

Is it difficult to make any alloy? It seems that not. Theoretically, it should be enough to heat two components (e.g. elemental solids) above their melting points and to mix the resulting liquids and finally to cool the mixture. However, as practice shows, the described procedure does not always work for any two components. It may happen that the liquids do not mix with each other and the resulting product may consist of two different phases. Even if the liquids can be mixed, it often happens that the resulting solid phase has a complicated crystal structure, not having too much in common with the crystalline structures of the starting elements. This type of new phase depends on several parameters, primarily on the types of alloying elements as well as their proportions and temperature (very often there are several such phases appearing simultaneously). One can guess that the attempt to melt three or more components may result in even greater complexity of the obtained products. Therefore, the big surprise was the fact that the melting several (but at least five) of the chemical elements in comparable quantities often leads to the preparation of the alloy, having the simplest possible structure, i.e. body centered cubic (*bcc*), face centered cubic (*fcc*) or sometimes hexagonal close-packing (*hcp*). Simple explanation of this fact has been based on the extremely high values of configuration entropy achieved in this type of systems. Therefore, these alloys have been called high entropy alloys (HEA).

For the crystal structure of the phase, which is the result of the connection of the several mixtures (as liquids) is responsible Helmholtz free energy  $F = E - TS$ , where  $E$  is the energy of the phase formation (that measures the energy needed to build the phase from the free atoms of individual elements),  $T$  is the temperature, while  $S$  is the total entropy. It is known that amongst the enormous number of potential phases, in principle that one is formed for which the function  $F$  reaches the lowest value. As is clear from the above formula, the influence of the term associated with the entropy decreases  $F$  with increasing temperature and for a sufficiently large  $T$  may even dominate energy  $E$ . In other words, at high temperatures,  $TS$  rather than  $E$  determines, which phase is formed.

What is the entropy? In the simplest approximation it is a measure of the disorder of a system, a measure of the potential 'mess'. The greater the chance of mixing of different objects, the greater the entropy is. Objects, that create the mess are the atoms of different elements, which are arranged in many ways (then we are talking about configuration entropy), but also their magnetic moments can form many orderings (magnetic entropy), the ways of their vibrations in the crystal lattice (phonon entropy) and finally free electrons can be distributed in space in many ways (electron entropy). One can demonstrate that in the case of several components the highest configuration entropy is obtained when their amounts are the same (stoichiometric alloys). Any attempts of ordering (e.g. the complication of structure by defining sublattices) always leads to a reduction of the entropy of the system.

High-entropy alloys are intensively studied for about 20 years, and the amount of published articles devoted to their properties is growing rapidly. It is connected first of all with their interesting technological parameters (e.g. hardness), but in recent years it has also become the subject of intense theoretical and experimental studies of a fundamental nature. For example, we do not know, why in some systems HEA does not appear, although the overall conditions of their formation are satisfied. In other systems (e.g. FeCrNiCoAl), the melting produces two simple structures (*fcc* and *bcc*) at the same time, and their relative contribution is highly sensitive to small changes in the concentration of aluminum. Additionally, the detailed studies showed that within the resulting simple structure, one can however detect various types of orderings of atoms.

In this project authors will intend to explain the aforementioned issues related HEA properties, both in theoretical and experimental ways. Because the typical alloys - as the name suggests - are obtained by alloying, the kind and contribution of the obtaining phases are determined by the dominant configuration entropy, at the stage of the alloy's formation, in high temperatures. However, it is possible to get an alloy directly from the solid phase by heating the mixtures of pure metal powders at temperatures well below the melting point of the alloy and most of its components. In this case, homogenization of the alloy occurs by diffusion of atoms in solid phase. Thus obtained HEA may have some other properties (for example the phase structure or magnetic properties) from that prepared by melting, since they have been determined by a large configuration entropy in much smaller extent. It is therefore a good subject for testing of real influence of formation energy values and other types of entropy on the phase composition of the HEA. Experimental studies rely here upon determination of the parameters of crystal structures (types of arrangement, the phase contributions, sublattice occupations) obtained mainly using X-ray and neutron diffraction techniques. It is also planned to use electron microscopy (EDX technology), which will allow to characterize the spatial distribution of the investigated phases, their stoichiometry and uniformity. Especially important technique to realize the purpose of the project is using the Mössbauer spectroscopy on  $^{57}\text{Fe}$  nuclei that should bring a lot of precise information about a neighborhood of the iron atoms in the structures, not available from diffraction techniques. Studies of magnetization as a function of the external magnetic field or a function of temperature will allow for the determination of the average magnetic moments as well as the magnetic ordering temperatures (similar information, but limited to of the iron atoms only are available applying Mössbauer spectroscopy).

In parallel to the ongoing measurements, ab initio electronic structure calculations of the experimentally investigated systems will be performed. Such calculations for disordered alloys will be performed using the KKR method with the coherent potential approximation (CPA), which would give the average values of various important parameters, independently available from different experiments. The second way of the theoretical analysis will be based on calculation of many ordered approximants with different distributions of atoms using e.g. KKR code. Statistical analysis of

such results allows for comparison with the average values obtained using the KKR-CPA technique, however, allows also a precise analysis of different atomic configurations and their influence on the properties of the phases. Since computational results are often the subject to some ambiguities of employed models on one hand, and the results obtained experimentally are the subject to the experimental systematic errors or the results can meet some problems with unambiguous interpretation on the other, parallel running of measurements and calculations may allow for more reliable explanation of the observed phenomena.

On the whole, the common investigations, carried out using state-of-art experimental and theoretical tools, should allow for obtaining novel, consistent and high-quality results.