Room Temperature Crystallographic Phase analysis of (1-x) $KNbO_3$-x$CaZrO_3$ Lead-free Piezoelectric Materials.

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Since the formation of the RoHS and REACH in 2006 and 2007 respectively, there has been an increase in research into lead-free piezoelectric materials. This research has mainly focused on finding an alternative to the piezoelectric materials market leader, PZT, by attempting to replicate the MPB it possesses. This is done by doping a lead-free base perovskite to produce a coexistence of phases in the desired operating temperature range. It is therefore necessary to understand the effect doping has on the phase transition temperatures of the base perovskite.

In this work, Reitveld refinement analysis was carried out to deduce the crystallographic phase of (1-x) $KNbO_3$ – x$CaZrO_3$ for $0 \leq x \leq 0.15$. With an increase in x, the single orthorhombic phase of pure $KNbO_3$ is replaced with a coexistence of an orthorhombic-tetragonal-rhombohedral phase. A further increase in x leads to a reduction in the orthorhombic and tetragonal phases, and the introduction of a cubic phase, leading to the coexistence of a rhombohedral-cubic phase. This is attributed the incorporation of the calcium and zirconium ions into the perovskite structure increasing the rhombohedral-orthorhombic phase transition temperature $T_{O-R,}$ whilst decreasing the orthorhombic-tetragonal phase transition temperature T_{O-T}, and the tetragonal-cubic phase transition temperature T_{T-C}.