Due to the increasing demands from modern industry (for example nuclear) there is a constant need for development of engineering alloys. The possibilities to improve conventional alloys (Ni-based superalloys or austenitic steels) are limited, thus materials scientists are trying to develop the new concepts of metallic materials.

One of the most promising is called high entropy alloys (HEA) which is different from conventional approach of alloying the main element with small amounts of other elements for tuning properties. In HEA at least four components are mixed together with similar proportions. In this situation, the crystal lattice of the alloy is built by random distribution of elements which feature various properties. Thanks to unusual architecture the basic properties are expected to differ from the conventional alloys due to disturbed crystal lattice. This features makes scientists all over the world to work on the design of HEA.

The properties of HEA strongly depends on the atomic scale interactions between elements. Despite seemingly random distribution of atoms, in certain situations like in CrMnFeNi alloys, the chemical short range ordering of atoms is expected to happen. Short range ordering is a local configuration of elements (with sizes below 1 nm) which is stable and could appear regularly within the random distribution of elements in HEA. The presence of such local order may positively influence mechanical strength. Another approach to improve the performance which will be tested within this project is strengthening by additional atoms which are not located in the regular array in the crystal lattice (interstitials). They disturb regular arrangement of atoms and introduce strong elastic stress field. This effect is achievable with non-metallic elements like oxygen or nitrogen. The project will focus on designing an alloy in which both strengthening mechanisms will operate simultaneously.

Since there are no experimental techniques enabling precise studies on interatomic interactions, the fundamental understanding of such systems must be studies using computer simulations. On the basis of techniques such as density functional theory, cluster expansion or Mote Carlo it is possible to investigate how neighbouring elements within the crystal structure of HEA will interact and what kind of properties could be achieved. With use of such tools, the exact chemical composition of alloy will be designed. The experimental part of the project will focus on casting alloys and developing heat treatment which enable to tailor microstructure with short range ordering for enhanced strength. The properties of experimental alloys will be evaluated on the basis of mechanical tests and differential scanning calorimetry. The advanced characterization methods like transmission electron microscopy will be used to understand the real crystal structure of alloys and compare it the simulations as well as understood the real microstructural conditions for properties.

As a final outcome of the project, it is expected that an approach including simulations and thermo-mechanical treatments will be develop to design new materials from CrMnFeNi system. Mechanical properties of the new alloy will benefit from chemical short range ordering and strength from interstitials.