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Raman scattering, structural, electrical studies and conduction mechanism of Ba_{0.9}Ca_{0.1}Ti_{0.95}Zr_{0.05}O₃ ceramic

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Abstract

Ba_{0.9}Ca_{0.1}Ti_{0.95}Zr_{0.05}O₃ BCZT (10%, 5%) ceramic was prepared via solid state route. BCZT (10%, 5%) presents a coexistence of orthorhombic and tetragonal structures. By Raman spectroscopy the ferroelectric-paraelectric phase transition (T_C) is detected. So as to investigate the electrical transport, a complex impedance spectroscopy is highlighted. With the Debye theory-based analysis and a series of Arrhenius relations, the Nyquist diagrams (Z" versus Z') are well suitable to an equivalent circuit model. The relaxation was argued to be related with the hopping motions of charge carriers between Ca²⁺ and Zr⁴⁺ ions. At various temperatures, the dielectric datum was analyzed using complex electrical modulus M*. The plot of modulus versus frequency presents a peak of relaxation. Using the universal Jonscher's power law, the AC conductivity for grain contribution is interpreted. Activation energies, determined from conductivity (E_a = 1.23eV) and complex modulus (E_a = 1.06 eV) are different, which confirms that the transport is ensured by an ion hopping mechanism. However, a dispersion of the conductivity was observed at medium frequencies and was explained using the correlated barrier hopping (CBH) model.

Keywords: Ceramic; Dielectric; Nyquist; Modulus; conductivity.

1. Introduction

Recall that $BaTiO_3$ (BT) has an environmentally friendly material with similar ferroelectric and piezoelectric performance compared to lead-based ceramics (Pb) [1]. BT-based solid solutions are being studied because of their potential applications in various fields such as piezoelectric transducers, dynamic random access memories (DRAMs) and microwave tunable devices such as antennas, etc...[2-8].

In particular, the ferroelectric materials of compositions derived from BT have strong dielectric constants; they are well known for their applications as dielectrics for low frequency capacitors. Substitutions of either ions for host cations at the A or B site in BT lead to significant changes in its characteristics [5]. BT exhibits three successive structural phase transitions with increasing temperature: rhombohedral(R) –orthorhombic (O), orthorhombic (O)-tetragonal (T) and tetragonal (T)-cubic(C) at -173K, 273 K and 393 K, respectively [6].

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