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

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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