D2C - a unifying approach towards analyzing, comparing, and validating arbitrary dislocation microstructure

Stefan Sandfeld* and Dominik Steinberger

* Institute for Material Simulation, Department Materials Science, Friedrich-Alexander University of Erlangen-Nuremberg, 90762 Fürth, Germany

e-mail: stefan.sandfeld@fau.de, web page: http://matsim.techfak.uni-erlangen.de

ABSTRACT

The mechanical behaviour of metallic materials is governed by properties of the underlying microstructure. Understanding and predicting the structure-property relation is central to experimental and computational materials science. Over the last decades a large number of different simulation methods on various time and length scales has evolved. At the same time, advanced experimental characterization methods with high resolutions are able to reveal a rich variety of details about microstructural features. This offers a number of interesting possibilities, e.g. to use experiments for validating computational results on a microstructural level, or to use microstructure data from a 'lower scale' method (e.g. atomistics) - directly or indirectly - as input or for validation purposes for simulation method on larger scales. Up to date, however, systematic and detailed methodologies for comparing and validating data from different methods are still lagging behind.

In this presentation we introduce our D2C (=discrete to continuous) approach, which can be used as novel 'language' for computationally characterizing dislocation microstructures: using orientation distributions we can mathematically compress dislocation data by means of a continuum description and the maximum information entropy principle. This data format can be tuned w.r.t. the level of compression and allows to directly compare dislocation microstructures from very different methods, e.g. MD simulations, TEM microscopy or tomography, continuum or DDD simulations. We show how our approach might serve as the foundation for a unified approach towards dislocation data, where one of the strengths of the D2C framework is that ensemble averages of statistically equivalent simulations/experiments can easily be performed. This is ideal for validation and data mining of in particular discrete methods (simulations as well as specialized experiments), whose microstructural data are often not easily accessible.

REFERENCES