measurements of the momentum distribution via X-ray Compton scattering. By measuring the energy distribution of X-ray photons which have been inelastically scattered by the electrons in the sample, it is possible to measure their momentum distribution.

The momentum distribution contains information about the occupied momentum states, and therefore about the Fermi surface. Results are presented of recent Compton scattering measurements [1] performed on optimally Co-doped $BaFe_2As_2$. When compared to *ab initio* calculations which have been adjusted through small shifts of the bands with respect to the Fermi energy, the Compton scattering results can only be understood if those calculations were performed at the LDA-relaxed As position, rather than at the experimental one [2].

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Keywords: X-ray, compton scattering, fermi surface

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Resonant X-Ray Magnetic Scattering for transition-metal ferrites

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Recent developments in synchrotron radiation research make it possible to use the resonant X-ray magnetic scattering (RXMS) for crystals with complicated structures. Since RXMS has element selectivity and sensitivity to magnetic moments, it is a useful tool to determine the magnetic structures associated with specific electronic states such as 3d-4p interactions. Although various magnetic resonant experiments have been carried out, there are only a few reports on an X-ray crystallographic approach to use Bragg reflections with a wide range of reciprocal space. Taking advantage of single-crystal analysis, three-dimensional magnetic structural analyses have been developed in a combination of RXMS and least-squares refinement or Fourier syntheses. The combined technique allows us to perform element-specific and site-specific analyses on the magnetic structure. The refinement technique has been applied for Ti^{4+}/Co^{2+}-substituted $BaFe_{12}O_{19}$ to determine the canting of magnetic moments in the ferrimagnetic structure [1].

Transition-metal ferrites, having incompletely filled *d*-electron shells of iron, show useful electronic and magnetic interactions related to transition-metal and neighboring oxygen atoms. Magnetite Fe_3O_4 is a typical example to have various physical properties such as metallic behavior, mixed valence and electron hopping material. In the inverse-spinel structure geometrically frustrated, ferric and ferrous ions show a characteristic preference between tetrahedral "A" and octahedral "B" sites occupied by Fe^{3+} and equally by Fe^{2+} and Fe^{3+}, respectively. One of our RXMS studies has been focused on the estimation of magnetic electrons of Fe_3O_4, which pinpoints the electronic transition related to unpaired spins.

Energy-selective intensity measurements were carried out by using four-circle diffractometers at BL-6C of Photon Factory. Circularly-polarized X-rays were produced by a transmitted-type phase retarder of diamond (111). X-ray magnetic circular dichroism (XMCD) at the Fe *K* edge was used to select the X-ray energy of the spectrum, which was connected with the RXMS experiments with left- and right-polarized diffraction data.

The difference in crystal structure factors between left- and right-circular polarized measurements was calculated to synthesize a difference-Fourier map for targeting only magnetic electrons within energy resolution of 0.5 to 1 eV. The difference-Fourier synthesis is superior in eliminating the other effects such as charge scattering and experimental errors. In the calculation of $[\Delta\rho_{obs}(\boldsymbol{r})^{left} - \Delta\rho_{obs}(\boldsymbol{r})^{right}]$ maps, the formalization of electron density to extract individual magnetic effects is given by $\Delta\rho(\boldsymbol{r}) = V^{-1}\Sigma\Sigma\Sigma\{|F_{obs}(hkl)^{left}| - |F_{obs}(hkl)^{right}|\}\exp(-2\pi i\boldsymbol{k}\cdot\boldsymbol{r})$, where $F(hkl)$ and $\boldsymbol{k}$ are the crystal structure factor and scattering vector, respectively. With some replacements of calculated F_{calc} for observed one, difference-Fourier maps of magnetite were obtained from the usual difference-Fourier formalism for $\Delta\rho(\boldsymbol{r})$. Positive and negative peaks appeared around the A and B sites, which may be caused by magnetic unpaired 3*d* electrons of Fe atoms associated with neighboring oxygen and the outer Fe atoms.

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High resolution compton scattering as a new tool for imaging dopants and probing metal-insulator transitions

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We discuss two recent applications of high resolution Compton scattering as a new bulk-sensitive tool for probing electronic structure and momentum density of complex materials [1], [2].

Imaging holes in cuprate high-temperature superconductors: We have carried out first-principles electronic structure computations to analyze Compton scattering measurements from a series of $La_{2-x}Sr_xCuO_4$ single crystals in which the hole doping level varies from the underdoped (UD) to the overdoped (OD) regime. Holes in the UD system are found to primarily populate the O-2p orbitals. In contrast, character of holes in the OD system is very different in that these holes mostly enter Cu d orbitals. In this way, we establish that high-resolution Compton scattering can provide a new probe for directly imaging dopants in complex materials. Moreover, our analysis of the momentum density reveals clear existence of a large Fermi surface in the OD system in agreement with band theory predictions [3].

Metal-insulator transition in $La_{2-2x}Sr_{1+2x}Mn_2O_7$: We have studied the [100]-[110] anisotropy of the Compton profile in the bilayer manganite. A quantitative accord is found between band theory predictions and the measured anisotropy in the two metallic phases (i.e., the low temperature ferromagnetic and the colossal magnetoresistant phase under a magnetic field of 7T). Robust signatures of the metal-insulator transition are identified in the momentum density for the paramagnetic phase above the Curie temperature. The number of electrons involved in this transition is estimated. Our study demonstrates the sensitivity of the Compton technique for investigating metal-insulator transitions in complex materials. Work supported by Basic Energy Sciences, United States Department of Energy.

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