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Structural investigation of Ca/Zr co-substituted $BaTiO_3$ through XRD and Raman spectroscopy

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Abstract

The present work reports the synthesis of Lead free $(Ba_{1-x}Ca_x)(Zr_yTi_{1-y})O_3$ with x = 0.13, y ≤ 0.15 (i.e. BCTZ) piezoceramics by semi-wet route and effect of additives viz., Ca^{2+}, and Zr^{4+} on phase formation, microstructure, piezoelectric and electromechanical properties. Detailed structural analysis suggests the formation of tetragonal perovskite phase with P4mm symmetry, which was also confirmed by Rietveld refinement and Raman spectra. SEM micrographs showed that the average grain size decreased with Zr^{4+} which acts as grain growth inhibitor. Composition with x = 0.13 and y = 0.10 exhibited the optimum piezoelectric and electromechanical properties (d_{33} = 367 ± 2 pC/N and kp = 0.39 ± 0.01) and showed higher densification (relative density ~ 98 %).

Keywords: Lead-free ceramics; Microstructure; Dielectric properties; Piezoelectric properties

1. Introduction

In the past few years, lead-free piezoelectric ceramics have received considerable attention due to its environmental friendly nature and alternatives to lead-based compositions such as $Pb(Zr,Ti)O_3$ (PZT) [1-2]. In continuous search for lead-free piezoceramics, barium titanate ($BaTiO_3$; BT) is one of the potential candidates [3] showing typical ferroelectric characters with three phase transitions: rhombohedral to orthorhombic (R-O) ~ –80 °C; orthorhombic to tetragonal (O-T) ~ 5 °C; and tetragonal to cubic (T-C) ~120 °C [1]. Barium titanate has been widely studied material because of its high dielectric constant, ferroelectric properties and