

Abstract of the PhD thesis

**„Research on the crystal structure and surface composition  
of cobalt catalysts for ammonia synthesis”**

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The ammonia synthesis process is one of the most energy-intensive industrial processes – it uses about 1% of global energy production. For this reason, research on efficient catalysts for this process is an important topic in modern chemical technology. Cobalt catalysts, due to the ease of synthesis and high availability of raw materials, are a group of materials that can be applied in industry.

As part of the doctoral thesis, cobalt catalysts for ammonia synthesis, deposited on mixed magnesium-lanthanum oxide, were studied. In the first stage of the work, catalysts containing 10 wt.% of cobalt, differing in the method of introducing this element onto the carrier were investigated. The cobalt was introduced by deposition-precipitation (DP), deposition-precipitation with urea (DPU), co-precipitation (CP) and wet impregnation (WI). The crystallographic structure of precursors and catalysts after the activation process was determined. The presence of a regular magnesium oxide phase and two phases: hexagonal and monoclinic lanthanum(III) carbonate phases were confirmed in the precursors. However, no cobalt-containing phases were observed. The activation process was carried out at high temperature, in a hydrogen atmosphere. It induced the phase composition change. A regular phase of magnesium oxide, a hexagonal and a regular phases of lanthanum(III) oxide were detected. For the co-precipitated (CP) and wet impregnated (WI) catalysts, a metallic cobalt with a regular structure was also detected. The surface composition was investigated by X-ray photoelectron spectroscopy (XPS). It was confirmed that the ratio of the cobalt atoms in the metallic state to the total amount of cobalt atoms on the catalysts' surface increases for a examined preparation methods in the following series: DP < DPU < CP < WI. The catalytic activity tests confirmed that the catalyst where the cobalt was introduced by the wet impregnation method (WI) showed the highest activity.

In the second part, systems containing 10, 20, 30, 40, 50 wt.% of cobalt introduced onto a magnesium-lanthanum support by wet impregnation method were investigated. After the activation process, only three crystallographic phases: cubic magnesium oxide, hexagonal lanthanum(III) oxide and cubic metallic cobalt were identified in all catalysts. Examination of the surface composition by X-ray photoelectron spectroscopy during the activation process showed that, for catalysts containing 20-50% of cobalt, there is a complete reduction of cobalt compounds to the metallic form of cobalt. Catalytic activity tests indicated that the highest activity in ammonia synthesis process was observed for catalyst containing 40 wt.% cobalt.

The method of catalyst preparation affects its activity in the ammonia synthesis process. During the activation process, significant changes in the structure of the catalyst occur, leading to the formation of new crystalline phases, in particular metallic cobalt. Performed studies indicated systems with the most promising properties for use as industrial catalysts for the ammonia synthesis.