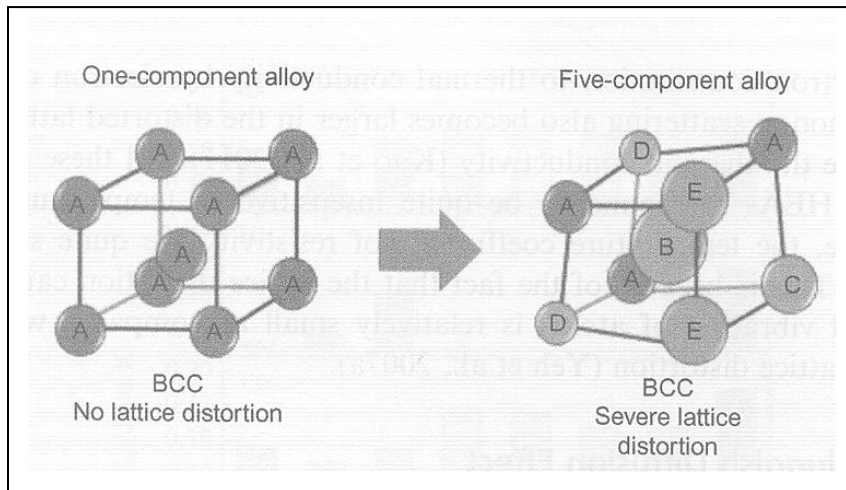


Preparation of Novel High Entropy Alloys

Ladislav Kalvoda, Jakub Skočdopole

HEAs (High Entropy Alloys) are multicomponental metallic alloys composed of 5 or more constituting elements of approximately equal relative weight fractions, forming a homogenous solid solutions. Basic concept of such alloys dates back to German scientist Karl Franz Achard (*April 28, 1753 – † April 20, 1821) and has been “re-vitalized” much later by prof. Cantor (University of Sussex) and prof. Yeh (University of Taiwan) at the end of the 20th Century.

The main idea behind HEAs lies in stabilization of a multi-elemental solid solution by the entropic contribution to its total free energy of mixing: $\Delta G_{\text{mix}} = \Delta H_{\text{mix}} - T\Delta S_{\text{mix}}$. Here H and S is enthalpy and entropy of mixing, respectively, and T is absolute temperature. Comparing “classical” alloys, HEAs usually adopt a severely disordered cubic structure (see figure below) leading, in combination with complex composition, to the unusual and potentially practically



important physical properties, such as sluggish diffusion, high mechanical strength and hardness, high wear, corrosion and radiation resistance, and significant thermo-stability of many other properties.

The proposed master / doctoral project aims on design and preparation of HEAs of novel composition, and examination / characterization of their properties. Arc melting furnace (AMF) available at the DSSE workplace will be used as the

main techniques in preparation of the proposed HEAs from elemental powders. Advanced simulation tools (CalPhad, Molecular Dynamics, DFT) and composition libraries prepared by IJD method are supposed to be utilized in the design process.

The general goal of the research is to develop novel materials suitable for contemporary heavy duty applications, such as coatings and barriers with high radiation and thermal resistance, construction materials for airplanes, fusion reactors and plasma facing materials, energy storage materials, easily recycled materials and magnetic conductors.

References

- B.S. Murty, J.W. Yeh, S. Ranganathan: High Entropy Alloys. Elsevier, 1st Ed 2014, 2nd Ed 2019.
- D.B. Miracle a, O.N. Senkov: A critical review of high entropy alloys and related concepts. Acta Materialia 122 (2017) 448-511.
- Lu Xie, P. Brault, Anne-Lise Thomann, Jean-Marc Bauchire: AlCoCrCuFeNi high entropy alloy cluster growth and annealing on silicon: A classical molecular dynamics simulation study. Applied Surface Science 285 (2013) 810-816.
- Lu Xie, Pascal Brault, Anne-Lise Thomann, Xiao Yang, Yong Zhang, GuangYi Shang: Molecular dynamics simulation of AlCoCrCuFeNi high entropy alloy thin film growth. Intermetallics 68 (2016) 78-86.
- O.N. Senkov, et al.: Microstructure and elevated temperature properties of TaNbHfZrTi alloy. J. Mat Sci. 47(9) (2012) 4062.