lany

diamond

Chemicals

CASE STUDY

Towards a better understanding of ZnO to enhance its functionality

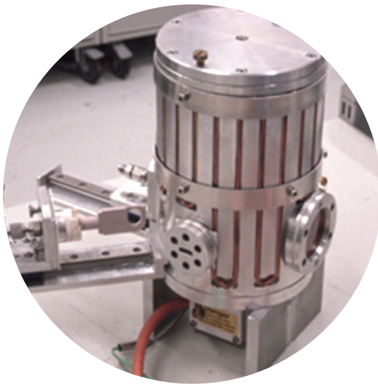
Zinc oxide (ZnO) is a highly desirable multifunctional material possessing superior electronic, structural and morphological properties which also exhibits high chemical stability, a broad range of radiation absorption and high photostability. For this reason, ZnO is used in n-type semiconductors, solar cells, photocatalysts, sensing materials and antiseptic additive compounds.

Many believe that the defects present in ZnO's structure are a key factor in influencing aspects of its performance and control of specific defect types could be used to enhance its functionality.

JM
Johnson Matthey
Inspiring science, enhancing life

The Challenge

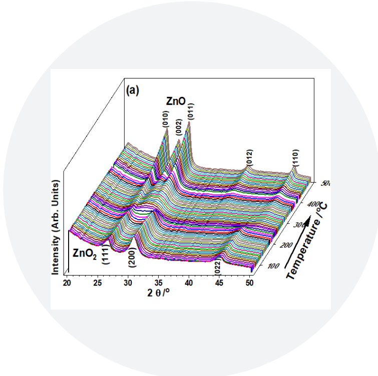
Defects in the ZnO structure are complex and hard to control during synthesis; they can influence both its chemical and physical performance. To study ZnO, scientists therefore need to use advanced characterisation techniques to help monitor changes in both local site symmetries and defective structures of ZnO. The results of this study will help scientists to understand the multifunctional properties and performance of ZnO.



The Solution

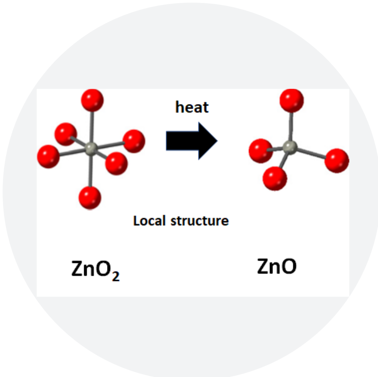
A collaboration of scientists from Johnson Matthey, UCL and Diamond carried out an *in situ* Zn K-edge experiment on B18 beamline using both extended X-ray absorption fine structure spectroscopy (EXAFS) and X-ray diffraction (XRD) via a controlled thermal decomposition of zinc peroxide (ZnO_2).

Respective *in situ* EXAFS and XRD datasets were collected in a combined time of less than one minute. This rapid time resolution allowed scientists to determine the pathway for the conversion of ZnO_2 to a defective ZnO, and then an ordered ZnO material, in an air atmosphere at temperatures up to 500˚C.



The Benefits

By combining two techniques with both a short-range order of sensitivity (EXAFS) and a long-range order of crystallinity detection (XRD) under *in situ* conditions, the team were able to acquire high quality data, enabling them to determine the pathway for the thermal decomposition of ZnO_2 to ZnO. Combining these results with those from thermogravimetric analysis (TGA), the team were able to identify a region where amorphous or very poorly crystalline ZnO solid is formed and monitor the defects forming in the ZnO structure.



"Johnson Matthey through our research efforts has developed an in depth understanding of zinc oxide materials properties under industrially related conditions. The ability to probe with fast time resolution at multi-length scales via *in situ* combined diffraction and spectroscopy at Diamond B18 has proven an essential component to this process." **Dr Tim Hyde,** Johnson Matthey

For further information

Diamond Industrial Liaison Team

+44 1235 778797
industry@diamond.ac.uk
diamond.ac.uk/industry
@DiamondILO

CS-CHM-JM-084-1

© Diamond Light Source Limited 2022