resolution single-crystal X-ray diffraction studies at 100 K analysed within the atoms-in-molecules (AIM) framework gave detailed information on the charge density distribution.

Keywords: dithiadiazolyl, organic Ferromagnet, spin density

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Observation of spin densities by the X-ray magnetic diffraction

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Observation of density distribution of magnetic moment in ferromagnets has been performed solely by the neutron magnetic diffraction which utilizes interaction between the neutron spin and the magnetic moments. Recently intense elliptically-polarized X-rays of synchrotron radiation have come to be available, and the observation of magnetic moment is becoming possible by the X-ray magnetic diffraction (XMD) which utilizes interaction between the photon helicity and the magnetic moment through pioneering researches [1-4]. The XMD, that is nonresonant X-ray magnetic Bragg scattering, is a peculiar experimental method which enables us to measure separately spin and orbital component of the magnetic moments of ferromagnets. Physical quantity directly observed by this method is spin and orbital component (or mixture of them) of the magnetic form factor. By inverse Fourier transform of the spin or orbital magnetic form factor, the real-space density distribution of spin or orbital magnetic moment can be obtained. We have constructed an XMD experimental system on the BL3C of KEK-PF at Tsukuba in Japan, and have been performing the XMD experiments. In this lecture three dimensional spin density of an orbital-ordering perovskite $YTiO_3$ obtained by the XMD is shown, which reproduced the electron distribution of 3d-t2g electrons of Ti atoms. This result would prove that the XMD method is a useful tool to observe spin density of ferromagnets.
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Keywords: X-ray magnetic scattering, spin density, titanates

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Coherent diffractive imaging: A new tool for high resolution X-ray imaging

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The increased availability of high coherence X-ray sources, such as 3rd generation synchrotrons and more recently X-ray free electron lasers1, has driven the development of many new forms of microscopy. Among these techniques coherent diffractive imaging (CDI) is one of the most promising, offering very high-resolution lensless imaging of non-crystallographic samples. The method computationally derives an image of a sample from a single measurement of its diffraction pattern. Image reconstruction has hitherto only been possible for isolated samples fully contained within the illuminating beam, presenting what has been seen as a fundamental limitation on the CDI method. We demonstrate here a form of CDI that can image objects of arbitrary size and which can be used to create a well-defined field of view within a complex environment. A diverging beam created by a focusing optic is used to define the region of interest, allowing it to be imaged within a much larger sample. We test the concept using visible light and then use x-rays and a high resolution test pattern to demonstrate a diffraction-limited spatial resolution of 16 nm. A key requirement of the method is that the wavefront have significant curvature over the region of interest and this is determined by the size of the focal spot. As x-ray focal spots approach 10 nm in size2, imaging of a single quantum dot or of a small virus located within a complex host environment will be possible. Thus, the technique lends itself to high-resolution structural imaging of samples previously inaccessible to CDI.

Keywords: imaging, diffraction, coherence

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Diffractive imaging and serial crystallography

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The inversion of single particle diffraction patterns offers aberration-free, diffraction-limited, three-dimensional images without the resolution and depth-of-field limitations of lens-based tomographic systems. Radiation damage becomes the main limiting factor for diffractive imaging of organic molecules. To overcome this limitation, two schemes have been proposed: femtosecond diffraction of single molecules with a FEL and serial diffraction of laser aligned molecules. In both cases the 3D charge density is reconstructed from the diffraction patterns via iterative phase retrieval algorithms. Our work on iterative phase retrieval and possible applications to serial crystallography will be reviewed.
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