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

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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

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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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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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