Report on Research in Groups

Materials structure and behavior: From atomistics to continuum

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Organizers: Isaac V. Chenchiah, Kaushik Dayal, Gero Friesecke, Richard D. James, Celia Reina

Topics

The scale transition between atomistic behavior and continuum response remains a tremendous challenge from a mathematical perspective. This is even more true in the presence of inelastic processes where the mathematical descriptions transitions from a conservative structure to a dissipative one. Yet, the importance of rigorous coarse-graining is unquestionable, as it enables physically-based macroscopic models, which can highly strengthen their predictive capability.

The program focused on three topics:

- Elasticity-dominated diffusion in two-phase solids (lead by I. Chenchiah).
- Twisted X-rays for the visualization of atomic structures with certain symmetries (lead by D. James and G. Friesecke).
- Mathematical coarse-graining of dislocation activity to the continuum scale (lead by C. Reina).

Goals

The specific goals for each of the three research thrusts are outlined below

- Elasticity-dominated diffusion in two-phase solids. Consider a two-phase solid whose phases may arrange freely, i.e., diffuse, and are elastically indistinguishable. Thermodynamically, the time evolution of such systems can be described by minimising the Helmholtz free energy

ψ that contains also a gradient term to model the interfacial energy. This gradient term automatically introduces a length scale. Mathematically, the time-evolution of such systems can be modelled by the Cahn-Hilliard equation. As is well known, in the Γ-limit of vanishing interfacial thickness, it converges to the Mullins-Sekerka problem.

However in almost all systems of technological importance the evolving phases are not mechanically identical and the elastic interaction may have a very strong effect. This is the case, for example, in steels, or for coarsening in superalloys, for instance, in turbine blades.

Both the Cahn-Hilliard and the Mullins-Sekerka equations have been extensively studied, by mathematicians, physicists, material scientists, and others. There have been several attempts in the engineering community to augment the Cahn-Hilliard equations with ad-hoc linearised-elasticity. Our efforts were aimed at formulating and analysing a system that would rigorously incorporate the effect of microstructure to elasticity, e.g. how the geometry of the phases on small length scales affects the mechanical properties macroscopically.

- Twisted X-rays for the visualization of atomic structures with certain symmetries. Nearly everything we know about the structure of matter (where the atoms lie, and what are the species) comes from X-ray analysis. The working principle is based on the pattern of the reflected radiation when the geometry and the frequency of the reflected radiation are right, in the sense that they match the symmetry of the crystal. However, there are many important emerging materials that do not crystallize, like buckyballs, carbon nanotubes and graphene, and, more recently, black phosphorus and the the dichalcogenides. Yet, they do exhibit some symmetries that James has characterized with his theories of Objective Structures (OS) [3]. The goal of this effort is to make use of these other symmetries to design X-rays that enable the visualization of OS, in the same way that classical X-rays are used to visualize crystals.

- Mathematical coarse-graining of dislocation activity to the continuum scale. Most continuum models of finite plasticity are based on assuming that the net change in shape, given by the macroscopic deformation gradient F, can be decomposed multiplicatively into a change in shape due to elastic deformation F^e and a change in shape due to dislocation motion F^p, i.e. $F = F^e F^p$. This assumption was heuristically proposed in the 1960's and is currently considered as the standard modeling strategy within the engineering community. However, a rigorous justification of this assumption and its connection to lower-scale theories have since remain open. This has lead to vivid arguments in the literature concerning the existence and validity of this kinematic assumption. In a recent effort [5], physically based and mathematically consistent definitions of the different tensors F, F^e and F^p from the dislocation microstructure and their evolution were first provided. The specific goal of this effort was to provide a rigorous proof of the relation $F = F^e F^p$ at the continuum scale from the definition of the individual tensors, and to show that det F^p=1, and that G =Curl F^p represents the so-called dislocation density tensor (measure of the dislocation content in the material).

Organization

The program provided a very stimulating and collaborative atmosphere, which included the participation of both local scientists from the University of Bonn (Sergio Conti, Barbara Zwicknagl), visitors to the University of Bonn (Patrick Dondl, University of Durham), as well as external visitors to the program (Anja Schlömerkemper, University of Würzburg and Thomas Blesgen, Bingen University of Applied Sciences). The organizers and external visitors had access to individual office space in a shared room, which provided a perfect environment for enabling goal-oriented research progress as well as cross-fertilization between the individual thrusts. For instance, organizers Chenchiah and Reina, initiated a new research direction during the program on the modeling of viscoelastic polymers, which continues to this date.

Results

Various important results have been obtained thanks to the program.

We were able to make considerable progress in addressing the coarsening problem. A model first formulated in [1] (shown in [2] to be consistent with experimental evidence) is being extended in multiple ways; we highlight the three most important here: (i) Existence of solutions, proved for a special case in [1], is being extended to all cases by exploiting the quasiconvexity of the elastic energy. (ii) The analysis, earlier limited to two dimensions, has been extended to three dimensions (for materials with isotropic or cubic symmetry). (iii) We are close to being able to show that our results qualitatively hold also for polycrystals.

Promising results have also been obtained in the thrust of twisted X-rays, which have been summarized in a publication [4]. The manuscript, recently published in Acta Crystallographica, contains a new exact solution for the visualization of helical structures with twisted X-rays. The key point for this accomplishment is the realization that Maxwell's equations, which govern the propagation of light, allow for a much broader family of symmetries than the translational symmetries of plane waves, used in standard X-waves. If these symmetries match those of the objective structures that one is interested in visualizing, this will result in strong spots in the far-field radiation that can be used for structure determination. The feasibility of this idea has been demonstrated analytically for helical structures. The fabrication of a machine capable of producing these twisted X-rays, would an able the visualization of helical structures, that appear, for instance, in the Ebola virus, and in some amyloid proteins that are believed to cause Alzheimer's, Parkinson's and Creutzfeldt-Jakob disease. These new forms of light could have other completely different uses (in optics, photonics, radar and communications) that James is now exploring.

The plasticity thrust made was also highly successfully, and the research progress has culminated in the first rigorous proof of the equality $F = F^e F^p$ from the underlying plastic activity, which was recently published in the Journal of the Mechanics and Physics of Solids [6]. This result is the main accomplishment of our research, and was complemented by other interesting results. This result is the main theorem of the paper, although other interesting results are contained in it. In particular, it was shown that the mesoscopic description, where individual dislocations are visibles and the displacement field associated to material deformation is discontinuos, leads in the macroscopic scale to a continuous formulation. Furthermore, the dislocation content in the body, usually measured in the so-called dislocation density tensor, was rigorously derived, and the plastic deformation tensor was shown to be isochoric. These results are no minor feat, as the specific expression of the dislocation density tensor has been the source of various debates in the literature, and determinant of the measure F^p is in principle ill-defined. Various uniqueness and regularization arguments were needed to achieve the aforementioned results.

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