

direction. However, a tilt range of 10° would cover 17.4 % of reciprocal space, and if it is possible to collect high quality diffraction data up to 1 \AA resolution, this would still be much more than 1 independent reflection per non-hydrogen atom.

In contrast to precession electron diffraction (PED) [5] LARBED includes all tilt angles within the limits of the tilt range and thus records diffraction intensities at the Bragg condition for a large range of diffraction conditions. Averaging over all these different Umweg excitations allows one to reconstruct quasi-kinematic diffraction intensities for part of 3D reciprocal space, as shown in Figure 1 for the example of $\text{K}_2\text{O} \cdot 7\text{Nb}_2\text{O}_5$ [6], in a random $[\text{hk}0]$ orientation. $\text{K}_2\text{O} \cdot 7\text{Nb}_2\text{O}_5$ has space group $P4/\text{mbm}$ (No. 127) and unit cell vectors of length $a = b = 27.5 \text{ \AA}$ and $c = 3.94 \text{ \AA}$. The data was automatically acquired using the QED DM-PlugIn by HREM Research [7].

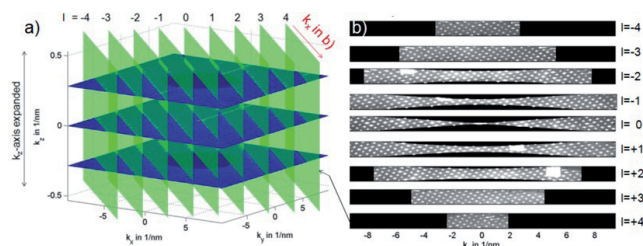


Figure 1: a) 3D reciprocal space reconstructed from the data shown in Fig. 2. Because of the tilt range of only $\pm 4^\circ$ the missing wedge is rather large. The vertical component spans a range of $-0.5 \text{ nm}^{-1} \leq k_z \leq 0.5 \text{ nm}^{-1}$. The green slices correspond to the vertical cuts through this 3D space shown in b). b) Positions of diffraction spots in 3D reciprocal space at different parallel planes. The intensities are the mean intensities averaged over a large number of diffraction patterns for which the Ewald sphere cut through that voxel in k -space. The contrast has been adjusted to reveal all reflections, not just the very bright ones. (White areas are due to the CCD read-out streak of very intense peaks.)

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Structure analysis of charge-orbital ordered phases in A -site ordered $\text{SmBaMn}_2\text{O}_6$ using CBED

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A structure analysis method using convergent-beam electron diffraction (CBED) developed by Tsuda and Tanaka [1] enables us to directly determine crystal structures and electrostatic potential distributions from nanometer-scale specimen areas. Using the method, sp^3 bonding electrons of silicon [2] and an ordered state of $\text{Fe } 3d \text{ } 3z^2-r^2$ orbitals of spinel oxide FeCr_2O_4 [3] were successfully observed. In the present study, the CBED method has been applied to an A -site ordered perovskite-type oxide $\text{SmBaMn}_2\text{O}_6$. The A -site ordered $\text{SmBaMn}_2\text{O}_6$

contains the alternate stack of SmO and BaO sheets along the c -axis with intervening MnO_2 sheets. This material undergoes a structural phase transformation at 190 K from a room temperature (RT) phase with charge- and orbital-ordering (COO) to a low-temperature (LT) COO phase [4]. Some different COO models have been proposed for the RT and LT phases. We aim to determine the crystal structures and COO patterns of the RT and LT phases and examine the relations between microscopic crystal structures and macroscopic physical properties. It is noted that the influence of the A -site randomness on CBED patterns can be excluded unlike the A -site disordered phase.

CBED patterns of $\text{SmBaMn}_2\text{O}_6$ were obtained at 293 K and 90 K using an energy-filter transmission electron microscope JEM-2010FEF operated at an accelerating voltage of 100 kV. The space groups of the RT and LT phases were determined by the CBED method. Based on the determined space groups, atom positions, atomic displacement parameters and low-order structure factors were refined by nonlinear least square fitting between the CBED patterns and dynamical diffraction calculations using our analysis software MBFIT [1].

From the symmetries of CBED patterns taken with five different incidences, the point group of the RT phase was determined to be mmm . The lattice type was determined to be primitive because no extinction by lattice type was observed. Dynamical extinction lines (DELs) were seen in the $h00$ ($h=\text{odd}$) zeroth-order Laue zone (ZOLZ) reflections and $0kl$ ($k+l=2n+1$) higher-order Laue zone (HOLZ) reflections, which indicate the existence of an a -glide symmetry perpendicular to the b -axis and an n -glide symmetry perpendicular to the a -axis, respectively. Thus, the space group of the RT phase of $\text{SmBaMn}_2\text{O}_6$ was uniquely determined to be $Pnam$ (No. 62). There are two different models were reported for the RT-COO phase. From the space group, an allowed COO model was selected.

Similarly, the space group of the LT phase was also determined to be $Pmam$ (No. 51) and a possible COO model was also selected.

The result of the refinement of crystal structural parameters will be presented.

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Electric field induced deformation in piezoelectric LiH_2PO_4 and LiH_2PO_3 crystals

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LiH_2PO_4 and LiH_2PO_3 crystallize in space group symmetry $\text{Pna}2_1$ and show piezoelectric properties. Single crystalline plates have been investigated under external high-electric field to study structural changes due to the internal deformation. The experiments have been performed using a four-circle diffractometer at D3 beamline @ DESY in ω scan mode combined with an open X-ray point detector. Diffraction curves of LiH_2PO_4 crystal ($a_1=6.253$, $a_2=7.656$, $a_3=6.881$, $Z=4$)[1] with orientations $[011]$ and $[201]$ were under an external electric field ($\pm 3 \text{ kV mm}^{-1}$). The measured peaks shifts reproduce the piezoelectric constants d_{ijk} of the material, the internal changes of atomic positions are deduced from changes of integrated intensities. The internal deformation was calculated to be larger for the Li-O bond compared to that of the P-O bonds. Normalized to an applied electric