Charge-density distribution in calcium titanate perovskite $CaTiO_3$

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Introduction

Calcium titanate perovskite $CaTiO_3$ is one of the most important compounds in materials science and engineering and in earth science. Here I report the charge distribution in the $CaTiO_3$ obtained by the MEM (maximum entropy method)/Rietveld analysis using synchrotron radiation powder data.

Experiments and data processing

To obtain higher angular resolution as possible with good counting statistics, we performed synchrotron X-ray powder diffraction experiments at 25°C for $CaTiO_3$ at the beamline BL-4B2 at the Photon Factory, High Energy Accelerator Research Organization (KEK), Japan (Toraya *et al.*, *J. Synch. Rad.* **3** (1996) 75). A monochromatized 1.2 Å X-ray was used for the measurement. The electron-density distributions were determined by the MEM/Rietveld technique. Computer programs *RIETAN*-2000 (Izumi and Ikeda, *Mater. Sci. Forum* **321-324** (2000) 198) and *ENIGMA* (Tanaka *et al., J. Appl. Cryst.* **35** (2002) 282) were utilized for the calculation.

Results and discussion

Figure 1 shows the fitting result of a preliminary Rietveld analyses in the MEM/Rietveld method of *Pbnm* $CaTiO_3$. Sample spinner during the synchrotron radiation diffraction measurement was very effective to obtain accurate Bragg intensity data. The reliability factors were R_{wp} = 16.10%, R_I = 8.26% and R_F = 4.44%. Goodness of fit was 1.46. Refined unit-cell parameters were a = 5.44322(3) Å, b = 7.64185(5) Å and c = 5.38113(3) Å. Refined structural parameters were x(Ca)=0.03579(7), z(Ca)=-0.00675(12), B(Ca)= 0.323(6)Å^2, B(Ti)=0.059(6) Å^2, x(O1)=0.4838(3), z(O2)=0.0721(3), B(O1)=0.47(3) Å^2, x(O2)=0.2902(2), y(O2)=0.0380(2), z(O2)=0.7101(2), B(O2)=0.40(2) Å^2.

Figure 2 shows the MEM charge-density distributions in $CaTiO_3$. Almost no overlapping electron distribution was observed between Ca-O bonding, indicating an ionic bonding nature. On the contrary, the Ti and O had overlapping electron distributions between them, indicating the covalent feature for the Ti-O bonding.

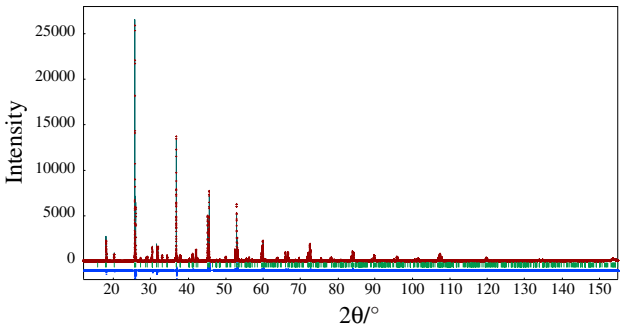

Fig.1. Rietveld pattern of $CaTiO_3$ measured at 25°C.

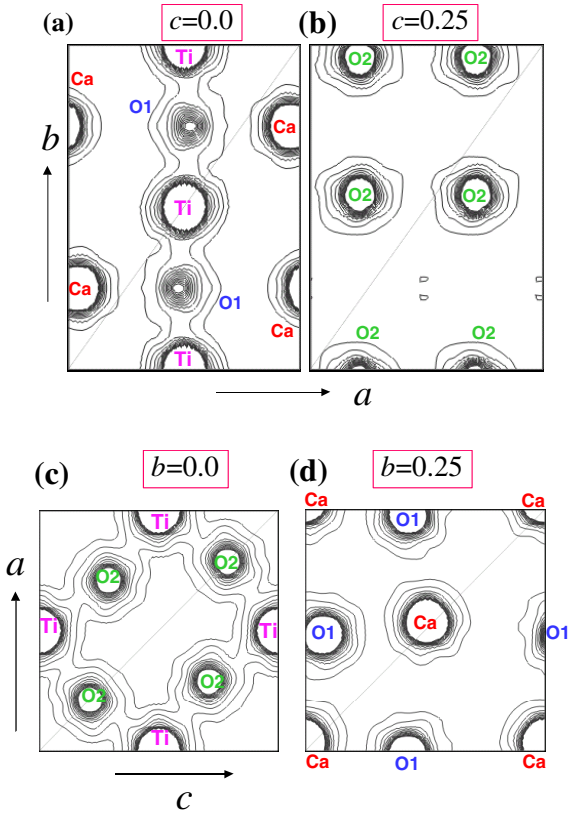

Fig.2. MEM charge-density distributions of $CaTiO_3$; on (a) (001), (b) (004), (c) (010) and (d) (040) planes. The contour lines are drawn from 0.4 to 4.0 e Å^{-3} with 0.2e Å^{-3} intervals.

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