techniques utilzing selected area or microdiffraction modes will be discussed. Examples include dispersed metastable phases that are common in alloy systems.

Keywords: electron diffraction, precession technique, precipitate phases

KN19

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Combined methods: Small-angle scattering with NMR and crystallography

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Small-angle scattering from macromolecules in solution yields low-resolution structural information that complements higher resolution information from crystallography and NMR. The ever increasing desire to understand more complex and often dynamic biomolecular systems, has brought about a surge in interest in the technique, greatly facilitated by recent developments in sources, instrumentation, and the availability of 3D modelling capabilities. Modelling 3D structures from solution scattering data does not always lead to a uniquely determined solution, and there are inherent limits to the information content of a scattering profile beyond the issue of resolution. The inclusion of scattering data with contrast variation can increase the information content, especially for biomolecular complexes with components having distinct scattering densities. We have combined small-angle X-ray scattering and neutron contrast variation data with crystallographic and NMR results to study protein complexes involved in signalling and regulation; specifically looking at the regulatory mechanisms controlling bacterial responses to environmental signals (1) and the actions of heart muscle proteins (2). In parallel we have been developing methods to improve the accuracy of structural analysis of individual protein structures in solution by co-refinement of NMR and small-angle X-ray scattering data (3). This presentation with describe the strengths and limitations of these approaches in the context of understanding bio-molecular function.

1. Whitten et al (2007) J. Mol. Biol. 368, 407.
2. Jeffries et al (2008) J. Mol. Biol. 377, 1186.
3. Grishaev et al. (2008) J. Biomol. NMR 40, 95.

Keywords: small-angle scattering, neutron contrast variation, combined methods

KN20

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Advances in high-pressure neutron scattering

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High pressure is a window to view matter in unusual states. In this talk I will show what neutron scattering is able to contribute to a better understanding of matter under extreme pressures. I will discuss the considerable efforts made recently by various groups to extend the capabilities of high pressure neutron scattering, i.e. to achieve higher pressures and better data quality, and to make it available to a broad scientific community. The methods involved are all based on opposed-anvil techniques which allow sample volumes of up to 100 mm^3. I will give a few illustrations which will cover structural studies of molecular systems, both at high and low temperatures, disordered as well magnetic systems. This talk will be dedicated to the memory of Igor Goncharenko, a pioneer in high pressure neutron scattering who passed away in November 2008.

Keywords: high pressure, neutron scattering, extreme conditions

KN21

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Charge flipping

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The talk is a brief review on charge flipping, a recently developed algorithm of ab initio structure determination. Its iterative scheme is based on the simplest Fourier cycle, where constraints are alternately prescribed in dual spaces. While the basic Fourier scheme is extremely sensitive to stagnation, charge flipping breaks it by introducing weak perturbations. The name-giving step is the most straightforward example of a fine balance: the sign change of electron density below a small positive threshold simultaneously forces positivity and a nearly orthogonal perturbation of structure factors. The method requires high-resolution data but no other information, like atom types, chemical composition or symmetry. Such a working principle significantly differs from that of classical direct methods and offers complementary applications. The new method has been successfully applied in practice: examples are periodic and aperiodic crystals using single crystal and powder diffraction data measured with X-ray and neutron radiation. Charge flipping can be used in different ways and at different stages of the structure solution process. It can either operate in a truly ab inito manner, can be applied to complete a partially known structure, it can check the stability of a solution, but can also be adapted to work as an ingredient of other dual-space schemes. Development of the algorithm is still very active. The list of various improvements will be discussed, as well as future prospects and the availability of user programs where the principles can be put into action. Finally, we emphasize the role of charge flipping in crystallographic teaching, now students can easily write their own code and experience firsthand success. This research was supported by OTKA 67980K.

Keywords: *ab-initio* structure determination, direct methods, software

KN22

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Neutron protein crystallography, beyond the folding structure of biological macromolecules

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Neutron diffraction provides an experimental method of directly locating hydrogen atoms in proteins, a technique complementary to ultra-high-resolution X-ray diffraction. 1) Three different types of neutron diffractometers for biological macromolecules have been constructed in Japan, France and the U.S.A., and they have been

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

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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

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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

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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