

Heterogeneous catalysis, i.e. catalysis in which the reactants and the catalyst are in different states of matter (e.g. gas reactants and solid catalyst), is one of the main branches of chemical industry. The presence of catalyst allows gas reactants to combine and form products that would not form without the catalyst. This property is widely used to convert/neutralize environmentally harmful products of incomplete fuel combustion (such as for example CO or NO) to compounds less harmful (e.g. CO₂, N₂ and O₂). Another common application of heterogeneous catalysis is the synthesis of chemicals, for example synthesis formaldehyde from methanol.

The catalytic activity of the material mainly depends on the structure and properties of its surface. To investigate the mechanisms of catalytic reactions and optimize the catalysts, especially in terms of their yield and "lifetime", it is necessary to perform basic studies on the so called model catalysts. Model catalyst studies combine the analysis of structural changes that occur in the catalyst and investigation of the reactivity of the system and allow to study reaction between individual molecules of gases under idealized conditions of ultra-high vacuum (UHV).

The main aim of this project is to carry out model studies of a catalytic activity of a catalyst consisting of ultrathin films of iron oxide FeO(111) grown on Ru(0001) single crystal support. Model catalyst investigations will be conducted in an ultra-high vacuum laboratory located at the NanoBioMedical Centre of the Adam Mickiewicz University in Poznan, Poland. Heterogeneous catalysis studies carried out under ultra-high vacuum conditions are a multidisciplinary scientific field on the borderline of chemistry and physics which fits perfectly the idea and scientific objectives of the NanoBioMedical Centre.

Poland has a significant tradition in research in the field of catalysis, both heterogeneous and homogeneous, as well as surface science. In the context of the proposed project, the leading centers engaged in research of catalytic properties of heterogeneous model catalysts are the Institutes of the Academy of Sciences: the Jerzy Haber Institute of Catalysis and Surface Chemistry in Krakow and the Physical Chemistry Institute in Warsaw. In addition to that, one should not forget the achievements of the Polish universities in the research in studies of homogeneous and heterogeneous catalysis, including the academic units located in Warsaw, Krakow, Gdansk, Wroclaw, Lodz or Poznan.

The main principle of model catalyst studies is the analysis of surface structure of the catalyst before and after the catalytic reaction and correlation of structural changes with catalytic activity of the system. Nowadays, model studies of thin oxide films in catalytic oxidation reactions of gases are of great interest. It has been demonstrated that ultrathin films of metal oxides grown on single crystal supports have much higher catalytic activity than the commonly used metal catalysts. The best example is the ultrathin iron oxide FeO(111) film grown on Pt(111) single crystal support. Model studies carried out in UHV have demonstrated that at approximately 450 K the system exhibits high catalytic activity in the oxidation of carbon monoxide (CO) to carbon dioxide (CO₂), where the activity was much higher than the activity of commonly used platinum catalyst. In addition, recent reports point to high activity of the edges of the FeO islands, at room temperature. All these studies emphasize the significant role of the substrate which determines the structure and catalytic properties of metal oxide.

The working hypothesis of this project is that ultrathin films and islands of iron oxide FeO can be also grown on other single crystal supports, including Ru(0001). Using different substrate significantly affects the structure of the oxide which may result in different catalytic properties. It was observed that the FeO(111)/Ru(0001) exhibits a large number of defects which may act as catalytically active centers. Due to this, it is expected that the system FeO(111)/Ru(0001) can exhibit higher catalytic activity than FeO(111)/Pt(111). At the moment, there are no literature reports on the activity of ultrathin films or islands of FeO(111) grown on Ru(0001). The results obtained within the project will provide an added value in the field of model heterogeneous catalytic studies and an important comparative value for the well-known FeO(111)/Pt(111) system. In order to achieve the goals of the project, it is planned to combine the experience of the project team in iron oxide films preparation on Pt(111) and Ru(0001) with the experience of the project's supervisor in model catalytic studies of such systems, gained at one of the world's leading scientific institutions in heterogeneous catalytic studies - the Fritz Haber Institute of the Max-Planck-Society in Berlin, Germany.