Solving the crystal structure of novel complex materials with X-ray diffraction

The Polish chemical company FAMAR in Dankowice produces chemical catalysts for industrial processes which limit emission of harmful gases and also are useful for storage of gases. To understand the crystal structure of these novel materials, high resolution Xray Diffraction (XRD) was performed at the P02 beamline at DESY in Hamburg.

CHALLENGE

Important challenges of the 21st century include the reduction of CO_2 emissions to combat climate change, as well as the development of new materials for hydrogen storage for future energy technologies. The company FAMAR's chemical catalysts imit the emissions of harmful gases and also are useful for storage of gases. However, many of the catalysts produced are of an unknown structure and are a complex mixture of metals or metal clusters connected by rigid organic groups, for example $Mo_3O_{10} \cdot (C_6H_5NH_3)_2$ and $ZnBr_2.(NH_2\text{-}C_2H_4\text{-}NH_2)_2$. Knowledge of the structure enables the identification of possible reaction pathways of the catalyst and the reactants of the desired reaction. Such would help also in the development of new and more efficient catalysts.

METHOD

To understand the crystal structure of these novel materials, high resolution X-ray Diffraction (XRD) was performed at the P02 beamline at DESY. XRD is a technique used to measure the crystal structure of ordered materials – and information about the space groups, lattice constants and atomic positions can be extracted. The unique nature of the synchrotron radiation of produced by the PETRA III storage ring as well as the special features of the diffractometer setup at P02 enabled very high resolution XRD patterns to be obtained.

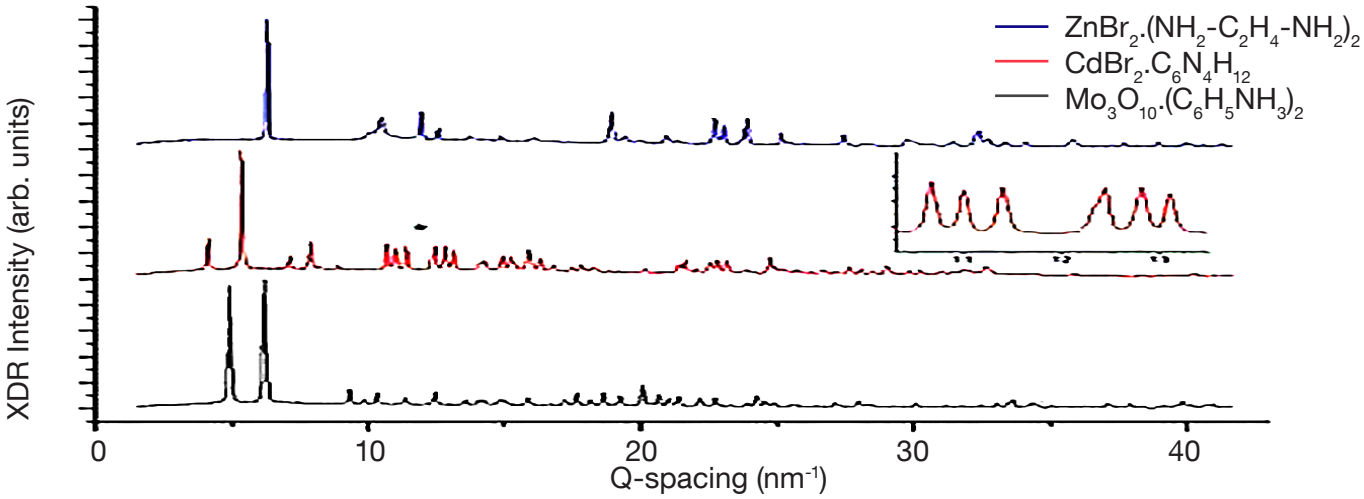

Figure I High resolution X-ray diffraction patterns for several compounds, produced by FAMAR in co-operation with scientists from Jagiellonian University, measured at beamline P02 at DESY.

INSIGHTS AND ANALYSIS

The measurements have been instrumental in solving the crystal structure of many complex materials, and many features of the measured diffraction patterns were superior to those measured using conventional laboratory diffractometers. Some peaks which are very close together and would usually overlap were made distinguishable with the synchrotron source (see figure above), as well as crystal phases which were present in a mixture of amorphous phases which are undetectable with conventional sources.

BENEFITS

The XRD technique and especially the setup at the Beamline P02 allowed FAMAR to get the full structural information of their catalyst. Due to the high x-ray energy and hence superb resolution, structural information was revealed that was formerly hidden in lab-based experiments. With this knowledge FAMAR is one step closer to produce new catalysts for greener chemistry.

SCIENCE LINK

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FOR MORE INFORMATION PLEASE CONTACT:

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