Research on the iron/ammonia/hydrogen system is important because industrial processes based on processes occurring in them, i.e. catalytic synthesis of ammonia and nitriding process (hardening) of metal surfaces has been carried out in the industry for about 100 years, and research is still ongoing and discussions about its functioning.

The iron catalyst consists of nanocrystalline iron, the surface of which is covered with promoter oxides (mainly Al_2O_3, CaO, K_2O) and under the conditions of technological processes is in a state of chemical equilibrium. The NC-Fe/NH_3/H_2 system is used as a model one to study surface phenomena in reactions between a nanocrystalline solid and a gas phase. In 2007. Professor G. Ertl was awarded the Nobel Prize from chemistry "for investigations of chemical processes occurring on the surface of solids", which was based on the mechanism of catalytic synthesis of ammonia on the surface of iron. In his considerations, he did not take into account the possibility of equilibrium states.

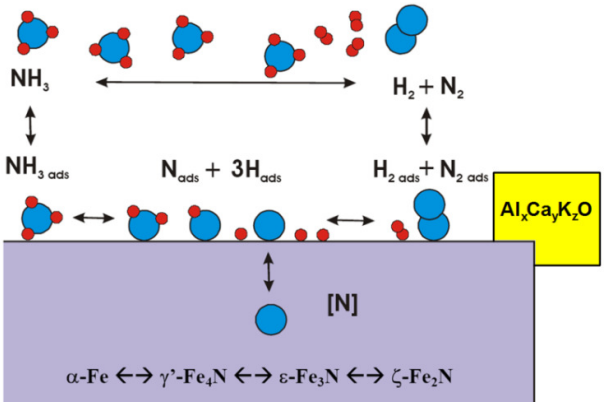

Figure 1. Processes occurring in the NC-Fe/NH_3/H_2 system

During the chemical process involving nanocrystalline iron with an ammonia-hydrogen atmosphere, the following are determined: (1) stationary states (Figure 2) in which the degree of conversion of a nanocrystalline substance depends on the temperature and chemical potential of the gas phase; and (2) states of chemical equilibrium between the gas phase and the solid, only the catalytic decomposition of ammonia takes place on the surface. In steady states in the two-phase system, the occurrence of the hysteresis phenomenon was observed (Fig.3) for chemical processes of nitriding of nanocrystalline iron and reduction of nitrides. Until now, the phenomenon of hysteresis has been associated with physical phenomena. Our research shows that the structure of nanocrystalline iron subsidized with hard-to-reduce metal oxides is the effect of determining the state of equilibrium.

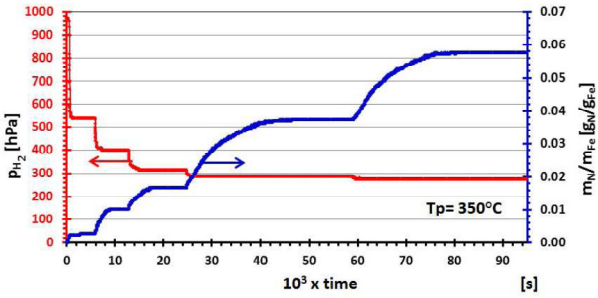

Figure 2. Changes in the degree of iron nitriding (blue line) and hydrogen concentration (red) during nitriding

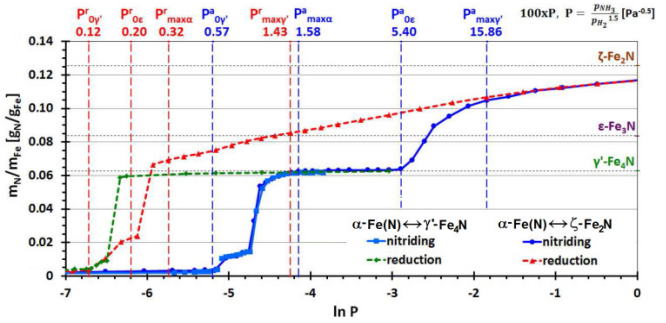

Figure 3. Dependence of iron nitrate degree on the nitriding potential - HYSTERESIS

The aim of this project is to understand the kinetics and thermodynamics of the catalytic decomposition of ammonia and nc-Fe recrystallization taking place in parallel with the nitriding process in the nanocrystalline iron/ammonia/hydrogen system. The research work undertaken in this project will allow to determine the thermodynamic relationships of physicochemical, magnetic and electrical properties of nanomaterials from the chemical potential of the gas phase with which they react in equilibrium or close to equilibrium states.

Currently, correlations between the properties of nanomaterials and the parameters related to the process of their preparation (temperature, resilience, etc.) are determined experimentally by trial and error. Lack of knowledge in the field of thermodynamics of nanomaterials prevents the conscious conduct of synthesis of these materials in a controlled manner. Understanding the thermodynamic basis of processes involving nanomaterials will enable the design of technology for the production (control and control of the synthesis process) of nanocrystalline materials with the desired, previously designed properties.