diffuse scattering intensity around and between diffraction spots.

The collected data of high quality can be used for further determination of a 3D crystal structure. For example, it was possible to identify all oxygen atoms in the calculated three-dimensional potential map after the crystal structure analysis of the experimental 3D data, collected using the rotation diffraction tomography method applied to $K_2Nb_{14}O_{36}$ sample (space group *P4/mbm*, unit cell is $a = b = 27.5$ Å, $c = 3.94$ Å). This is the first time for the given structure when the oxygen atoms have been localized and identified in the 3D potential map using electron microscopy.

The use of cryo-TEM specimen holder allowed us to collect a data set and perform a partial reconstruction of a small part of reciprocal space for a *sucrose* sample. It was possible to maintain the data collection for ~12 min covering 16.5° in reciprocal space using 3D tomography.

[1] D. Zhang, P. Oleynikov, S. Hovmöller and X.D. Zou. *Z. Kristallogr*., **2010**, *225*, 94–102.

Keywords: Electron_diffraction, Tomography, Reciprocal_Space

MS.79.5

Acta Cryst. (2011) A**67,** C176

Electrostatic potential analysis of the rhombohedral phase of ferroelectric $BaTiO_3$ using CBED

Kenji Tsuda, Rikiya Sano, Michiyoshi Tanaka, *IMRAM, Tohoku University, Sendai (Japan).* E-mail: k_tsuda@tagen.tohoku.ac.jp

A CBED structure analysis method using convergent-beam electron diffraction developed by Tsuda and Tanaka [1, 2] enables accurate determination of crystal structural parameters such as atom positions, atomic displacement parameters (ADPs) and low-order structure factors from nanometer-sized specimen areas. From the refined parameters, electrostatic potential and electron density distributions are reconstructed. Recently, the method was successfully applied to the electrostatic potential analyses of silicon [3] and the orbital ordered phase of spinel oxide $FeCr_2O_4$ [4].

The method is particularly advantageous for the analysis of ferroelectric materials: (1) Reliable diffraction intensity data are obtained from a single ferroelectric-domain area of specimens containing minute ferroelectric domains. (2) The direction of ferroelectric polarization can be readily identified from the symmetries of CBED patterns through strong dynamical diffraction effect. (3) Electric polarization can be evaluated from the electrostatic potential distribution directly determined by the CBED analysis.

In the present study, the structure analysis method has been applied to the rhombohedral phase of ferroelectric $BaTiO_3$. CBED analysis of the tetragonal phase of ferroelectric $BaTiO_3$ at room temperature has not yet been successful enough. This could be attributed to the existence of partial disorder, or local fluctuations of atomic displacements which cause electric polarizations [5]. Such fluctuations are expected to be much smaller in the rhombohedral phase below 183 K.

Energy-filtered CBED patterns of the rhombohedral phase were obtained at 90K using a JEM-2010FEF energy-filter transmission electron microscope operated at an accelerating voltage of 100 kV and a liquid-nitrogen cooling specimen holder. Two dimensional intensity data of reflection disks of the energy-filtered CBED patterns were quantitatively compared with dynamical diffraction calculations based on a nonlinear least squares fitting using our analysis software MBFIT [1], [2]. Atom positions, anisotropic ADPs and some low-order structure factors were refined with a much better agreement between the experimental data and theoretical ones than that of the tetragonal phase. Detailed comparison between the result of the present analysis of the room-temperature tetragonal phase and that of the tetragonal phase will be presented.

[1] K. Tsuda, M. Tanaka, *Acta Cryst.* **1999**, *A55*, 939-954. [2] K. Tsuda, K. Takagi, Y. Ogata, T. Hashimoto, M. Tanaka, *Acta Cryst.,* **2002**, *A58*, 514-525. [3] Y. Ogata, K. Tsuda, M. Tanaka, *Acta. Cryst.*, **2008**, *A64*, 587-597. [4] K. Tsuda *et al*., *Phys. Rev.*, **2010**, *B81*, 180102-1-4. [5] R. Comes, M. Lambert, A. Guinier, *Solid State Commun.* **1968,** *6*, 715-719.

Keywords: convergent beam electron diffraction, ferroelectrics, electrostatic potential

MS.80.1

Acta Cryst. (2011) A**67,** C176

Photomechanical motion of molecular crystals

Hideko Koshima, *Department of Materials Science and Biotechnology, Graduate School of Science and Engineering, Ehime University, Matsuyama 790-8577 (Japan).* E-mail: koshima.hideko.mk@ehime-u.ac.jp

Scientific and technological communities are interested in molecules that generate mechanical motion with physical stimuli such as photon impingement. In particular, interest exists in linking the motion to macroscale mechanical work of crystals. Such machines are amenable to remote operation with external stimuli and do not require direct contact. We would like to report mechanical bending of photochromic crystals.

Azobenzenes are typical chromophores that undergo trans–cis photoisomerization. We found that platelike microcrystals of *trans*-4-(dimethylamino)azobenzene bent away from the light when irradiated at 365 nm, reaching a maximum deflection angle of 180° in half a second [1]. The crystals returned to the initial flat shape 30 seconds after stopping irradiation. The bending motion was repeatable. Trans-cis photoisomerization of azobenzene chromophores has never been observed in the crystalline state because of the large geometric changes that would be required in such densely packed crystal lattices. The molecular-level shape changes of azobenzenes near the crystal surface can be translated to the macroscale mechanical motion in crystals.

[1] H. Koshima, N. Ojima, H. Uchimoto, *J. Am. Chem. Soc.* **2009**, *131*, 6890-6891.

Keywords: mechanical bending, photochromism, crystals

MS.80.2

Acta Cryst. (2011) A**67,** C176-C177

Structural Studies on Photoactivated Transition Metal Complexes

Paul R. Raithby,[a] Simon K. Brayshaw,[a] Sara Fuertes,[a] Lauren E. Hatcher,[a] Stefanie Schiffers,[a] Anna J. Stevenson,[a] Mark R. Warren,[a] Christopher H. Woodall,[a] David R. Allan,[b] Simon J. Teat,[c] [a]*Department of Chemistry, University of Bath, Bath (UK).* [b]*Diamond Light Source Ltd, Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire (UK).* [c]*Advanced Light Source, Lawrence Berkeley National Lab., Berkeley California 94720 (USA).* E-mail: p.r.raithby@bath.ac.uk

Solid state photochemical processes can be placed in two general categories: (i) reversible processes where, without continued light