DFG Schwerpunktprogramm / Priority Programme Compositionally Complex Alloys – High Entropy Alloys (CCA-HEA)

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Design and mechanical properties of compositionally complex alloys from twinning-induced towards bidirectional transformation-induced plasticity (MULTI-TRIP CCAs)”

The transformation induced plasticity (TRIP) effect has been successfully introduced into interstitially alloyed face centered cubic (FCC) CrCoNiMnFe-based HEAs utilizing a combined ab initio-experimental approach. Three quinary HEAs have been selected from ab initio calculations, experimentally prepared and investigated. The atomistic calculations allowed us to interpret the different observed deformation modes and highlight the high efficiency of the developed coupled ab initio-experimental approach developed within the first project for developing mechanically high-performing, low-SFE, interstitially alloyed CCAs.

Further opportunities lie in the exploration of thermodynamics and properties of such near-zero SFE HEAs. In these alloys, the matrix could possibly assume both the hexagonal closed packed (HCP) and FCC structure, in adjacent regions of the same bulk microstructure, owing to the energetic equivalence of the coexisting phases. The similarity in phase energy can lead to a bidirectional TRIP effect, in which FCC-structured matrix portions transform under load into HCP regions and vice versa, depending on the local, micromechanical stresses. This effect can lead to an extreme microstructure refinement down to the nanometer regime and enhanced mechanical properties.

Project MULTI-TRIP CCAs builds on the successful first project phase and aims at further significantly enhancing the strength-ductility combination of quinary CCAs by introducing the bidirectional TRIP effect into interstitially alloyed CCAs. This will be achieved by combining state-of-the-art ab initio calculations and multiple experimental techniques such as rapid alloy prototyping (RAP), digital image correlation (DIC) assisted tensile testing, electron backscatter diffraction (EBSD), X-ray diffraction (XRD), transmission electron microscopy (TEM) and atom probe tomography (APT). Ab initio calculations will be used to screen a large compositional HEA/CCA phase space for promising low-SFE candidate alloys. Key quantities linking the quantum-mechanical calculations and experiment are, e.g., the generalized SFEs and HCP, FCC, and DHCP phase energies. Non-equiatomic quinary CoCrFeMnNi alloys with near-zero SFEs will be developed by fine-tuning the concentrations including interstitial C, N and H. Each principal element will have a concentration between 5 and 35 at. %, and the content of minor interstitial alloying elements (C, N, H) will be low (less than 1.5 at. %). In relation to the first project phase MULTI-TRIP CCA explores a larger compositional phase space including also variations of Cr and Co. The ab initio simulations will allow us to identify promising alloys, design rules and physical interpretations. The above-mentioned advanced experimental techniques will be utilized to demonstrate the superior mechanical properties of the new materials and reveal the underlying mechanisms via micro- and nanoscale microstructural investigations.