kim was interested in the wrinkling of compressed thin films bonded to compliant substrates (a recent area of interest for me, which occupies about 1/3 of my talk). Fortunately I learned of his interest by chance, in a discussion over dinner on Sunday. We decided not to wait for our respective talks (which are on Thurs and Fri), and instead had a great 2-hour discussion Mon evening, which revealed a number of potential areas for possible collaboration.

(2) Talking with Ekhard Salje over dinner one night, the discussion turned to Barkhausen noise. Basically, I expressed frustration that there seems to be lots of experimental work but almost no theory. I didn't know (till I asked) that this was a major interest of his (though not a focus of his talk). He agreed that there is great need for theory, but also suggested that the time might be ripe for making progress, and has given me some suggestions of things to read in the area.

Both examples highlight the interdisciplinary character of the workshop. Kim and Salje are mechanics people, who go to a whole different set of meetings than I do. Their presence here is due to the Organizers' concept of the meeting (consciously interdisciplinary), to the Organizers' good judgement (choosing speakers from whom synergy can be expected though not predicted), and to BIRS' willingness to host a meeting that isn't "just" mathematics.

Schryvers Four identifiable progress matters:

- several members of the mathematical community showed interest in the new evolution of electron vortex beams. I was actually hoping for this when adding this item in my lecture, since I know our colleagues are struggling with solving some complicated equations, so maybe some further contacts will develop.

- concrete steps were agreed upon between Dick's group and ours for future research on NiTiNb and cofactor alloys. We will search for different transformation strains in the former, and start the TEM work on the latter. Possibly Xian Chen will visit EMAT in the near future.

- I received some more info from Ekhard on the precision of his XRD measures of lattice parameters in NiTiNb so we have a better idea on how to apply those in the context of changing hysteresis versus lambda2.

- I promised Irene to contact the applied math people in Antwerp to see if they can increase their interaction with SIAM.

Elliot I had a very helpful discussion with John Ball about Lyapunov functions for thermomechanical problems. He sent me a paper that I expect to be very useful in my research and teaching.

Meeting Reidun Twarock was very exciting. The work she is doing has many connections with the Objective Structures theory that Dick James has developed and I have worked on. Her presentation has given Dick and I a new idea that may allow us to generalize the theory and identify a new class of structures and materials with interesting properties.

Abeyaratne Very useful discussion about the role of Langevin Dynamics in dissipative processes with Celia Romo. Useful "tutorial" on cell mechanics from Antonio DeSimone.

Bannerjee a) Discussions with Prof. Tim Healey revealed that there might be a somewhat better way of carrying out (Symmetry adapted) Branch Following and Bifurcation studies on Objective Structures. We are looking to implement this in the near future. b)Prof. Vikram Gavini suggested some improvements/enhancements to our current implementation of the Objective Density Functional Theory code. c) Other useful discussions with Prof. Tim Healey, Prof. Robert Kohn, Prof. Reidun Twarock, Prof. Samantha Daly.

Romo 1. Discussions with Felix Otto were very helpful to get a better understanding of different kinetic evolution equations and their variational formulation. 2. Contacts: Discussions with Anja Schlomerkemper set the basis of a potential collaboration.

Daly A better understanding of mathematical modeling for phase transformations, and also for a host of other applications ranging from the study of virus-cell interactions (particularly the concept of objective structures) to density functional theory and its applications. Interesting and useful scientific discussions with attendees including Dick James, Ryan Elliot, Celia Reina Romo, Anja Schlomerkemper, Petr Sittner, and Manfred Wuttig.

K.S. Kim I have made new connections with Bob Kohn, John Ball and Tim Healey.

S. O. Kim All talks inspired me. Mathematical approaches, e.g. the use of group theory, differential geometry, and combinatorial methods, computational methods, in the study of materials confirms again that there are no border lines in disciplines.

Especially I liked the talk by Reidun Twarock about "Biomaterials Science: Structural Transitions in Viral Capsids". Yes, I made a new contact with Reidun and we discussed about Icosahedral Group and Hamilton Path from Graph Theory and possibility of collaborations with my research groups. As an abstract algebraist and a computational mathematician, the use of group theory and graph theory in the study of biological structures bring me back to quest for joint works with other disciplines.

Twarock (1) There is an interesting link between the theory of "objective structures" with our affine extensions of noncrystallographic groups (in particular affine extensions of the icosahedral group which are relevant for viruses, but the procedure can also be applied to other noncrystallographic symmetries such as 7-fold rotational symmetry). In particular, the requirement that the affine extension leads to a group with nontrivial identities fixes the translation lengths in the construction. It will be interesting to explore if the projection method that is used in the construction of these groups can also be used to generalise objective structures to a non-periodic setting.

(2) I had an exchange with Bob Kohn regarding the modelling of the structural transitions in viral capsids. He has drawn my attention to his article "Energy-driven pattern formation" which shows how a stochastic term can be introduced in the equation describing capsid dynamics (in particular (26) on p.17), and we discussed the possible consequences of this. I am planning to follow this up and generalise our models along these lines.

4.2 Education

Given the diversity of the participants, a discussion was held on the nature of mathematical eduction that a graduate student in the physical sciences should receive. While there were diverse opinions and perspectives, an overall consensus on the following lines: Mathematical courses provides two things to graduate students specializing in physical sciences and engineers:

1. A way of critical thinking that is universally useful for any scientific research. This can be inculcated through any number of courses (a number of participants felt that Linear Algebra is a good means of doing this). This is best taught by faculty in mathematics departments, and in a rigorous manner that it would be taught to advanced undergraduates specializing in mathematics.

2. Specific mathematical methods that are analyzing problems. These of course are discipline specific, and also evolve with time. Therefore, the faculty teaching these courses should be aware of the evolution of these disciplines.