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Light for Science

Chemical Engineering

overview

Catalysis is estimated to be involved in 90% of all chemical processes, and the creation of 60% of the chemical products available on the market, and yet it is rarely analysed on the atomic scale. The need to understand catalysis at this level is driven by both economic and environmental concerns, and consequently there is a global interest in rationalising the synthesis of new catalysts.

Other chemical processes such as combustion can be studied in situ in real time using synchrotron light. The detection of minute levels of fine airborne particulate matter can be studied, as synchrotron light has the ability to detect fine particles less that 2.5µm in size. This allows chemical companies to refine their industrial processes whilst ensuring compliance with environmental regulations.

Key Challenges

- **Understanding the fundamental process of catalysis**
  To refine catalytic mechanisms and develop more efficient and selective catalysts
- **In situ processes in real time**
  This allows chemical processes to be tracked as they happen, over the full range of relevant length scales, and enables the detection of transient compounds which would otherwise not be observed.
- **Analysing and reducing waste**
  Ensuring compliance with regulation and minimising environmental impact.
- **Protecting product properties**
  Detailed chemical analysis can ensure that product patent infringements can be detected.

The Synchrotron Solution
Synchrotron X-rays can often yield more in-depth information on a material's structural, electronic, and catalytic properties than laboratory techniques, and can carry out experiments under operating conditions. Small and wide angle x-ray scattering (SAXS and WAXS) allow the collection of data from fast industrial processes in purpose built environmental chambers.

Techniques
Total X-ray Reflection Fluorescence, X-ray absorption fine structure spectroscopy (XAFS), powder diffraction, Surface X-ray diffraction, small angle scattering, Photo Emission Electron Microscopy (PEEM)

Beamlines: I06 Nanoscience, I07 Surface and Interface Diffraction, I11 High Resolution Powder Diffraction, I18 Microfocus Spectroscopy, , I19 Single Crystal Diffraction, I20 X-Ray Spectroscopy, I22 Non-Crystalline Diffraction

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case studies

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Predicting Plastic Properties

Injection moulded polymers have a tough life. The polymers do not flow easily, and so forcing plastic into moulds has to be carried out at extreme pressures. It is difficult to predict the mechanical properties of the plastics at the end of the injection moulding process. Current software models are limited, and they are unable to provide information on the toughness or surface appearance of the finished product.

To improve their predictive capabilities Australian scientists used synchrotron radiation at the Australian National Beamline in Japan to study how polymers behave as they are injected into the moulds. These results are used to refine the modelling software to gain more accurate predictions.

Although this work could potentially have been carried out in a laboratory, according to scientist Graham Edwards "We take days to complete work that would take months in the laboratory, and the synchrotron results are more accurate."

The predictions from the computer models so far show good agreement with observations of real polymers.

Source: Australian Beamline Facility, Photon Factory, Japan.

Website: www.synchrotron.vic.gov.au

Understanding Catalysis

Zeolites are valuable catalysts in industrial processes. The zeolites found in nature meet the properties needed for a large variety of applications but for new processes new combinations of characteristics are desired. By understanding catalysis on the atomic scale it is possible to synthesise zeolites with properties required for specific applications.

Scientists at the European Synchrotron Radiation Source (ESRF) used synchrotron light to investigate the formation of zeolites, with an underlying goal of coming closer to their rational design. Using a combination of techniques including SAXS and WAXS scientists were able to follow the crystallisation process of zeolite synthesis over the complete range of relevant length scales for the assembly process. They were also able to identify transient compounds that could not be detected without the real-time data provided by the synchrotron.

This work demonstrated that synchrotron light can be used to analyse industrial catalysts with less than 1% of active agents.

Source: ESRF

Website: www.esrf.fr

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