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

J. Manuel Perez-Mato
Universidad del Pais Vasco,, Fisica de la Materia Condensada, Apdo. 644,, BILBAO, (Bizkaia), 48080, Spain, E-mail：jm.perez-mato@ehu.es

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

Cristian Mocuta[1], Hartmut T. Metzger[1], Kiran Mundboth[1,2], Baerbel Krause[1], Julian Stangl[2], Guenther Bauer[2], Christoph Deneke[3], Oliver G. Schmidt[3], Ana Diaz[1,2], Angelo Malachias[1,3]
[1]European Synchrotron Radiation Facility (ESRF), 6, rue Jules Horowitz, Grenoble, -, F38043, France, [2]Johannes Kepler University, Linz, Austria, [3]Max-Planck-Instiutut fuer Festkoeperforschung, Stuttgart, Germany, E-mail：mocuta@esrf.fr

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

Gervais Chapuis
EPFL, laboratoire de cristallographie, BSP/Cubotron, Lausanne, Vaud, 1015, Switzerland, E-mail：gervais.chapuis@epfl.ch

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