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Understanding Dislocation Flow and Avalanches: From Digital Twins of In-Situ TEM Experiments and Data-Mining of High-Entropy Alloys to Machine Learning-assisted Theory Development

This presentation focuses on a topic that is at the core of materials science and engineering: understanding the microstructure-property relation. As this relation does not describe a fixed "state" of the material but rather a time and history-dependent, complex interaction of many different details and aspects, this poses still a significant challenge to the materials community.

In this talk we elucidate how data mining strategies can be used to extract otherwise inaccessible information from experiment and simulation and how this can be used to shed some light on the microstructure-property relationship in metals and alloys. In particular, our goal is to understand some of the many open questions concerning the underlying structure-property relations in single crystalline metals and High Entropy Alloys (HEAs).

Although in-situ Transmission Electron Microscopy (TEM) allows high-resolution studies of
the structure and dynamics of moving dislocations and -- in a way -- makes the local obstacle/energy "landscape" directly visible through the geometry of dislocations; a truly three-dimensional analysis and high-throughput data-mining of the resulting images or movies is still not possible. To this end we introduce a novel data-mining approach that is based on spatio-temporal coarse graining of TEM dislocation movies, making ensemble averaging of a large number of snapshots in time possible.

Furthermore, we show how Data Science approaches can be used to extract information from molecular dynamics and discrete dislocation dynamics simulations. In particular, we demonstrate that such machine learning approaches have the potential to aid theory development of a continuum theory of dislocations even on a conceptual level.