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Identification of the intrinsic deformation mechanisms of single phase body-centered cubic high entropy alloys

Body-centered cubic (BCC) refractory high-entropy alloys (HEAs) have been studied as novel metallic systems for high-temperature applications due to their, for example, superior strength, excellent thermal stability, and oxidation resistance even at elevated temperatures. To date, the research emphasis in the field of refractory HEAs has been upon the development and evaluation of the resulting microstructure. However, the intrinsic deformation mechanisms of the single-phase BCC HEAs are still under debate. For example, a mean field solute-strengthening model severely underestimates the critical stresses for dislocation motion in single phase BCC HEAs, whereas the later solute-strengthening model is consistent with experimental yield strengths of face-centered cubic single phase HEAs. In general, the mechanical behavior of BCC HEAs depend on intrinsic properties, such as the chemical composition, microstructures, and the interaction of defects with the different microstructural components, as well as extrinsic parameters, such as temperature, and strain rate. The proposed project aims at determining the intrinsic deformation mechanisms of singlephase BCC HEAs and at characterizing the chemical/microstructural stability under deformation with the goal to predict their structural integrity at roomtemperature and in the transition to the high-temperature regime at 700K. The deformation kinetics and dislocation slip systems are determined and linked to the characteristic deformation signatures of the macroscopically ductile Ta-Nb-Hf-Zr-Ti HEA and the macroscopically apparently brittle NbMo-Cr-Ti-Al HEA in the proposed synergistic approach, which combines atomistic simulation methods and advanced temperature-dependent nano and micromechanical experiments. The mechanical tests are supplemented by multiscale and extended spatiallyresolved microstructural and chemical analysis. Electronic structure calculations simulate explicitly disordered HEAs using special quasi-random structure and provide a chemical accurate prediction of the intrinsic fluctuations of materials parameter, e.g., ideal shear strength and generalized stacking fault energies. The possible slip systems and the associated screw/edge dislocation anisotropies are determined on the basis of simulationinformed dislocation theory. A kinetic Monte Carlo method is developed to elucidate elementspecific segregation trends during deformation. The combined simulations-and-experiment ansatz will allow to formulate a verifiable phenomenological model for the deformation processes in single-phase BCC HEAs at room-temperature