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Thermomechanical properties and microstructure of fcc and bcc high-entropy alloys

The goal of this collaborative proposal is to study the influence of lattice structure and microstructure on the thermomechanical properties of two families of HEA, fcc and bcc including their coexistence, each represented by a model alloy in a concerted approach including experiment, theory and simulation. We deliberately focus on these well-studied single-phase model alloy systems, namely the fcc CoCrFeMnNi and the AlCoCrFeNi system, which undergoes an fcc-bcc transition depending on the Al content, and the bcc HfNbTaTiZr alloys, in order to profit from available literature data, e.g. on stability ranges in temperature and/or composition. Based on these stable fcc and bcc lattices, we will explore in a continuous approach the chemical parameter space in between these model alloys as well as in the direction of subset compositions. The results that we shall obtain will thus not only contribute to the understanding of a specific alloy system, but also to HEAs in general. Processing of the alloys will involve systematic thermomechanical treatment including diffusion couples and severe plastic deformation of the alloys with subsequent heat treatment. Tracer diffusion will present an important tool for analysing the atomic mobilities in the bulk HEAs but also specifically in the grain boundaries, providing important input concerning the general characteristics of HEA but also concerning highly relevant properties such as stability, oxidation resistance or hightemperature creep. The alloys will be analyzed with respect to their mechanical properties using macroscopic and small scale mechanical testing approaches, from RT up to 500 °C at various strain rates and under in-situ observation, both SEM and TEM. Microstructure investigations on all relevant length scales from the atomic (TEM) to the micron scale (high resolution EBSD) shall reveal defect structures, lattice strain and the characteristics of internal homophase (grain boundaries) and heterophase interfaces such as segregation, dislocation pile-ups or strain fields. In-situ experiments inside the TEM will analyse the formation of specific defects such as nano-twins in strained fcc-HEA but will also allow analysing microstructure-defect interactions, like dislocation storage and dislocation-solute as well as the dislocation-grain boundary and solute-grain boundary interaction. The experimental studies are closely interlinked to atomistic modelling, which provides additional insight into the lattice stability, basic deformation mechanisms, diffusion mechanisms, defect structures, and particularly defect formation and defect interactions in HEAs. The interconnected questions outlined above shall be addressed in a collaborative research effort that benefits from the complementing expertise of the involved partners.