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Analyzing dislocation nucleation and multiplication in atomistic nanoindentation simulations

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Analysis of large scale molecular dynamic (MD) simulations is a challenging topic, due to the huge data sets generated by these simulations.
During simulations of a nanoindentation process large numbers of dislocations are created and interact with each other, making it difficult to trace their individual movements and interactions. In order to investigate these effects, or to detect the nucleation of additional dislocations, the dislocation network in the crystal underneath the nanoindenter has to be identified in a very high time resolution. Without reducing the complexity of the results on-the-fly during a simulation, the amount of data for such high resolutions becomes difficult or even impossible to handle.

For this purpose a new fully automated method has been developed to detect dislocation cores inside the atomistic system of MD simulations and transform them into compact vectorized representations, directly resembling the concept of dislocations as an one-dimensional line defect.
The new method first filters out all atoms related to dislocations and then reduces this set of atoms into dislocation cores, each one described as a vectorized curve. These curves are connected at dislocation nodes to fully describe the dislocation network in the crystal.
The amount of data to describe the dislocation network after this transformation at a certain time step of the simulation is minimal compared to the full atomistic system in MD simulations. Combined with a highly efficient implementation, where all time consuming operations can be executed in parallel on-the-fly, this method allows observations and advanced analyses of dislocations in high time resolutions.

As a proof of concept, this new method has been applied to investigate the nucleation of additional dislocations in advanced stages of a nanoindentation simulation in copper. At this stage a large number of dislocations already exists inside the single crystal. By investigating a time sequence of extracted dislocation networks, multiple spots close to the free surface have been identified, where additional dislocations nucleate frequently. Although the precision of the vectorization method is significantly reduced close to the surface, due to a large number of defect artifacts and a possibly high dislocation density, these nucleations are still visible.

Additionally to the results obtained from visualization of the vectorized dislocation networks, local stress values have been calculated. Stress-peaks, indicating dislocation nucleation, have been monitored at the same spots, previously identified by the vectorization method, thus building the link between mechanical description of nanoindentation with the evolution of dislocation microstructure.