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Electron density contour maps via Rietveld-MEM analysis using HR-XRD for the polycrystalline ferroelectric BCZT

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Abstract

The maximum entropy method in combination with the Rietveld refinement method applied to the analysis (Rietveld-MEM analysis) of high-resolution x-ray diffraction (HR-XRD) is an important tool to elucidate the electron density distribution and chemical bonding nature of materials. In this work, we present the comparison of electron density distribution obtained from the Rietveld-MEM analysis for polycrystalline perovskite BaTiO3 (reference sample) and Ba0.9Ca0.2Ti0.9Zr0.1O3 (BCZT). To perform this task, HR-XRD patterns using synchrotron radiation at the beamline 7.1 MCX of Elettra sincrotrone were acquired. Tetragonal phase with P4mm (No. 99) space group and pseudo-Voigt function were considered to model the HR-XRD peaks by the Rietveld method using the profile fitting Fullprof suite program. VESTA software was used to visualize 3D, 2D electron density distribution maps and line profiled to monitor the chemical bonding nature between Ba-O and Ti-O interactions and to visualize the off-center displacement of Ti cations by the incorporation of Zr and Ca cations. The interaction between Ti contours with O contours in the electron density distribution and the minimum electron density values revealed the enhancement of covalent nature and predominant ionic nature between barium and oxygen ions in the BCZT. To monitor the ferroelectric hysteresis behavior, polarization versus electric field curves complement the characterization of these samples.

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