Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5]Symposium A-5

Chair: Sinisa Dj Mesarovic(Washington State University, United States of America)
Wed. Oct 31, 2018 9:45 AM - 11:00 AM Room6

[SY-A5]Data Mining of Indentation Induced Dislocation Microstructures

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In general, data mining is the process of discovering patterns in large data sets, with the most common tasks being, anomaly detection, association rule learning, clustering, classification, regression and summarization. Within materials science, the most popular application so far is materials discovery, one of the goals of the well-known Materials Genome Initiative (https://www.mgi.gov).

In order to understand the convoluted interactions of dislocations that define the mechanical properties of metals to a large degree, a lot of data has been and is being generated, be it via experiments or simulations. Due to the complexity of the dislocation microstructure and its discrete nature aforementioned algorithms can not be applied ad-hoc. Thus, developing methods that enable their use are highly desirable.

In this presentation we want to outline the key aspects of the data mining framework for dislocation microstructures that we are currently developing. Among others, we will show examples of how quantitative comparisons of dislocation data—be it from experimental or computational methods—can be done. Aforementioned framework will be applied to a dataset consisting of hundreds of realizations of a numerical indentation experiment realized with discrete dislocation dynamics. Rate coefficient beneath the indenter will be extracted for the dislocation densities commonly found in continuous dislocation dynamics models. The resulting microstructures will be analyzed for common patterns and their correlation with the intially emerging structure to enable predicting the characteristics of the final state from the first initial steps.