equilibrium leading to a range of interesting and decisive crystal chemical features including nanometric domains, polytypism and miscibility gaps. Such features must be investigated using a combination of crystallographic probes - neutron, X-ray, electron - that can examine the waste forms at different scales to give a complete understanding of the distribution and chemical state of waste metals

Keywords: mineral wasteforms, wasteform design, crystallochemical modification

KN12

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Imaging of nanostructures at diffraction-limited resolution from electron diffraction patterns

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Elucidation of the atomic order of complex nanostructures requires a local probe and sub-Å resolution. High resolution structural information can be obtained from diffraction patterns, in principle, which is not subjected to the resolution limitation of imaging lenses and their aberrations. But the use of diffraction patterns for imaging requires the solution of the phase problem without the 3-D periodicity of crystals. Here we report the coherent electron nanoarea electron diffraction technique and diffractive imaging of individual nanostructures using iterative phase retrieval and phase extension techniques. We demonstrate this technique using examples of nanometer-sized CdS quantum dots and Au nanoparticles imaged at sub-Å resolution with an electron microscope of nominal resolution of 2.4 Å and information limit of 1.1 Å. We show that in the diffractive images atoms at sub-angstrom distances are clearly resolved. Significant contrast improvement is also obtained compared to high resolution electron micrographs. The issues critical to the image reconstruction will be discussed in the talk. The high sensitivity of electron diffractive imaging promises a general imaging technique for ultrafine particles and nanocrystals. The contributors to the work reported here include Weijie Huang, B. Jiang, K.W. Kwon, M. Shim. The work is supported by DOE BES and NSF DMR.

Keywords: high resolution electron imaging, nanocrystals, phase determination

KN13

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Structure and function of multifunctional channels

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Water permeation through biomembranes should be strictly separated from the movement of ions in biological cells. The water channels must therefore be highly specific for water to prevent any ions. Aquaporin-1 can permeate 2 billion or more water molecules in a second without proton permeation. For accomplishing the function, structure analyzed at a resolution of 3.8 Å by electron crystallography showed peculiar structural determinants including an unusual fold for which we named aquaporin fold [1]. After finding of aquaporin-1, thirteen water channels, aquaporin-0 to 12, were identified in human body. By analyzing structure of aquaporin-0 at a resolution of 1.9 Å, we discriminated water molecules [2]. Aquaporin-4 is the predominant water channel in brain. By the two-dimensional crystals, showing the same molecular packing *in vivo*, its structure was analysed to 3.2 Å resolution and revealed weak but specific interactions suggesting a structural role for the water channel in the adhesion of membrane layers in glial lamellae. The aquaporin-4 molecule acquired cell adhesive and channel functions. We named this type channels as “Adhennel” family [3]. Structure of another Adhennel family protein, a Gap Junction channel, connexion 26 was analyzed by electron crystallography and we proposed a plug gating model [4]. By focusing on multifunctional channels, I would like to introduce recent results in structural biology of membrane proteins by utilizing our cryo-electron microscope with helium cooled specimen stage [5].

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Keywords: channel proteins, electron microscopy, membrane protein crystallization

KN14

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Experimental charge density modeling: Some frontier examples

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Experimental charge density research is now a very mature field which attracts many crystallographers and other scientists: hence, one can now handle difficult problems with success like interesting materials, proteins (1), host guest compounds , large molecules, which may contain transition metals or rare earths..It contributes to better a understanding of electronic structures, reactivity, inter or intra molecular interactions (2). The interplay between X-ray charge density results and complementary ab initio or DFT calculations also allows both experimental and theoretical fields to progress. These studies may be performed at home, on synchrotron facilities, coupled or not to other experiments like diffraction of polarized neutron, Compton scattering, NMR, and NQR to provide a thorough model of the electronic structure. Recent experiments also show the possibility to model the charge and spin density of long living metastable states (3) This lecture will illustrate these new results and draw some lines for the future.

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(2)On the accurate estimation of intermolecular interactions and charge transfert :the case of TTF-CA, Pilar Garcia, Slimane Dahaoui, Claudine Katan, Mohamed Souhassou and Claude Lecomte,Faraday Discussions,135,2007,217-235
(3) Sebastien Pillet, Vincent Legrand ,Mohamed Souhassou, Claude Lecomte et Al Out-of-equilibrium charge density distribution of spin crossover complexes from steady-state photocrystallographic measurements: experimental methodology and results Z. Fur Kristallographie 2008,000

Keywords: electron density models, photocrystallography, intermolecular interactions

KN15

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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

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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.

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

KN17

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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

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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