

MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

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**Mini-Workshop: Inelastic and Non-equilibrium Material  
Behavior: from Atomistic Structure to Macroscopic  
Constitutive Relations**

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ABSTRACT.

The workshop brought together 15 scientists, which included leaders in the fields of mathematics (partial differential equations, statistical mechanics and calculus of variations) and mechanics (continuum mechanics, computational mechanics, microstructure and material science) as well as mid- and early-career participants. We addressed the themes of modeling crystal plasticity, crystallization and fracture, and non-equilibrium thermodynamics.

*Mathematics Subject Classification (2010):* 74, 35, 82, 49.

**Introduction by the Organisers**

The workshop *Inelastic and Non-equilibrium Material Behavior: from Atomistic Structure to Macroscopic Constitutive Relations* addressed two key problems in the multiscale characterization of materials undergoing large inelastic deformations: (i) the understanding of non-equilibrium deformation of materials and nanostructures, and (ii) the atomistic-to-continuum limit of inelastic processes such as dislocation induced plasticity, crystal formation, and fracture. The diverse background of the participants made it possible to have a vibrant and open exchange of ideas in this intrinsically interdisciplinary problem of scale bridging in materials.

On the materials science side of the topic, we had presentations from areas of computation and modeling, in particular regarding the topic of objective structures and their thermodynamic behavior, phase field models for modeling phase transitions and crystallization. The mathematical topics covered included relaxation

in models for crystal plasticity, crystallization and fracture, as well as modeling thermodynamic processes far from equilibrium in both particle systems and the continuum. In all presentations we had a lively discussion that usually already started during the lecture and continued during the afternoon and evening breaks, sparking many ideas for improvements and further research and collaboration. The discussions in the mini-workshop atmosphere exceeded our expectations.

Complementary to the lectures on current research we had evening sessions where experts in the respective fields provided introductions to specialized topics. These sessions covered three areas: models for crystal plasticity, with a particular focus on kinematics derived from atomistics, the Boltzmann equation, and gradient flows. These lectures proved to be very successful and further facilitated the interdisciplinary exchange within the workshop.

In the feedback we solicited from the workshop participants, the high scientific standard and the benefits of informal structure and the small group, leading to long and in depth discussions during and after the presentations were explicitly mentioned. The more tutorials were also praised by the participants, especially their focus on open questions. This even lead to some new collaborations.

The workshop participants came from the US, Germany, and the UK, with a diverse mix of established researchers and early career scientists as well as PhD students. The excellent working and living conditions at the institute were vital for the lively and productive scientific atmosphere. The organizers thank the NSF for contributing to the travel expenses of two doctoral students and two professors from the US.

## Mini-Workshop: Inelastic and Non-equilibrium Material Behavior: from Atomistic Structure to Macroscopic Constitutive Relations

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