



Mechanism of depolarization with temperature for $\langle 001 \rangle$ $(1 - x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$ single crystals

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Abstract

The temperature dependence of polarization for $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})_{1-x}\text{Ti}_x\text{O}_3$ single crystals poled in the $[001]$ -direction has been investigated. During the application of a temperature increase, the percentage of switched domains and the distortion of the crystalline lattice in $(1 - x)\text{PZN} - x\text{PT}$ single crystals were evaluated by X-ray diffraction (XRD) patterns. Using this method, intrinsic and extrinsic contributions to polarization variations were separated in the temperature range from 25 °C to the Curie temperature (T_c). Experimental polarization variations were simulated from microscopic data and details on micro–macro relationships were given. It was found that polarization variation with temperature is caused by the variation of the distortion of the crystalline lattice for temperatures below the Curie temperature and that only 90° domain switching occurs in the vicinity of the Curie temperature. Moreover, the hysteretic behavior of the polarization with temperature is due to motion of domain walls. The understanding of mechanisms of depolarization with temperature and the hysteresis associated with are of interest for the enhancement the pyroelectric properties of the material for detection and energy harvesting applications.

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1. Introduction

Due to their extremely high dielectric and piezoelectric constants compared to lead zirconate titanate (PZT) ceramics, single crystals of solid solutions of $(1 - x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$ (PZN–PT) are candidate materials for future high-performance piezo-devices such as medical ultrasound imaging probes, sonar for underwater communications, high-sensitivity sensors and actuators [1–3]. Some of the applications, such as those in space, involve environments where the temperature varies over a wide range. It is therefore necessary to characterize the behavior of these ceramics over a wide range of possible operating tempera-

tures. Temperature variations will result in significant non-linear behavior of the material's coefficients and will therefore affect its overall performance [4–6]. This nonlinearity occurs due to the material composition, dopants and internal defects and is dependent on the magnitude of the temperature variations. Aside from the hysteresis and non-linearity discussed above, ceramics are also useful in many applications for enhancing the pyroelectric and electrocaloric effects of piezoelectric materials used for energy harvesting and refrigeration [7–12].

Several investigations on the temperature dependence of piezoelectric coefficients in polycrystalline PZT ceramics have been carried out. Cook et al. indicated that heating of poled ceramics below T_c caused a change in the preferred domain orientation without affecting the piezoelectricity [13]. Thus, in the pioneering work of Jaffe and

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Berlincourt [14], the increase of the piezoelectric d_{33} coefficient with temperature was discovered. Most of the more recent results are related to the low temperature range. Zhang et al. found an increase in d_{13} by a factor of ~ 2.5 when the temperature was increased from 50 to 300 K [15]. This large change in the piezoelectric constant with temperature is due to the change in the domain-wall activities of the materials.

The variations in dielectric and piezoelectric properties of a material with temperature have two distinct origins: the variation of the distortion of the crystalline lattice, or intrinsic contribution, and the motion of domain walls (mobility and/or switching), or extrinsic contribution [16]. However, the separation of intrinsic and extrinsic contributions based on experimental data is difficult. In reality, the two contributions are weakly coupled, but such separation is useful because it highlights mechanisms of polarization variations. Currently, two methods are commonly used in separating the extrinsic and intrinsic properties in ceramics. One is based on the frequency dispersion characteristics of the dielectric constant, and the second is based on the properties measured at low temperatures where the domain wall is frozen [11,15,17].

Diffraction [18–20] has been used in several studies to observe modifications in the domain organization under an electric field [21–24] or compressive stress. This method can be used in the case of temperature to separate the two contributions (intrinsic and extrinsic).

In this article, we propose a microscopic method allowing simulation of the temperature effects and correlating the microscopic parameters and macroscopic properties. X-ray measurements were carried out on tetragonal $(1-x)\text{PZN}-x\text{PT}$ (with $x = 0.12$ and 0.14) single crystals in order to quantify domain switching as a function of temperature. Using this method, the intrinsic and extrinsic contributions were separated for both tetragonal compositions PZN–12PT and PZN–14PT in the temperature range from 25 °C to T_c .

2. Experimental procedure

2.1. Single crystal growth

Crystals of $(1-x)\text{PZN}-x\text{PT}$ were grown using the high temperature flux technique. High purity ($>99\%$) powders of Pb_3O_4 , ZnO , Nb_2O_5 and TiO_2 were used, and Pb_3O_4 was added as the flux. The powders were mixed in alcohol, dried, and loaded into a platinum crucible. The platinum crucible was covered with a platinum lid, which had a hole of $\sim 200\text{ }\mu\text{m}$ in order to equilibrate the pressure, and placed on a pedestal on an alumina column inside a vertical furnace equipped with a gas cooling arrangement under the crucible. The bottom of the crucible was cooled by oxygen gas to establish a preferential nucleation point and to protect the platinum crucible [25,26]. The platinum crucible was placed in a tube furnace and held at a soaking temperature of 1180 °C, followed by slow cooling to 850 °C at a rate of 1 °C/h. The crucible was then furnace cooled to

room temperature. Hot nitric acid was used to separate the crystals from the melt. Typically, crystal sizes ranged from 15 to 35 mm. Crystals were then oriented by plotting their pole figure corresponding to the desired crystallographic direction.

The dielectric constant K and dielectric loss factor ($\tan \delta$) were determined on polarized samples ($[001]$ single crystals) using an HP 4284 LCR meter at 1 kHz, and the piezoelectric coefficient d_{33} was determined with a Berlincourt meter 24 h after poling. Dielectric and piezoelectric properties are given in Table 1.

2.2. X-ray diffraction measurements

X-Ray diffraction data were taken with an X'Pert Pro MPD Panalytical diffractometer using $\text{Cu-K}_{\alpha 1}$ radiation ($\lambda = 1.5406\text{ }\text{\AA}$) with an incident-beam monochromator and a real time multiple strip X'Celerator detector. X-ray reflection profiles of $(1-x)\text{PZN}-x\text{PT}$ crystals (i.e., 001, 002, 003 and 004 reflections; tetragonal indexing) were recorded in symmetrically coupled $\theta-2\theta$ scan mode. The diffraction patterns were recorded over the angular range $20-110^\circ$ (2θ) with a step length of 0.016° (2θ) and a counting time of 100 s step^{-1} . X-ray studies were performed on plate samples ($10 \times 6 \times 0.7\text{ mm}^3$), which were silver paste electroded and poled when necessary. In this case, the electrodes were removed with solvent before X-ray diffraction measurements.

For non-ambient studies, the diffractometer was equipped with an Anton Paar HTK16 high-temperature chamber, in which the sample was put directly in intimate thermal contact with a heating metal strip. So, as the single crystal was heated by thermal diffusion, it was necessary to use a previously performed temperature calibration. The X-ray diffraction was performed on the surface perpendicular to the poling direction. Several isothermal scans were operated under ambient atmosphere (air) between room temperature and 300 °C. Before each scan, the temperature was stabilized for 15 min. Diffraction patterns recorded on poled single crystals for several temperatures were analyzed via a numerical fit of individual observed profiles using a pseudo-Voigt function. The positions, full widths at half maximum and integrated intensities of the Bragg reflections have been refined using a likelihood optimization. For the description of domain configuration, only the Bragg reflections in the angular domain $43-47^\circ$ in 2θ (step size of 0.016°) have been studied. The temperature depen-

Table 1
Characteristics and properties of $(1-x)\text{PZN}-x\text{PT}$ single crystals.

	PZN–12PT	PZN–14PT
ϵ_r	860	820
$\tan \delta$	1.2	2
d_{33} (pC N ⁻¹)	570	485
a (Å)	4.0163(3)	4.0149(2)
c (Å)	4.0992(4)	4.1156(2)
P_{spont} (C m ⁻²)	0.41	0.43
μ (C m)	2.71×10^{-29}	2.85×10^{-29}

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