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Microstructures in Solids: From Quantum Models to Continua

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Abstract. The mathematical theory of solids was studied from the modern perspective of materials with microcstructures. The discussed topics ranged from experimental findings, via numerical simulations and mathematical modeling to the analysis of models with microstructures. A special emphasis was given to theories providing rigorous insight into and justification of the limit passage between different scales.

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Introduction by the Organisers

The design of modern materials, like multifunctional materials, and devices needs a deeper qualitative and quantitative understanding of material properties. However, the material behavior is influenced by effects on different length scales. For instance, the formation of single dislocations in a crystal is dominated by quantum and atomistic effects on a subnano-scale, whereas single-crystal plasticity has its origin in the motion and generation of thousands of dislocation lines on the micron scale. Similarly, phase transformations in shape-memory alloys or domain-wall formation in micromagnetics is generated via microstructures on different spatial scales. Formation of microcracks is one of the main origins of material failure, and the modeling of a crack tip involves length-scales over several decades.

The workshop brought together mathematicians and applied scientists and enabled them to discuss the relevant physical effects and their pertinence for the understanding of materials as well as the mathematical methods modeling the formation of microstructures and the effective description of small-scale effects on larger scales. The talks concentrated on the following three main topics with special emphasis on their interaction:

- mathematical models for solids, in particular involving damage, fracture, plasticity and multifunctional materials;
- multiscale techniques, evolution of microstructures;
- computational and experimental aspects.

The discussed mathematical methods for multiscale problems included (two-scale and high-contrast) homogenization and analytical relaxation for models of crystal plasticity. Moreover, a new "uniformly Γ-equivalent" continuum theory for fracture was derived from a discrete model based on Lennard-Jones type interactions. For rate-independent systems the theory of Γ-convergence was shown to predict the creation and the evolution of microstructure from macroscopic states as well as providing a rigorous link between damage models and delamination of Griffith type. The passage from viscous kinetics to rate-independent dynamics was investigated via spatially random models, which give rise to a microscopic stick-slip motion.

The theory of dislocations was discussed from several points of view, namely as obstacles to crystallization in 3D, as a discrete origin to strain-gradient plasticity, and as a continuous transport theory for dislocation densities. Furthermore, a macroscopic model for non-associative plasticity in cam-clay was discussed analytically.

Effective descriptions of microstructures in nematic elastomers, elastoplastic materials, magnetic shape-memory alloys, solids undergoing phase transformations and ferroelectric materials were discussed in the framework of dissipative materials or using a special evolution law for simple or double laminates. The influence of rapid heating and cooling on microstructure formation was reported on the basis of recent experiments.

Size effects for microstructures in solids become relevant below the micron scale. The relevant multiscale modeling of the mechanical properties of metallic and biological polycrystals (e.g. chitin) was investigated using ab initio theory in conjunction with continuum homogenization. Similarly, progress in the understanding of interfacial cracks was obtained by combining quantum theory with macroscopic adhesion and strain-gradient models.

The foundations of such numerical approaches were investigated at several examples, like the statistically equivalent representative volume elements, a comparison of force-based atomistic/continuum hybrid models and the quasi-continuum methods and an effective numerical approach to gradient Young measures.

The stimulating discussion between the different research communities created many interesting links between previously disconnected research topics. The workshop initiated several new collaborations which will foster the progress of our understanding microstructures in solid materials.