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

KO 5080/2-1
RA 659/29-1

Interstitial transformation-induced plasticity-assisted quinary compositionally complex alloys: Design, structure and mechanical behavior (TRIP-iCCAs)

Pursuing outstanding mechanical properties in high entropy alloys (HEAs) and compositionally complex alloys (CCAs) have drawn great interest in the past several years due to immense compositional opportunities inherent to CCAs/HEAs. A novel design strategy has recently been proposed to introduce the transformation induced plasticity (TRIP) effect into HEAs. The resulting CCAs consist of dual-phase HEAs and reveal both exceptional strength and ductility.

The proposed TRIP-iCCAs project aims at significantly enhancing the strength-ductility combination of quinary HEAs and/or CCAs (with 5 main alloying elements) by simultaneously introducing interstitial C/N (as minor alloying elements) and the TRIP effect. Thus, a new class of alloys, namely, interstitially alloyed TRIP-assisted quinary (five-component) CCAs (TRIPiCCAs), will be developed.

This will be achieved by combining state-of-the-art density functional theory (DFT) 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). The DFT calculations will include finite-temperature excitations and will be used to screen the large compositional space of HEAs/CCAs to identify promising candidate alloys. The key quantities linking the quantummechanical calculations and experiment are the intrinsic stacking fault energy (SFE) and HCP-FCC phase stabilities. Nonequiatomic quinary CoCrFeMnNi alloys with TRIP effect will be developed first, followed by introducing interstitial C and N. Each principal element (Co, Cr, Fe, Mn and Ni) will have a concentration between 5 and 35 at. %, and the content of minor interstitial alloying elements (C and N) will be low (less than 1.5 at. %). Finite-temperature DFT simulations will provide atomistic insights (C,N impact on SFEs, partitioning of interstitial elements, thermal excitations, lattice distortions) allowing 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.

The success of TRIP-iCCAs will greatly advance the development of a new class of CCAs/HEAs with superior mechanical properties. The combined theoretical and experimental efforts will result in a thorough scientific understanding of the unusual phenomena in the novel quinary TRIP-iCCAs