



INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION

## MMM Seminar

AMS seminar room 3.06, Universitätsstr. 90a

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### **Defect Identification and Indexing Algorithms for Molecular Dynamics Simulations of Crystals**

The increasing size and complexity of molecular dynamics simulations of crystals pose a challenge: The data analysis requires powerful computational tools and indexing algorithms, which can identify (and quantify) interesting features in large datasets and connect the original atomistic description of crystal defects with higher-scale models and theories.

I will present new computational techniques that facilitate the transformation of the original atomistic representation of a solid into a more abstract, high-level description of a microstructure in terms of grains, interfaces, and other defects such as dislocation lines.

One key element in this transformation is the robust identification of characteristic atomic arrangements. Using advanced pattern matching algorithms, taking into account medium-range atomic order, the range of identifiable structures can be considerably extended. The structure identification provides the foundation for our definition of purely elastic deformation at the atomic level. For instance, we may compute the incremental elastic and plastic deformation gradient fields  $F\Delta e$  and  $F\Delta p$  given an initial and a final simulation snapshot. These fields (and their variation with time) can provide valuable insights into the number, mobility, and localization of defects, and link atomistics to continuum models of crystal plasticity.

As a recent application of this framework, I will describe the fully automated identification of grain boundary dislocations from the incompatible elastic displacement field that surrounds them.