MS19.O02

Importance of multiple diffraction avoidance for charge density observation

T. Sakakura[1], T. Nakano[1], H. Kimura[1], Y. Noda[1], Y. Ishikawa[2], Y. Takenaka[3], K. Tanaka[4], S. Kishimoto[5], Y. Tokura[6], S. Miyasaka[7]

[1]Tohoku University, IMRAM, Sendai, Japan, [2]High Energy Accelerator Research Organization, KEK Tokai Campus, Tokai, Japan, [3]Hokkaido University of Education, Hakodate Campus, Hakodate, Japan, [4]Nagoya Institute of Technology, Omohi College, Nagoya, Japan, [5]High Energy Accelerator Research Organization, KEK-PF, Tsukuba, Japan, [6]The University of Tokyo, Department of Applied Physics, Bunkyo, Japan, [7]Osaka University, Department of Physics, Toyonaka, Japan

It might not be well recognized, most reflections are contaminated by multiple diffractions (MD). Therefore high redundancy data could not coincide with high accuracy data when MDs are not avoided. We collected both data set of MD-avoided and no MD-avoided ones and investigated its effectiveness in electron density measurement. For data collection, four-circle diffractometer at KEK-PF BL14A (Tsukuba, Japan) was used. In MD-avoided measurement, each reflection is collected at angle setting of least of MD contamination which calculated by psi-scan simulation software MDC [1]. In no MD-avoided measurement, usual bisect setting were used. In no MD-avoided measurement, intensities of forbidden reflections of YMn2O5 are more than 10 times largely observed than for MD-avoided one, and resulting residual density map is also highly contaminated reflecting the tendency of Fo>>Fc which is typical for reflections of weak intensity. Figure 1 shows this situation. Figure 2 is the deformation density of YTiO3 for MD-avoided data. Where model density of without Ti-3d1 valence electrons is subtracted from experimentally observed electron density. In the figure, quenching of angular momentum of Ti-3d1 electron is clearly observed. Although Rint could not be an ideal indicator of data accuracy since it cannot perceive Fo>>Fc, Rint(F) of MD-avoided measurement for YTiO3 is significantly reduced to ~0.5%. For no MD-avoided one, Rint(F) is ~1.2%. Since accuracy of MD-avoidance technique is confirmed, the next step is to exploit informations of only a few numbers of valence electrons among F(000) electrons. To accomplish this, wave function based refinement such as XAO [2] should be applied and studied.

[1] *K. Tanaka et al., Acta Cryst. A50, 246-252 (1994).,* ***[2]*** *Kiyoaki Tanaka and Yasuyuki Takenaka, Recent Advances in Crystallography, Chap. 11, Intech, ISBN 978-953-51-0754-5 (2012).*

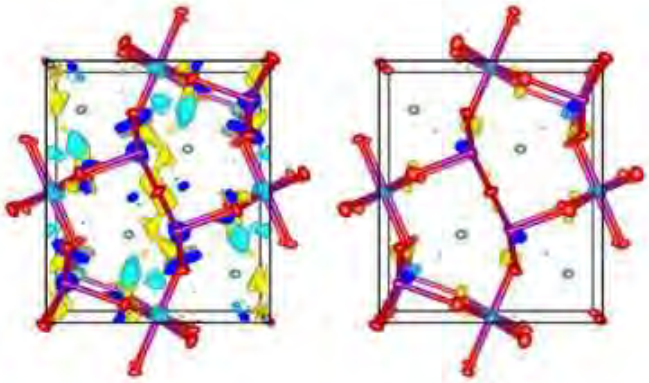

Figure 1. The residual density map of YMn_2O_5 for no MD-avoided (a) and MD-avoided (b) measurements.
Isosurface level is $\pm 0.28 e Å^{-3}$ for both (a) and (b).
$\Delta\rho_{min}$=-0.56eÅ^{-3} and $\Delta\rho_{max}$=+0.70eÅ^{-3} for (a),
$\Delta\rho_{min}$=-0.42eÅ^{-3} and $\Delta\rho_{max}$=+0.35eÅ^{-3} for (b).

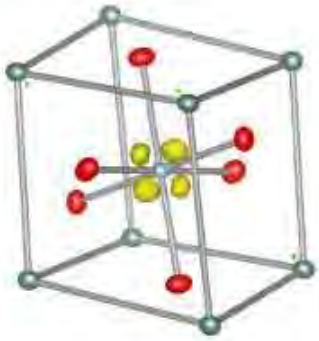

Figure 2. The deformation density map of $YTiO_3$. Y^{3+} are locates at corners and TiO_6 octahedron is shown in the center. Four embryos are observed Ti-3d^1 electron.

Keywords: multiple diffraction, electron density, 3d electron