used to determine the crystal structures of proteins up to resolution limits of 1.5-2.5 Å. Results relating to hydrogen positions and hydration patterns in proteins have been obtained from these studies. Examples include the geometrical details of hydrogen bonds, the role of hydrogen atoms in enzymatic activity, CH3 configuration, H/D exchange in proteins and oligonucleotides, and the dynamical behavior of hydration structures, all of which have been extracted from these structural results. These will open the new field beyond the folding structure of biological macromolecules such as:
1) Recognition of proteins and nucleic acids through the network structure of water molecules surrounding bio-macromolecules, and
2) The nature of chemical bond in proteins and nucleic acids elucidated by the accumulation of accurate structural information of hydrogen atoms.
Other techniques, such as the growth of large single crystals and a database of hydrogen and hydration in proteins, will be given.
Reference:
1) Nobuo Niimura and Robert Bau, Acta Cryst. A64 (2008) 12-22

Keywords: neutron protein crystallography, hydrogen and hydration, protein crystal growth

KN23

Acta Cryst. (2008). A**64**, C9

Crystallography and mechanisms of structural phase transitions: The use of symmetry-adapted modes

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When symmetries in a phase transition are group-subgroup related, as in ferroic materials, the transition mechanism can be treated within a perturbative approach. The distortion relating both phases can be decomposed into contributions from different modes with symmetries given by irreducible representations of the parent space group. This is the starting point of the well known Landau theory, based on the identification of the order parameter, i.e. the mode(s) driving the stabilization of the distorted phase. In general, a structure description in terms of symmetry modes separates the correlated atomic displacements which are fundamental for the phase stability from those which are marginal. The resulting parameter hierarchy can be very valuable when determining complex structures. In this talk I will present several examples illustrating the power of this approach for pure crystallographic purposes, and also combined with ab-initio calculations for studying transition mechanisms. Despite its advantages, the use of symmetry-adapted distortion modes is still scarce among crystallographers. Only rigid-body considerations (equivalent to a partial intuitive use of some symmetry-mode arguments) are used. A probable reason is that a full symmetry-mode decomposition required a deep familiarity with group theory. This has now changed drastically. A new program (AMPLIMODES) at the Bilbao Crystallographic Server (www.cryst.ehu.es) [1,2], allows to perform automatically such analysis for any pseudosymmetric structure, and a program with similar functions is also available at the website of Stokes et al. [3].
[1] M. I. Aroyo et al., Acta Cryst. (2006) A62, 115
[2] M. I. Aroyo et al., Z. Krist. (2006) 221, 15
[3] B.J. Campbell et al., J. Appl. Cryst. (2006) 39, 607

Keywords: structural phase transitions, ferroics, symmetry modes

KN24

Acta Cryst. (2008). A**64**, C9

X-ray scattering on nanostructures: From ensemble average to single object properties

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X-ray diffraction is a versatile tool to determine the structural properties of nanostructures (size, spatial distribution, chemical composition and strain state), and it can be applied to buried as well as uncapped objects. So far, in most x-ray studies, ensembles of nanostructures have been investigated. Consequently, the obtained parameters are those of an average structure, thus meaningful only if the ensemble is monodisperse. We present here local probe x-ray diffraction experiments on inhomogeneous systems: focused x-ray beams are used to localize nanostructures and analyze their strain and composition, identifying and probing individual objects one by one. In a scanning mode, an image of the sample surface is recorded, which allows the reproducible alignment of a specific nanostructure for analysis. Two examples will be shown:
i) SiGe islands on Si(001). The structural properties of specific islands are measured in diffraction and compared to the results of scanning electron microscopy on precisely the very same object.
ii) Rolled Up NanoTubes [Phys. Rev. Lett. 96, 165502 (2006)]. We will show microdiffraction results on a single particular tube on a macroscopic sample. The lattice parameter distribution and strain were measured and modeled using elastic theory.
By addressing shape, strain and composition at the nanoscale, the spatially resolved microdiffraction from low-dimensional systems is expected to play an important role in the understanding of the structure of nanomaterials, and provide a better control on their fabrication and functionality. In the outlook it will be shown that this approach can be complemented by coherent (diffraction) imaging methods and phase retrieval, allowing for a model-free direct reconstruction of the nanostructure in real space.

Keywords: X-ray microdiffraction, X-ray microscopy of small structures, strain

KN25

Acta Cryst. (2008). A**64**, C9−10

Incommensurate, composite modulated structures and beyond

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The discovery of aperiodic crystals some four decades ago has ended a very longstanding paradigm of classical crystals exhibiting three-dimensional periodicity. Aperiodic crystals are characterised by discrete diffraction patterns whose intensities require additional indices to be fully described. This discovery has triggered new theoretical and experimental investigations, which have resulted in the creation of the superspace formalism, a conceptual environment in (3+n)D with n=1 to 3, where three-dimensional aperiodic crystals regain their periodicity. Within a short period of time, superspace has established itself as the common denominator between diffraction

specialists in order to investigate the structures of aperiodic crystals including incommensurately modulated crystals, composites and quasicrystals. Composite and modulated structures occur in almost every type of solids including organic and inorganic compounds, minerals, metals and alloys and even in proteins. The study of their structures has greatly contributed to identify and understand the interactions occurring in crystals. Numerous phenomena, which were partially understood, could be reinterpreted on the basis of the incommensurability of structures. The superspace formalism appears to be particularly suited for the description of modular structures, i.e. structures sharing common building units. This has been applied to a series of technologically important class of compounds including perovskites, ferrites and sheelites. In some favourable case, the full series of compounds can be described with a single parameter, characterising the chemical composition of each member. The presentation is intended to illustrate the evolution of the superspace concept since it was introduced some four decades ago.

Keywords: aperiodic crystallography, superspace symmetry, incommensurate structures

KN26

Acta Cryst. (2008). A**64**, C10

Materials research with scanning microfocus small-angle X-ray scattering

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Complex materials are often inhomogeneous at many length scales. This is true, in particular, for biological materials, such as bone, wood, arthropod or mollusc shells. More generally, graded functional materials in biology or in engineering require special characterization techniques to account for the fact that the structure at the nanoscale varies spatially on the scale of microns or larger. Scanning micro- and nano-focus small-angle x-ray scattering offers a unique tool for obtaining structural information from the molecular to macroscopic length scales, combining the powers of scattering analysis with scanning imaging. The lecture reports recent progress focussing on examples from biology and materials science.

Keywords: SAXS, microfocus, hierarchical structure, biological meterials

KN27

Acta Cryst. (2008). A**64**, C10

Using neutrons and synchrotron X-rays together: Looking at the full picture in condensed matter

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Neutrons and synchrotron xrays are truly complementary probes. The matrix elements for the scattering of neutrons are straightforward and diffraction and inelastic scattering provide quantitative information on magnetic and chemical structure. Hard xrays on the other hand can be considerably harder to interpret but provide very high wavevector accuracy and information on the electronic and magnetic states through resonant scattering. In the soft xray regime the matrix elements for charge and orbital scattering again can become simpler but with the challenges of limited wavevector ranges, surface effects, and the need to work under ultra high vacuum. In this talk I will present a few selected materials whose complex structure and behaviour is becoming clear by the coordinated use of multiprobe scattering techniques. From these examples areas of importance for the challenges of the future will be discussed.

Keywords: neutron and X-ray scattering, magnetic materials, transition metal-rare earth oxides & intermetallic

KN28

Acta Cryst. (2008). A**64**, C10

Structural pharmacology and drug discovery: Exploring biological and chemical space

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Knowledge of the three-dimensional structures of protein targets that is now emerging from structural proteomics and targeted structural biology programmes has the potential to increase our understanding of human genetic variation, as well as to accelerate drug discovery. Protein structures provide insights into human genetic variation, including both non-synonymous single nucleotide polymorphisms and somatic mutations and their relationships to disease. This is exploring biological space. Structural analyses can also be used to explore chemical space, to investigate the chemical molecules that proteins might bind. This can be defined by fragment-screening techniques, which inform not only lead discovery but also optimization of candidate molecules. A range of biophysicaltechniques can be exploited, buthigh-throughput X-ray crystallography focused on identifying several weakly binding small-molecule fragments from compound libraries consisting of hundreds of small-molecule fragments has huge strengths and is an effective way of defining the chemical space of potential ligands. The high-resolution definition of these binding interactions provides information-rich starting points for medicinal chemistry. The use of high throughput X-ray crystallography does not end there, as it becomes a rapid technique to guide the elaboration of the fragments into larger molecular weight lead compounds. I will describe such developments not only in industry but also in academia for diseases of poverty, rare diseases and difficult targets. A long-term objective must be to define the chemical space around all macromolecules in man and in pathogens, so as not only to facilitate lead discovery but also to identify potential off-target interactions and minimise side effects.

Keywords: structural biology, drug discovery, design

KN29

Acta Cryst. (2008). A**64**, C10−11

Metal-organic materials: Strategies toward functional porous materials

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The quest for functional materials targeted for specific applications is ever increasing as societal needs and demands mount with advancing technology. One class of inorganic-organic hybrid materials, metal-organic materials (MOMs), has burgeoned in recent years due, in part, to effective design strategies (i.e. reticular chemistry) for their synthesis and their inherent [and readily interchangeable] hybrid,