Dimagnesium iron hydride with the chemical formula Mg_2FeH_6 is the material characterized by the highest, among all known hydrogen compounds, volumetric hydrogen density - 150 kg/m³. This value is more than twice as high as for liquid hydrogen and seven times higher than for compressed hydrogen (at a pressure of about 20 MPa). The gravimetric hydrogen density in this compound is 5.46 wt.%. Due to the aforementioned properties, this material is one of the most frequently tested compounds with potential use as a material for the hydrogen storage and thermal storage (at temperature above 500 °C).

Unfortunately, the synthesis of this compound directly from pure elements is difficult. This is because in the Mg-Fe equilibrium system there is no intermetallic bond and there is no mutual solubility of these two elements. It is only in the ternary Mg-Fe-H system that hydrogen becomes a bonding component and contributes to the possibility of producing the Mg₂FeH₆ compound. For the first time, this hydride was produced in 1984 by a team led by J. Didisheim. However, the efficiency of this process remained at 50%. Several methods for the production of this hydride are already known and well-developed. It is, among others, sintering elementary powders Fe and Mg at elevated temperatures (about 500°C) under high hydrogen pressure (20 -120 bar) for a long time, reaching even a few days. Another method is mechanical alloying (MA), in the inert atmosphere, of MgH₂ and Fe powders and reactive mechanical alloying (RMA), in a hydrogen atmosphere, of powders of pure Mg and Fe elements. The last method is mechanical milling process, for a relatively short time, powders of magnesium hydride and iron and subsequent heating of the resulting mixture under hydrogen pressure. In this way, the efficiency of the process can increase up to 97%.

However, iron powder of high chemical purity is involved in each of the above-mentioned cases of preparation of a ternary hydride. The iron usually used for the synthesis process of Mg_2FeH_6 has a body centered cubic (BCC) crystal lattice. It is well known, iron also has another allotropic form with face centered cubic (FCC) crystal lattice structure, which is stable at temperatures above 910 °C. However, iron alloys with a stable A1 crystal lattice can be obtained by additions of a sufficiently large amount of elements favorable to the creation of the austenite phase. The chemical stability of the alloy austenite is exceptionally high and for this reason austenitic steels are used as stainless steel, heat-resistant steel and implantable materials. From a scientific point of view, a very interesting issue is to explore the possibility of producing Mg_2FeH_6 from the precursor (austenitic steel), which contains very high amounts of iron but in a form with very low chemical activity in relation to pure iron. The use of this phase for the synthesis of dimagnesium iron hydride has not been investigated, although there are reports of magnesium reactions with alloy austenite in the form of nanowires. In addition to the cognitive character of the examination reaction mechanisms, there is also the question of future practical using the above-mentioned concept of producing this hydride from steel. The use of steel from scrap can contribute to an increase in the recycling process of this type of materials and a significant reduction in the cost of production of ternary hydride, which in the present world are a very big advantages.

The main purpose of the proposed project is to investigate the effect of iron allotropy on the possibility and efficiency of the synthesis of the Mg_2FeH_6 and to compare the properties of the hydride thus obtained with the hydride obtained from pure chemical iron (alpha phase). For this aim, such research techniques will be used: X-ray diffraction (phase analysis of powders before and after hydrogeneration), scanning electron microscopy (microscopic observation and chemical analysis of both powders before and after the hydrogeneration process), differential scanning calorimetry, thermogravimetry and mass spectroscopy (these techniques will allow the observation of the nature of phase transition). Moreover, for samples after hydrogeneration hydrogen absorption and desorption isotherms will also be tested.

So far, preliminary studies have been made, which prove the possibility of synthesis of MgH_2 powder with austenitic steel powder (gamma phase). The research planned in the proposed project will allow to examine the mechanisms of creation and the impact of process conditions on its effectiveness.