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Ph.D Pre –Thesis Submission Seminar

Name of the Student	: N. S Kiran Kumar (Reg No. R190402)
Name of the Supervisor	: Dr. Koppole Chandrasekhar
Title of the Thesis	: **Development of Efficient Lead-free Ferroelectric Materials for Energy Storage and Solid State Refrigeration Applications**
Date and Time	: 4th April 2024 at 11:30 am
Venue	: Seminar Hall, First Floor, Department of Physics.

Abstract

Relaxor Ferroelectrics (RFE) have emerged as promising candidates for energy storage (ES) and electrocaloric (EC) effect applications, particularly in pulsed power technologies and solid-state cooling, respectively. However, most RFEs contain lead or lead based materials and canot be used in real time applications as per recent regulations from various governments all over world due to the toxicity of lead. Therefore, it is necessary to develop a suitable lead-free alternative RFEs.

Recently, $0.6Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.4(Ba_{0.7}Ca_{0.3})TiO_3$ (BZCT) ceramics have emerged as a potential candidate that competive with ferro and piezoelectric properties of lead based FEs. However, the low ES and EC parameters make them unsuitable for emerging applications. Therefore, the prime objective of present thesis is to introduce relaxor behaviour in BZCT and thus enhance the EC and ES properties of BZCT ceramics. To achieve this goal, we explore various doping strategies, including the addition of binary oxides like MgO, CuO and bismuth-based ternary oxides such as $BiZn_{0.5}Ti_{0.5}O_3$ and $BiTa_{0.5}La_{0.5}O_3$ into BZCT lattice. The studies on the effect of MgO doping content on BZCT ceramics revealed that the 0.99BZCT–0.01MgO ceramics exhibit optimal ES properties with a recoverable energy density (W_r) of 177.6 mJ/cm^3 and an efficiency (η) of 79%. Moreover, EC properties demonstrated an EC temperature change (ΔT) of 1.12 K at 45kV/cm are observed. In order to further enhance the ES parameter, the CuO binary oxide was introduced. The 0.5% inclusion of CuO in the BZCT shows a W_r of 398 mJ/cm^3, η of 90% and ΔT of 1.02 K at 30kV/cm. On the other hand, inclusion of bismuth-based ternary oxide ($BiZn_{0.5}Ti_{0.5}O_3$) in BZCT lattice shown a W_r of 197 mJ/cm^3, η of 92% and ΔT of 0.67 K at 45kV/cm for optimum composition of 0.98BZCT-0.02BZT. Further, the effect of $BiTa_{0.5}La_{0.5}O_3$ in BZCT boosed EC and ES properties with a W_r of 479 mJ/cm^3, η of 95% and ΔT of 1.06 K at 100kV/cm. These findings highlight that the addition of binary oxide strategies improved BZCT EC parameters, whereas the addition of bismuth based ternary oxide strategies improved ES parameters. Moreover, a strong correlation has been established between the microstructural, morphological and electrical properties.

List of Publications

1. **N. S. K. Kumar**, et al. "Effect of MgO doping on energy storage and electrocaloric properties of ferroelectric $0.6Ba(Zr_{0.2}Ti_{0.8})O_3$–$0.4(Ba_{0.7}Ca_{0.3})TiO_3$ ceramics" Materials Today Communications, 2023, 105754.
2. **N. S. K. Kumar,** et al. "Energy storage and electrocaloric properties of lead-free (1-x)($0.6Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.4(Ba_{0.7}Ca_{0.3})TiO_3$)–x$BiZn_{0.5}Ti_{0.5}O_3$ ferroelectric ceramics" Ferroelectrics, 2023, 20-32.
3. **N. S. K. Kumar**, et al. "Electrocaloric and energy storage properties of Pb-free 1-x($0.6Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.4(Ba_{0.7}Ca_{0.3})TiO_3$-x($BiTa_{0.5}La_{0.5}$)$O_3$ relaxor ferroelectric ceramics" Journal of Electroceramics, 2024, 1-13.
4. **N. S. K. Kumar** et al. "Effect of copper oxide doping on electrocaloric and energy storage properties of lead-free $0.6Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.4(Ba_{0.7}Ca_{0.3})TiO_3$ ceramics" Applied Physics A, 2024, (Ms. No. APYA-D-23-02745R1) (Accepted)