Elucidation of transport properties in high-entropy alloys with the use of a computational-oriented approach

During the last 15 years, the high entropy approach to the materials design became one of the most coveted topics in materials science. Originally, it was applied to the multicomponent alloys, known as high entropy alloys (HEAs), which today have grown into one of the most promising metallic materials. The general idea behind them is as follows - one should select 5 or more elements, characterized by relatively similar properties such as atomic radii and crystal structure, and mix them together in proportions close to equimolar. The configurational entropy of such a mixture reaches the maximum for the case of a random solid solution, in which every lattice site is randomly occupied by one of the elements, promoting the formation of simple crystal structures characterized by high symmetry. Described approach drastically differs from the one applied in conventional alloys, which are based on one, sometimes two main elements, with the rest of them playing a role of minor additions. As a result, the advent of HEAs opened a number of completely new opportunities and systems, suitable for the design of new, better materials.

From the very beginning of their development, the high entropy alloys were believed to possess extraordinary properties, which were categorized in 2006 into the so-called "four core effects". These are: high entropy effects (stabilization of simple solid solutions), severe lattice distortion (distortion of the crystal lattice due to random distribution of atoms characterized by different radii), cocktail effect (occurrence of new properties, not related to properties of the composing elements), and sluggish diffusion effect (diffusion slower than in conventional alloys and metals). These effects were a major driving force behind the development of HEAs during last decade. However, nowadays their existence is widely questioned, with the experimental data directly contradicting their assumptions, or being inconclusive. Nevertheless, already a number of extremely promising materials have been established within HEAs family.

After years of development, the HEAs are finally entering the stage, when their actual, industrial-level applications can be considered. At the moment, they are projected mainly as high-temperature structural materials, potentially replacing the nickel-based superalloys. However, it is already clear that the original, single-phase approach, especially for the most popular FCC alloys, does not provide the materials with sufficient mechanical strength. As a result, more and more studies are concentrated on the systems with prominent content of the much tougher BCC phase. This however, leads to the questions concerning the stability and kinetics of such systems, questions for which there is no data to provide us with an answer.

The aim of the proposed study is to design and carry out the first diffusion experiments in the BCC-structured high entropy alloys. Thanks to the most recent developments in this field, a number of new, stable BCC systems finally emerged, making such studies possible. A number of different alloys from the novel, previously not experimentally tested systems, will be designed with the use of thermodynamic databases and synthesized. The obtained materials will be then used to conduct interdiffusion experiments. The resulting data will be interpreted with the use of theoretical models, combined with the numerical analysis and advanced thermodynamic description. The applied methodology will allow determining diffusion coefficients, as well as their temperature dependence, providing us with the first data on the subject of diffusion kinetics in BCC-structured HEAs. This, in turn, will allow a much better understanding of the potential of these alloys, in the role of high-temperature structural materials, as diffusion directly affects the high-temperature mechanical properties of materials, through the creep phenomena. The experiments planned within the project will expand the number of studied systems more than two-fold, finally providing us with sufficient data to create a kinetic database that allows us to design transport properties of the diffusion in high entropy alloys.