

Description for general public

High-entropy alloys (HEAs) are multicomponent systems incorporating four or more elements in similar concentrations, in contrast with existing commercial alloys. The conventional concept behind HEAs is that the high configurational entropy inhibits the formation of brittle intermetallic phases in favour of multicomponent random solid solutions with unique properties, significantly different to the properties of pure constituents, such as high yield strength and hardness at elevated temperatures or outstanding irradiation properties. One of main technological problems related with HEAs is the difficulty with their casting, further processing and machining. Fortunately, due to inhibited formation of precipitations HEAs are promising candidates for additive manufacturing (AM) – an important novel technology which provides design flexibility, low cost of geometric complexity and low material waste. Up to now, there are just a few materials suitable for industrial AM applications. It is related with the unique conditions present in AM as rapid cooling and large thermal gradient, which induce thermal residual stresses and non-equilibrium microstructures. Rapidly cooled HEAs show a potential of replacing standard AM-grade alloys.

The main goal of this project will be to improve the knowledge about the microstructure evolution of HEAs at elevated temperatures, which may enable a better understanding of processes existing during AM as well as during an annealing of these materials. The investigation will be focused on alloys from the Ta-Ti-V-W system, which was chosen based on the theoretical and experimental investigations of Cr-Ta-Ti-V-W performed in the previous project.

Within this project, the theoretical investigation of microstructure evolution of Ta-Ti-V-W alloys will be performed by using a combination of DFT, machine learning (ML) methods and molecular dynamics (MD) simulations. Thousands of DFT calculations will be used to investigate the most important properties of HEAs, such as migration energies of vacancies in those alloys and the relative stability between bcc structures and liquid configurations as well as to create the input database for ML methods. The crucial and most challenging theoretical task related will be the development of an accurate interatomic potential for MD simulations for Ta-Ti-V-W alloys using ML methods. MD simulations with ML potential for Ta-Ti-V-W system will enable the investigation of time evolution of the microstructure and its elastic properties as well as the diffusion of atoms in HEAs as a function of alloy composition and temperature. They will allow also the investigation of formation of solid phases in the melted high-entropy alloys. The results of MD simulations will enable not only a better understanding of processes existing during an additive manufacturing as well as during an annealing of these materials but also will help in a design of alloy compositions and the choice of parameters for additive manufacturing.

The theoretical investigation will be supported by experiments. The samples of alloys will be synthesized using arc-melting. In order to investigate the evolution of the microstructure as a function of time and temperature, the samples will be annealed at different temperatures and next characterized. The samples of alloys with the best microstructure stability will be atomized using custom-made ultrasonic atomizer facility and obtained powders will be used for the 3D printing of samples of alloys via selective laser melting (SLM) method. The main goal of the experimental part of the project will be to try to design an alloy composition and the choice of parameters optimal for printing elements using additive manufacturing. The experiments will be also used to validate the developed theoretical models. In particular, the microstructure evolution (precipitations, changes in chemical composition) observed in as-received and annealed samples will be used to validate the ML potential for Ta-Ti-V-W alloy. Moreover, the comparison of results measured for samples produced using arc-melting and additive manufacturing will enable to understand how the choice of processing method influences the stability and properties of HEAs.