

local order in the new phases is required to understand what happens to the material. In the majority of the cases, x-ray diffraction can provide such knowledge of the local environment of the atoms. But in some cases the long range order does not exist (amorphous material, glasses or liquid) or is only an average of the local order. Therefore more local investigations, like X-ray Absorption Spectroscopy (XAS) are needed to follow the modifications of the short range order. Moreover, in case of dilute specie in a matrix, the local probes become unique tools to determine the effect of the phase transformation on the impurity.

After a short introduction to XAS and to high pressure technology, I will summarize the limitations due to the pressure set-up. Then I will illustrate the possibilities of XAS with few examples:

- Coordination change in glasses (GeO_2 , $\text{Ge}_{1-x}\text{Si}_x\text{O}_2$) under pressure

- Pressure induced phase transformation on perovskites PbTiO_3 , BaTiO_3 [1] and KNbO_3 [2]. For the last two samples, both XAS and diffuse scattering experiments have been performed under high pressure in order to check the relation between the off centre position of the Ti (Nb) atoms with respect to the oxygen octahedron and the observation of diffuse scattering lines in the diffraction pattern. For the Ti perovskite, XAS demonstrate that Ti atoms go to the centre of the oxygen octahedron, but at pressures well above the tetragonal-cubic transition. In the case of KNbO_3 , Nb atoms remain off centre in the whole pressure range studied.

- Phase transformation on $\text{Zn}_{1-x}\text{Mn}_x\text{O}$ [3] for $x=0.25$ and $x=0.05$. The effect of pressure on the Mn local environment is determined by the evolution of the XAS spectra. In particular the Mn is in substitution of Zn in both low pressure (zinc blend) and high pressure (rocksalt) phases and the local compressibility is identical to the bulk one although the Mn-O distances differ from the Zn-O ones. The transition is shown to be reversible for $x=0.05$ and irreversible for $x=0.25$.

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KN12

Molecular mechanisms of RNA degradation Elena Conti. EMBL, Heidelberg (Germany) and Max Planck Institute of Biochemistry, Martinsried, (Germany)

The life span of RNAs in the cell depends on the balance between the rate with which they are synthesized and the rate with which they are degraded. Degradation is fast in the case of messenger RNAs (mRNAs) coding for gene products that need to be active only transiently in the cell (cell cycle regulators, transcription factors, circadian regulators etc.), as well as in the case of aberrant mRNAs that need to be rapidly destroyed before being translated into aberrant proteins. Nonsense-mediated mRNA decay (NMD) is a surveillance pathway that detects and degrades mRNA with premature stop codons (PTCs). PTCs can arise from alternative splicing, from defects in mRNA processing, and are also present in an estimated 30% of inherited genetic disorders. The talk will focus on our current understanding of the molecular mechanisms of

NMD: how the PTC-containing mRNA is recognized, how it is targeted for rapid degradation and how it is degraded.

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Reviews:

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KN13

The future potential of neutron diffraction studies in small molecule crystallography. Chick C Wilson, *Department of Chemistry and WestCHEM Research School, University of Glasgow, Glasgow G12 8QQ, UK.*
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Keywords: Neutron Diffraction, Small-Molecule Crystallography, Instrument Development

There has been a recent quiet but substantial revolution in the applications of neutron diffraction in the area of chemical crystallography and molecular materials; many of these exploit the power of neutron diffraction in determining accurately the hydrogen atom parameters in materials. As a result of continuing instrument development at the facilities, along with an appreciation of the developing needs of the chemistry user community, neutron chemical crystallography has responded in a highly successful fashion to modern trends in structural molecular science.

The relevant instrumentation developments include improved single crystal facilities at ILL, Grenoble (notably LADI, VIVALDI and the upgraded D19) and at ISIS, UK (the upgraded SXD), with further instrumentation planned at both sources (notably at the ISIS Second Target Station). Exciting developments in single crystal neutron instrumentation for molecular structure are also taking place at new high power neutron sources in the US and Japan (for example the TOPAS instrument at the 1 MW SNS at Oak Ridge) and the possibilities of powder diffraction are also being explored. Some of the areas recently advanced in neutron studies of molecular materials include:

- studying structures on a shorter timescale, either to examine a series of samples or to study a single sample under a range of conditions;
- providing a rapid tool for defining the geometry of hydrogen bonds, including weaker hydrogen bonded interactions;
- studying smaller single crystals;
- studying materials under conditions of variable temperature and variable pressure.

Recent advances and the exciting potential in a range of these areas will be discussed, including studies of proton migration, investigations of thermal parameter trends, hydrogen atom disorder, polymorphism, weak hydrogen bonded interactions and studies of molecular materials under high pressure.

The potential for future developments in both science and instrumentation of relevance to neutron diffraction studies of molecular structure will also be discussed.

KN14

From Small Molecules to Extended Structures
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Nature embraces the principles of supramolecular chemistry by exploiting non-covalent interactions in a multitude of ways to facilitate all biological processes. The facile assembly of complex synthetic systems in both solution and the solid state is becoming increasingly feasible and there is significant interest in the encapsulation of chemical space. This often requires that known systems be modeled, explored and fine-tuned in order to develop further systems of even higher complexity. Examples include the construction of globular or spheroidal self-assembled molecular capsules, which have potential applications as drug delivery agents, van der Waals catalysts, nano-reactors and mimics of biological systems. Spheroidal assemblies are generally highly symmetrical and frequently assume the shapes of the Platonic or Archimedean solids. For example, the cowpea chlorotic mottle virus is comprised of 180 identical protein subunits assembled into an icosahedron. Under pH control the overall conformation of the virion changes, giving rise to pores in the outer shell, thus allowing the passage of molecular material between the interior of the viral cavity and its environment. Although gaining analogous control over the size, conformation and composition of synthetic systems is a formidable challenge, advances have been made in influencing both the volume and composition of enclosed chemical space within the shells of non-covalent capsules assembled mostly by means of hydrogen bonding. These and other extended assemblies will be discussed.

KN15

In situ examination of Li-ion battery materials Helmut Ehrenberg^{a,b}, Natalya N. Bramnik^b, Kristian Nikolowski^{a,b}
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Keywords: Lithium ion batteries, positive-electrode materials, in situ diffraction study

Electrode materials in rechargeable lithium ion batteries undergo significant structural changes during charging and discharging, i.e. lithium extraction and insertion. Both the local structural changes due to the accompanied redox-reaction and the global changes in volume for different charge states are of primary importance for the electrochemical performance of such materials. An investigation of the relationship between crystal structure and electrochemical properties requires *in situ* studies under real operation conditions, because the disassembling

of the battery will most probably affect the electrode materials and falsify the structural characterisation. We have developed dedicated test cells, which allow *in situ* studies in transmission geometry up to at least 150 charge-discharge cycles [1], so that correlations with the capacity loss due to limited cycle stability become accessible.

In this contribution we report on structural studies on the most relevant positive electrode materials for lithium ion batteries and the role of the underlying crystal structures for the resulting electrochemical properties. In addition to induced phase transitions during conditioning the importance of microstructural aspects for degradation phenomena will be emphasized.

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KN16

Multiprotein machines for gene transcription Patrick Cramer *Gene Center Munich, Ludwig-Maximilians-Universität München, Munich, Germany*.
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Keywords: Multiprotein complex, transcription, X-ray crystallography

The current state of our structure-function analysis of the mRNA gene transcription cycle will be discussed. The crystallographic structures of the complete 12-subunit RNA polymerase II in free form and with bound DNA and RNA have been determined as atomic models. The structure of the complete Pol II elongation complex bound by the transcript cleavage factor TFIIS explained how Pol II uses a single tunable active site for both RNA synthesis and RNA cleavage. Three structures of complexes of CTD-interacting proteins provided insights into the coupling of transcription elongation to mRNA processing and histone methylation, and into Pol II recycling. The first structure of a Pol II complex with an RNA inhibitor and the first atomic structures of subcomplexes of the Mediator of transcriptional regulation provided insights into gene regulation. A set of new structures of Pol II bound to damaged DNA together with complementary functional assays revealed unexpected mechanisms of lesion recognition during transcription-coupled DNA repair. Unpublished data show that we can use hybrid methods to obtain new insights into the structure and function of the two other RNA polymerases, Pol I and Pol III.

KN17

Reciprocal space phasing methods for reconstructed surfaces Jordi Rius, *Institut de Ciència de Materials de Barcelona (CSIC), Campus de la UAB, Catalunya, Spain*.
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Keywords: GIXRD, phasing methods, surface diffraction

In the last years the application of GIXRD to the study of reconstructed surfaces has experienced considerable progress. The principal reasons have been the easier access to 3rd generation synchrotron sources, the increasing computer power but also the development of new methods for the solution of reconstructed surfaces.