sets. Therefore, there are only two reports of high-resolution magnetic Compton experiments [2, 3] in this decade.

A new setup of the Cauchois-type x-ray spectrometer for Compton scattering experiments installed on BL08W at SPring-8 allows us to perform high-resolution experiments within a reasonable beam time. This spectrometer employs an X-ray image intensifier as a position sensitive detector. Using this spectrometer, a high-resolution magnetic Compton profile of iron single-crystal was measured with a momentum resolution of 0.14 atomic units. The statistical accuracy is approximately 4% at p_z=0. The experiment shows a good agreement with the theoretical prediction [1].

[1] Kubo Y., Asano S., *Phys. Rev. B*, 1990, **42**, 4431. [2] Sakurai Y. *et.al.*, *J. Condens. Matter*, 1994, **6**, 9469. [3] Cooper M. J. *et. al.*, *J. Phys. Chem. Solids*, 2000, **61**, 512.

Keywords: magnetic Compton scattering, momentum density, X-ray spectrometer

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The Effect of Fourier Series Truncation Errors on the Electron Density Distribution of $LiMn_2O_4$

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The effect of Fourier series truncation errors on the electron density distribution (EDD) of $LiMn_2O_4$ has been examined using the single-crystal synchrotron X-ray diffraction data and the molecular dynamics (MD) simulation[1]. The MD crystal structure factors obtained from each MD snapshot taken at 2fs intervals in real space were time-averaged and then reversely Fourier transformed to calculate EDD in a similar way to the X-ray data. The EDD thus obtained in the range $\sin\theta/\lambda < 3.33$ Å^{-1} was scarcely affected by the series truncation errors, indicating unambiguously that a small portion of Li does exist close to interstitial positions near the 16c site of the space group Fd3m. The residual EDD assuming a partial structure with eliminating Li atoms also reproduced a mostly correct picture about the distribution of interstitial Li atoms, even though the value of $\sin\theta/\lambda$ of the MD data was reduced to 0.80 Å^{-1}. The interpretation of EDD obtained from the single-crystal synchrotron X-ray diffraction data was thus verified and reinforced from the MD simulation, not only by looking at the real space distribution of atoms in the snapshots but also by a close examination of their Fourier transform.

[1] Tateishi K. *et al.*, *Annual Report of Ceram. Res. Lab*.,2005, **4**, *in press*.

Keywords: electron density distribution, Fourier methods, molecular dynamics

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Ultra-high Resolution Data for Charge Densities Studies

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X-ray diffraction is at present the main experimental technique to obtain the electron density distribution in crystals. Use of the new advanced area detectors allows measuring the ultra-high resolution data almost routinely. Speed of data collection and its quality is optimized when an integrated system for data collection, reduction and structure solution is used. The presented system allows for immediate control of the data quality in terms of such parameters as diffraction limit, completeness, and redundancy during the experiment. The experiment simulation module may minimize the influence of profile overlap and detector obstructions on data completeness. The further optimization can be accomplished by the use of specifically adjusted oscillation angle for each scan. The precise determination of diffraction intensities in the resolution shells between 0.7Å and 0.38Å is achieved by separate treatment of $K_{\alpha1}$-$K_{\alpha2}$ split. The ultra-high resolution, high quality data allow for precise analysis of interactions continua for all pairs of interacting atoms. The application of this approach to several systems will be presented.

Keywords: charge density, data collection, $K_{\alpha1}$-$K_{\alpha2}$ split

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Electron Density and Electrostatic Potential Study of an Organic Phosphate

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The electron density of the phosphate of L-histidinium phosphoric acid (LHP), experimentally obtained by X-ray and neutron diffraction data, is used for a detailed study involving *ab initio* calculations and topological analysis of both the electron density and the electrostatic potential [1][2].

As the L-histidinium presents a large dipolar moment and LHP crystals are non-centrosymmetric, this material has potential non-linear optical properties. These properties strongly depend on the crystal packing which, in this case, involve very short hydrogen bonds.

The results of this analysis on the LHP electron density allow a good characterization of the intermolecular interactions and a better understanding of the crystal packing. Moreover, the topological analysis of the electrostatic potential proves to be a useful tool to study the interaction of the molecules with its environment.

[1] Bouhmaida N., Dutheil M., Ghermani N.E., Becker P., *J. Chem. Phys.*, 2002, **116**, 6196. [2] Leboeuf M., Köster A.M., Jug K., Salahub D.R., *J. Chem. Phys.*, 1999, **111**, 4893.

Keywords: electron density studies, electrostatic potential, organic phosphates

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Accurate Charge Densities in under a Day with a Home X-ray Source

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The assembly and evaluation of a new in-lab facility for the rapid collection of charge density quality diffraction data will be presented. The system uses an 18 kW Mo rotating anode generator, graphite monochromator, large curved image plate, and an open flow helium cryostat. The rational for the choice and operating conditions of each of the components will be discussed. The need and application of a flood field correction will be demonstrated. Data integration with the program *VIIPP* [1] was shown to be superior to any other program available to us. Proof of principle experiments have been carried out in under a day. The quality of the diffraction data obtained at 15 K to $(\sin\theta/\lambda)_{max}$ = 1.32 Å^{-1} has been evaluated from the statistics provided by SORTAV [2], and by the quality of the multipole refinements [3] as judged by final R factors, residual maps, deformation density maps, etc. Although not as fast as a synchrotron experiment, a home source is always available, is more stable than most synchrotrons, and has no travel overhead associated with its use.

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Keywords: charge density, home X-ray source, rapid collection

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Topological Analysis of Charge Densities in Polymorphs of 3-acetylcoumarin

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