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X-Ray Diffraction Use fo PZN-PT Single Crystal's Synthesis and Microscopic Thermal Dilatation Coefficient Determination

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The performance of transducers can be significantly increased by the use of active materials with large piezo-electric coefficients (d_{ij}) and large coupling factors (k_{ij}) [1]. Recently, high levels of piezoelectricity have been published in $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$ (PMN-PT) and $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$ (PZN-PT) single crystals: $d_{33} > 2500$ pC/N, $d_{31} > -1500$ pC/N, $k_{33} > 90\%$, $k_{31} > 80\%$ and $kt > 60\%$ [1-5].

X-Ray Diffraction is an excellent technique to follow and analyze structures and crystallographic phases of solid materials.

In this paper we use the X-Ray powder Diffraction technique to control the different steps for the synthesis of precursors (PbTiO_3 and ZnNb_2O_6) and single crystals such as PZN-PT and PMN-PT.

X-Ray powder Diffraction was performed on ground single crystals with the help of a Philips X'pert Pro diffractometer using a monochromatic selecting $\text{CuK}\alpha$ radiation ($\lambda = 1.5418$ Å). Measurements for XRD characterization were realized by using a HTK16 high temperature chamber. The DRX diffraction patterns confirm a pure perovskite phase for the two crystals, within the X-ray powder diffraction's sensitivity. It means that $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ and PbTiO_3 have formed a perfect perovskite structure solid solution. Generally, XRD diagrams are carried out over narrow angular regions centered about the six pseudo-cubic reflections (100), (110), (111), (200), (220) and (222), from which it is possible to determine unambiguously the crystal's symmetry [6]. In the rhombohedral symmetry, the (h00) pics are all singulets while the (hhh) pics become doubled. In our case, from the peak profiles of the pseudo-cubic (200) and (222) reflections, the symmetry is clearly seen to be rhombohedral. The lattice parameters were determined in ambient and non-ambient conditions for the rhombohedral and cubic structure respectively. The plot of the lattice parameter and the lattice volume versus temperature in the cubic phase was performed to determine the dilatation coefficients α and ν by calculating the slope as indicating in the following equations:

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