

Strengthening model for edge dislocations in BCC Mo-Nb alloy parametrized with *ab initio* calculations

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Our objective is to advance the understanding of plasticity in body-centered cubic (BCC) concentrated alloys across a broad temperature range, with particular emphasis on high-temperature behavior, where plastic deformation is strongly affected by the presence of interstitial impurities, such as oxygen, nitrogen, and carbon.

Ab initio calculations based on density functional theory (DFT) are necessary to better understand the physical mechanisms controlling dislocation mobility in concentrated alloys. Ultimately, the combination of experimental data and atomistic modeling is expected to enhance our understanding of the origins of material performance, especially at high temperatures. This study focuses on the Mo-Nb BCC binary system, modeled using special quasi-random structures (SQS) method. To approach alloys of technological interest, a range of concentrated alloys is considered, with selected molybdenum concentrations of 0, 4, 8, 20 and 30 atomic percent in niobium, resulting in a solid solution.

To address the complexity of the mechanisms governing the interactions of dislocations with substitutional and interstitial solutes, a first step is to work on the strengthening model, following the approach of F. Maresca and W.A. Curtin [1] for edge dislocations in BCC high entropy alloys. *Ab initio* calculations of Mo-Nb alloy properties, including bulk parameters and relaxation volumes, allow the direct parametrization of the strengthening model for edge dislocations. A detailed overview of the methodology used to calculate the different parameters of the strengthening model, as well as the results of this developed strengthening model, will be presented, including the evolution of yield strength as a function of temperature and alloy composition. Next work will involve the study of screw dislocations strengthening and introducing dislocations into the SQS supercells for DFT calculations, in order to characterize the interaction energies between local concentration fluctuations (substitutional solutes) and the edge dislocations.