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

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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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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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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