Keywords: electron density models, photocrystallography, intermolecular interactions

KN15

Acta Cryst. (2008). A**64**, C7

Nanostructure refinement and solution

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A diverse array of complex materials and structures are driving the nanotechnology and molecular biology revolutions. To understand and design these materials, it is essential to perform high precision structural characterization at the nanoscale. Often,even sub-Angstrom changes in inter-atomic bond lengths have profound consequences for the chemistry and functionality of these structure-sensitive materials. Crystallographic methods are the gold standard for atomic structure determination, however a broad and growing class of materials and/or nanophase morphologies do not yield to a crystallographic analysis. The scattering is diffuse and Bragg-peaks become broad and overlapped. This is “the nanostructure problem” which currently has no robust solution. I will discuss recent developments using the atomic pair distribution function (PDF) analysis of x-ray and neutron diffraction data that results in quantitative structural information on the nanoscale. I will describe the data collection and modelling methods that allow this, using a number of examples from materials science, physics and chemistry.

Keywords: nanocrystalline materials, pair distribution function, complex materials structure

KN16

Acta Cryst. (2008). A**64**, C7

Structural insights into immune defense by the complement system

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The complement system is a regulatory pathway in mammalian plasma and tissues that enables the host to recognize and mark invading pathogens and altered host cells for destruction, while protecting healthy host tissue. We study the large multi-domain proteins and the molecular mechanisms underlying this regulatory pathway. Structures of the large multi-domain proteins (up to 13 domains) of the central opsonization step revealed intricate domain arrangements and marked conformational changes that lead to covalent labelling of the target membrane [1-3]. Most recently, we determined the structures of protein complexes involved in the central amplification and regulatory steps. These data provide unprecedented insights into formation, specificity, activity and regulation of the short-lived (half-life time ~90 s) protease complexes that amplify the complement response. One of the effects of complement activation is lysis of the targeted cell through the formation of 100-Ang wide pores in the membrane. The structure of the central domain of human C8alpha revealed a surprising structural homology to bacterial cholesterol-dependent cytolysins [4]. This similarity indicates a possible mechanism of membrane attack and pore formation of these immune defence proteins.

[1] Janssen, B.J.C. et al. Nature 437, 505-511 (2005).
[2] Janssen, B.J.C. et al. Nature 444, 213-216 (2006).
[3] Milder, F.J. et al. Nature Structural and Molecular Biology 14, 224-228 (2007).
[4] Hadders, M.A. et al., Science 317, 1552-1554 (2007).

Keywords: complement immune system, multi-domain plasma proteins, protein compexes

KN17

Acta Cryst. (2008). A**64**, C7

Some structure property relationships

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The lecture will outline methods and describe instrumentation used to study structure evolution as a function of temperature, time, pressure, light or other external stimuli. It will relate the changes, often subtle, in the molecular structures to the macroscopic properties observed, for example the magnetic, optical and electrical characteristics. One interesting class of compounds that undergo subtle structural transitions that do map closely to their interesting macroscopic properties are the Spin Cross Over compounds, containing primarily, but not exclusively, Fe (II) centres. These bi-stable compounds are of potential commercial application, but we are investigating the various structural types from a fundamental science point of view and from these results, we hope to extrapolate to the design of new materials. The majority of the high resolution experiments described in detail will relate to single-crystal-to-single-crystal transitions.

Keywords: inorganic organic compounds, iron complexes, low temperature single crystal diffractometry

KN18

Acta Cryst. (2008). A**64**, C7-8

Electron diffraction intensities and structure analysis

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Two basic principles for intensity measurement from crystals were known from Xray crystallography: integrated intensities - and the high resolution “rocking curve”. In electron diffraction the latter was established by P. Goodman in the 1960’s (following earlier work by G. Möllenstedt and others). The convergent beam technique, CBED, was found particularly suited to small, perfect regions of crystals with small unit cells. Precise refinement, including charge distribution, became an option based on extensive dynamical scattering calculations. Crystal symmetries were revealed by inspection af symmetry features in the patterns. Several attempts were made to establish a practical way to collect well-defined integrated intensities from crystals by electron diffration. In 1994 R. Vincent and P.M. Midgley introduced a precession technique based on a double conical scan in the electron microscope, that emulates the precession camera in X-ray crystallography. It has since been demonstrated thatthree-dimensional data can be collected by this technique. Dynamical scattering is supressed to an extent that alllows standard crystallographic procedures to be applied with confidence. Dynamical calculations can then be left to a refinement stage. Recent commercial development has made the technique generally available. Relations between these techniques, and with the parallel beam