

Structural and Charge-density Studies of Transition-metal Oxides using Convergent-beam Electron Diffraction

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We developed a method to refine crystal structural parameters and charge density using convergent-beam electron diffraction (CBED) [1,2]. The method is based on the non-linear least-squares fitting between full dynamical calculations and experimental intensities of energy-filtered two-dimensional CBED patterns of zeroth-order Laue-zone (ZOLZ) reflections and higher-order Laue-zone (HOLZ) reflections. The HOLZ reflections are essential for the determination of atom positions and Debye-Waller factors and the ZOLZ reflections are utilized for obtaining charge density distributions.

For this purpose, we developed an energy-filter transmission microscope JEM-2010FEF [1], and an analysis program MBFIT [1]. A problem of long computation time needed for dynamical calculations was greatly eased by implementation of parallel computation on a computer cluster [3].

A nanometer scale probe in CBED has great advantages and can be used extensively. Our current targets are perovskite-type transition-metal oxides and related materials with strongly correlated electrons, in which very small domains of twin structures exist and characteristic phase separation occurs easily. In the present talk, analyses of perovskite transition-metal oxides using the CBED method are demonstrated.

[1] Tsuda K., Tanaka M, *Acta Cryst.* 1999, **A55**, 939. [2] Tsuda K. et al., *Acta Cryst.* 2002, **A58**, 514. [3] Ogata Y., et al., *Acta Cryst.* 2004, **A60**, 525.

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