Computer Aided Design of Novel High Entropy Alloys

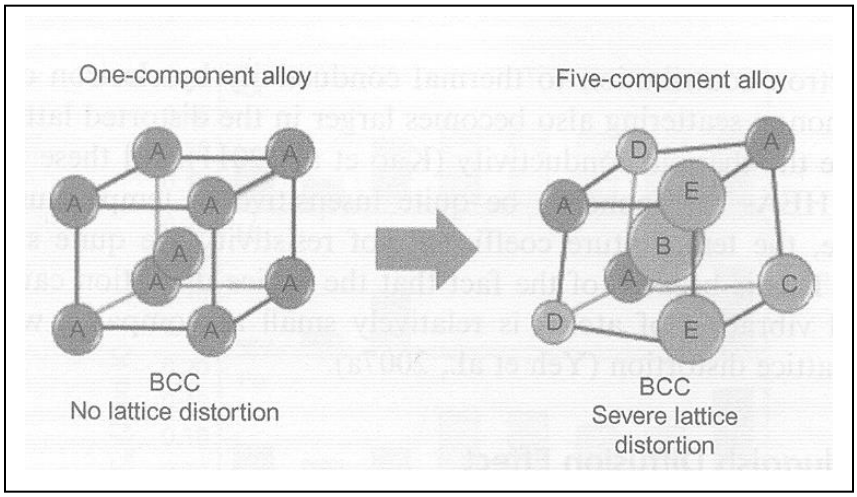
Master /doctoral project

Supervisors: Mgr. Jaroslav Hamrle, Ph.D., doc. Ing. Ladislav Kalvoda CSc.

There is steadily growing attention nowadays paid to development of novel high entropy alloys (HEAs), multicomponental metallic solid solutions composed of 5 or more elements, approximately equal in their relative weight fraction.

Concept of multicomponent alloys dates back deep in history, to german scientist Karl Franz Achard (18th Century), but became lost for a more then hundred years till it has been re-discovered 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: $\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$. Here H and S is enthalpy and entropy of mixing, respectively, and T is absolute temperature. Comparing "classical" alloys, such HEAs usually adopt a severely disordered cubic structure (see Figure 1) leading, in combination with the complex composition, to very unusual properties, involving among others, e.g. sluggish diffusion, high mechanical strength, high hardness, high wear resistance, high corrosion resistance, high thermo-stability of properties and high radiation resistance.



The proposed project aims to constitute and consolidate a simulation model applicable in design of HEAs with novel compositions, and simulate their structure and physical properties. The model is supposed to stem from thermodynamic (CalPhad method) and atomistic (quantum mechanical Density Functional Theory methods) approaches. The general goal of the research is to contribute to development of novel HEA materials optimized towards future 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 or magnetic conductors.

References

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