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Structural, Microstructural, and Dielectric Investigations of Lead-Free $Ba_{0.95}Ca_{0.05}TiO_3$ Ceramics Synthesized via Solid-State Route

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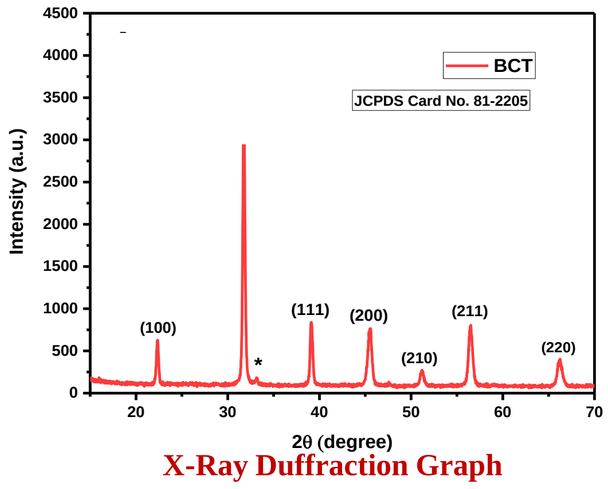
INTRODUCTION & AIM

Lead-free barium titanate ($BaTiO_3$) based ceramics have attracted significant attention as environmentally benign alternatives to lead-based ferroelectric and dielectric materials used in capacitors, actuators, and high-temperature sensors. Calcium substitution in $BaTiO_3$ plays a crucial role in improving phase stability, dielectric constant, and thermal reliability by stabilizing the tetragonal perovskite phase while suppressing secondary phases and extrinsic losses. However, a detailed correlation between microstructural parameters such as crystallite size and lattice strain with dielectric properties remains limited in the literature. Therefore, the present work aims to synthesize and investigate the structural, microstructural, and dielectric characteristics of $Ba_{0.95}Ca_{0.05}TiO_3$ (BCT) ceramics prepared through the conventional solid-state method. The objective is to establish a clear structure–property relationship through combined X-ray diffraction, Rietveld refinement, Raman, FTIR, and dielectric studies, thereby demonstrating BCT as a potential lead-free dielectric material for modern energy-storage and electronic applications.

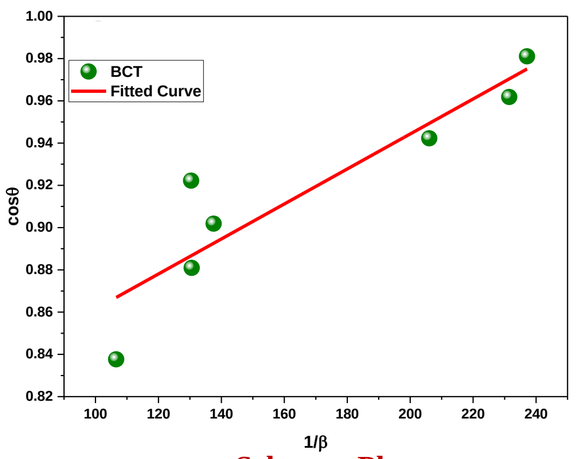
METHOD

$Ba_{0.95}Ca_{0.05}TiO_3$ ceramics were synthesized via the conventional solid-state route using high-purity $BaCO_3$, $CaCO_3$, and TiO_2 as precursors. The powders were mixed with ethanol, ground for 8 hours, and calcined at 850 °C for 7 hours to ensure phase formation. The calcined powder was blended with 2 wt% PVA binder, pressed into pellets at 85 MPa, and sintered at 950 °C for 8 hours for densification. Structural analysis was performed using XRD (Cu-Kα) and Rietveld refinement to determine phase and lattice parameters. Raman (532 nm laser) and FTIR confirmed tetragonal symmetry and Ti–O stretching vibrations. Dielectric and impedance analyses (100 Hz–1 MHz, 50–550 °C) using an LCR meter with silver electrodes were conducted to evaluate relaxation and electrical behavior.

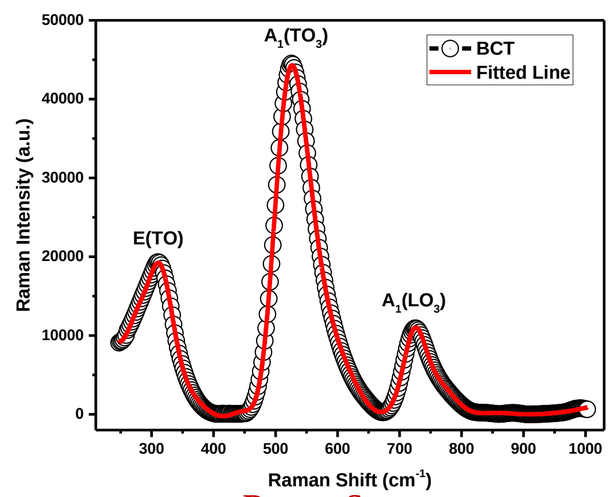
RESULTS & DISCUSSION



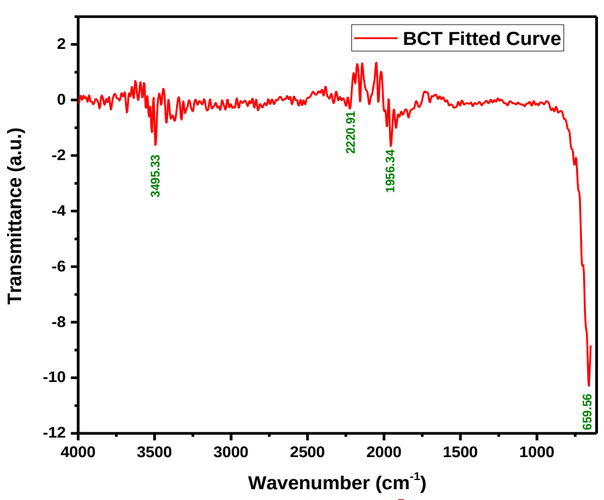
X-Ray Duffraction Graph



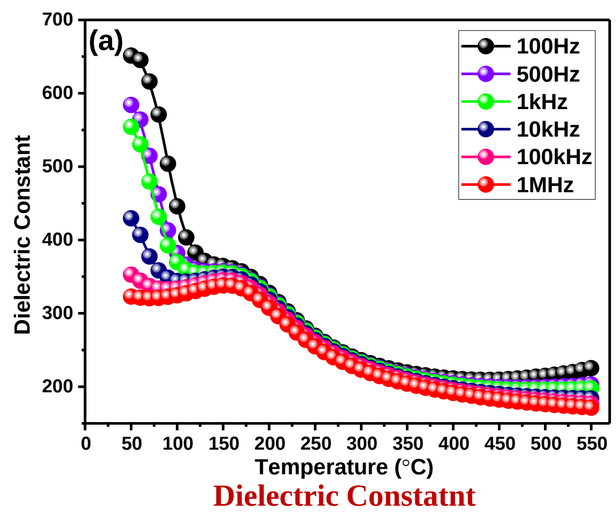
Scherrer Plot



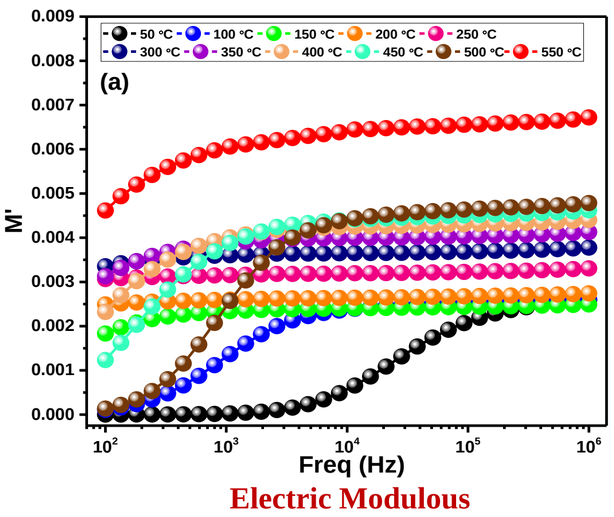
Raman Spectra



FTIR Graph



Dielectric Constatnt



Electric Modulous

XRD confirmed a tetragonal perovskite phase with **~26 nm** crystallite size from the Scherrer method. Raman and FTIR verified strong **Ti–O bonding and phase purity.** The dielectric constant **(~600)** remained **stable with low loss,** while electric modulus analysis indicated **non-Debye relaxation and excellent charge dynamics.**

CONCLUSION

$Ba_{0.95}Ca_{0.05}TiO_3$ ceramics showed a phase-pure tetragonal structure with excellent dielectric stability and low losses. Non-Debye relaxation and NTCR behavior confirmed efficient charge dynamics, making BCT a strong lead-free candidate for capacitors and high-temperature electronic devices.

FUTURE WORK / REFERENCES

Future studies will focus on integration of BCT in thin films and multilayer capacitors will also be explored for device-level applications.

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3. Rashwan G.M. et al., J. Sol–Gel Sci. Technol., 2024, 109(3): 707–719