The hardest cation, Li^+, shows a very large polarising power which is able to invert the deformations in the metal carbonyl geometry and produce stronger interion bonds.

Keywords: ionic metal carbonyls, electric field, intermolecular interactions

MS.68.5

Acta Cryst. (2008). A**64**, C118

XAO analysis of the 5d-occupation in rare-earth complexes with high potential as quantum

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The 4f and 5d electron density distribution (EDD) in MB_6 (M=Ce, Sm) were investigated by the X-ray Atomic Orbital analysis (XAO). In XAO each atom is divided into the groups of sub-shell electrons (s/p/d/f) and they are treated as an pseudo-atoms, which enables to analyze non-stoichiometric compounds keeping the crystal neutral. Since orthonormal condition is obeyed in XAO, the electron population on each AO is obtained reliably, which cannot be done by spectroscopic methods. The EDD of CeB_6 measured at several temperatures from 100 K to 535 K revealed the flow of Ce-4f electrons to B-B bonds connecting B_6 octahedrons below room temperature. However, above room temperature electrons are donated to Ce-5d orbitals and fill the 5d(j=5/2)Γ_8 and Γ_7 orbitals at 430 and 535 K, respectively[1]. On the other hand, SmB_6 exhibited electron flow from B_6 to Sm and filled 5d(j=5/2)Γ_8・orbitals below room temperature while 4f populations do not change significantly. The occupied 5d orbitals seem to be common among the rare-earth complexes. The energy difference between 4f and 5d states in $[Ce(OH_2)_9]^{3+}$ were 3.7-4.0 eV[2]. If electrons of fully occupied 5d orbitals are transferred to 4f orbitals, the emitted UV light can be an energy source getting energy from discarded heat below 473K. Rare-earth complexes can be effective quantum energy materials.

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Keywords: 4f and 5d EDD, XAO analysis, quantum energy material

MS.69.1

Acta Cryst. (2008). A**64**, C118

3D view of mesoscopic internal structure by coherent hard X-ray diffraction

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X-ray diffraction microscopy is a novel method of structural analysis in nanoscience. Diffraction limited sub-micrometer resolution becomes possible by reconstructing a sample image directly from the coherent diffraction data without aid of lenses. High penetration power of x-rays allows three-dimensional structural analysis for thick samples in a non-destructive manner. We have been performing x-ray diffraction microscope experiments by using hard x-rays from SPring-8 for a variety of samples in materials science and biology. Here, we report some recent results of our studies. In materials science application, we measured an aluminum alloy sample, and observed an internal high electron-density structure in the three-dimensional reconstruction [1]. We interpret that the high electron-density structure originates from sub-micrometer sized precipitates, which play an important role in practical applications in controlling the strength of the alloy. In biological application, we measured human chromosomes [2]. We, for the first time, succeeded in three-dimensional electron density mapping of a cell organelle by using hard x-rays. It is important because it is directly connected with x-ray crystallography, which is currently the most powerful method of the atomic structure analysis for proteins. Though electron cryo-tomography has been an almost unique method of cell structural analysis at high spatial-resolution, x-ray diffraction microscopy has definite advantage for thicker samples. Prospects for x-ray diffraction microscopy using future x-ray free electron laser are also discussed.

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Keywords: X-ray microtomography, nanostructures, phase reconstruction

MS.69.2

Acta Cryst. (2008). A**64**, C118-119

Femtosecond dynamic diffraction imaging: X-ray snapshots of ultra-fast nanoscale phenomena

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The ultrafast pulses from X-ray free-electron lasers are ushering in extraordinary new capabilities in X-ray imaging, including potentially the imaging of isolated objects at near-atomic resolution. Of particular interest is the the ability to study transient material dynamics, and ultimately determine the structures of proteins, viruses and macromolecules that cannot be crystallized. The FEL X-ray beam is sufficiently intense that the specimen can be completely destroyed by the pulse, but that destruction only happens after the X-ray pulse has passed through the object. The scattering pattern from the object will therefore give structural information about the undamaged object. An extensive program of research has been

undertaken at the FLASH soft-X-ray FEL at DESY, Hamburg, to develop the experimental methods for FEL diffractive imaging. We have reconstructed images from single-pulse ultrafast diffraction patterns that show no evidence of the effects of the FEL pulse on the structure even though the object was completely vaporized by the intense pulse. We also performed quantitative measurements of the explosion of test particles in the focused FEL pulse by recording their transient diffraction patterns. No motion occurred during the pulse and we followed the evolution of the explosion with a novel holographic time-resolved technique. Our results confirm the basic principles of flash imaging and provide clear demonstration of flash imaging with simultaneous nanometer spatial and femtosecond temporal resolution.

Keywords: XFEL, ultrafast imaging, phase retrieval

MS.69.3

Acta Cryst. (2008). A**64**, C119

Coherent X-ray diffraction microscopy of extended objects

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Coherent Diffractive Imaging (CDI) techniques use coherent sources of radiation - such as x-rays from high-brilliance synchrotrons and free-electron laser sources - to extract information on a specimen from its diffraction pattern. This approach can produce high-resolution images of both the absorption and the phase shift within the specimen. However, replacing the lenses with a reconstruction algorithm involves solving the notoriously hard phase problem and imposes strong constraints on the specimens' preparation. Scanning Transmission X-ray Microscopy (STXM) is an alternative imaging method that can yield high-resolution images through the raster scan of a focused x-ray beam on the specimen. STXM is fast, efficient, and does not require sophisticated data analysis, but it is resolution limited by the spot size at the specimen plane. This presentation will focus on how CDI and STXM can be combined into one method that bridges the gap between coherent imaging and scanning techniques. We will review the principles of this new Scanning X-ray Diffraction Microscopy (SXDM) approach and show first experimental results obtained with a coherently focused hard x-ray beam. For a buried nanostructure test specimen we demonstrate that the resolution can be improved by a factor of more than five beyond the focal size. In addition to providing the full complex-valued transmission function of the specimen, the new analysis procedure retrieves the complete structure of the wavefront incident on it.

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Keywords: phase problem, super resolution microscopy, X-ray imaging

MS.69.4

Acta Cryst. (2008). A**64**, C119

Fresnel coherent diffractive imaging with X-rays

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Coherent diffractive imaging (CDI) attempts to replace a resolution-limiting lens with a calculation on a Nyquist-sampled far-field diffraction pattern. In essence, this shifts the resolution limit of X-ray microscopy from the lens to the detector, promising images with resolution far below the spot size of even a modern zone plate. In Fresnel coherent diffractive imaging, one keeps the resolution limiting properties of CDI, but places a lens before the sample. This provides two important advantages: the iterative scheme used to recover an image is much more robust and the beam may be used to restrict the area to be imaged on the sample. Here, we present a collection of experimental results from biological and materials samples, demonstrating both high-resolution imaging and the ability to choose an arbitrary region of interest to image within a sample.

Keywords: coherent diffractive imaging, coherent X-ray scattering, X-ray imaging

MS.69.5

Acta Cryst. (2008). A**64**, C119

Coherent small angle scattering from polymer nanocomposites

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Polymer nanocomposites are a novel class of multifunctional hybrid materials which are obtained by appropriate mixing of nanoparticles and polymers leading to a wide range of potential applications in terms of their unique electrical, optical and thermal properties. However, to realize such potentials it is very crucial to understand their micro-structure and their microscopic dynamics. The enormous enhancement of surface-to-volume ration in such materials over conventional composites implies that interface morphology determines to a large extent the properties of these materials. Small angle x-ray scattering is a very powerful technique to probe the interface morphology of multi-phase materials. We have shown [1] using incoherent SAXS how interface morphology determines the glass transition in such materials. Using synchrotron multi speckle coherent SAXS or XPCS on gold nanoparticle embedded polymethyl methacrylate polymer nanocomposites we explore the rich phase behavior of their dynamics. We have performed temperature and wave vector measurements of the relaxation dynamics of such nanocomposite system and find a cross-over from compressed to stretched exponential relaxation with decreasing temperature from above the glass transition temperature of the composite. This is contrary to a recent observation in XPCS measurement on nanoparticles in supercooled liquids where compressed exponential relaxation was observed on cooling from above the glass transition of the liquid. We also find a wave vector dependence of the exponent of the relaxation which is similar to that observed for jammed systems.

Reference:
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2.C. Caronna et al, Phys. Rev. Lett. 100 055702(2008)

Keywords: X-ray small-angle scattering, nanocomposites, polymers