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Effect of chemical sublattice ordering on the slip systems in BCC High Entropy Alloys

High entropy alloys (HEA) are a new class of metallic alloys with more than four approximately equimolar elements and are promising structural materials with partially outstanding mechanical properties. To understand the mechanical behaviour of HEAs it is essential to investigate their intrinsic dislocation deformation mechanism and the associated kinetic signatures. Experimental results as well as theoretic calculations indicate chemical sublattice ordering (SLO) in HEAs at low temperature and sufficient time to be kinetically accessible during synthesis. The impact of SLO on different HEAs is evaluated by density functional theory (DFT). The respective implication on possible slip systems, which are crucial to describe the deformation mechanism, are predicted by dislocation theory with different levels of approximations. DFT is used to determine the needed material parameters to assess the elastic properties, the energetics of SLO and the generalized stacking fault energies.

Abstract (optional)

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