Analysis of domain switching and elastic lattice strain in ferroelectric ceramics

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Introduction

Poling in a ferroelectric material occurs by switching of electric domains. Domain switching leads to a change in the strain which can be defined as stress-free transformation strain or eigenstrain. The degree of switching, defined as a texture change, and its associated eigenstrain depend on the orientations of grains. Thus, poling causes internal or residual stress. High energy synchrotron X-ray is a powerful tool to examine the structure inside a (bulk) matertial. Texture can be detected by the relative intensity of diffraction peaks and elastic lattice strain due to internal stress can be measured by the shift of the diffraction peaks. In the present study, this advantage is used to investigate the residual stress and texture development in poled ferroelectic PZT (lead zirconate titanate) ceramics. The poling process is also studied in-situ diffraction measurements [1,2].

Methods and Materials

Beamline ID 11 at ESRF, Grenoble, was used with an energy of X-rays of 70 keV. The diffraction pattern was collected in the remnant state after poling to 4 kV/mm as well as during poling. The diffractions from the planes, the normal of which inclined by ψ from the poling direction, were recorded using the KUMA detector set-up. A tetragonal PZT and a rhombohedral PZT, made through a standard method of powder sintering, were used.

Results

In Fig. 1, the lattice elastic strain, $\varepsilon(111)$, measured for *{111}* planes and the texture for *{002}* planes of the tetragonal specimen are plotted against $\cos^2\psi$. The texture is defined by

$$R(002) = I(002)/(I(002) + I(200)), \qquad (1)$$

where $I(002)$ is, for example, the diffraction intensity of the (002) peak, and ε and R have linear dependence on $\cos^2\psi$, written as

$$\varepsilon(111) \approx (3\cos^2\psi - 1),\ R(002) \approx (3\cos^2\psi - 1). \qquad (2)$$

A similar dependence was found for the rhombohedral specimen, when the lattice elastic strain was measured for *{002}* planes and the texture was defined for *{111}* planes, the latter being defined as $R(111) = I(111)/(I(111) + I(-111) + I(1\text{-}11) + I(11\text{-}1))$.

In-situ measuremnts of the lattice elastic strain and texture during poling also showed similar results to Fig.1. The proportional constants increase sharply at a certain applied electric field, corresponding to the onset of domain switching. After this stage, the proprtional constants monotonically increased as the electric field increased.

Discussion

The above results are consistently understood by a micromechanics model. In the model, a grain is taken as a spherical inclusion embedded in an infinite medium. The inclusion has eigenstrain determined by the degree of domain switching. The surrounding medium has an overall poling strain equal to the average poling strain of all the grains. Eshelby's inclusion theory is used. With respect to the use of high energy synchrotron X-ray, it is important that the present study examined the domain switching and lattice elastic strain in grains *inside* a specimen. This contrasts with the method of using usual laboratory X-ray which detects grains only on the surface of a specimen. The surface is traction-free and, thus, the elastic state is different from that inside a specimen. This point has been confirmed experimentally and it is found that the laboratory X-ray analysis is misleading, when domain switching and associated elastic state of grains in a ferroelectric material is studied by a lab-based diffraction method.

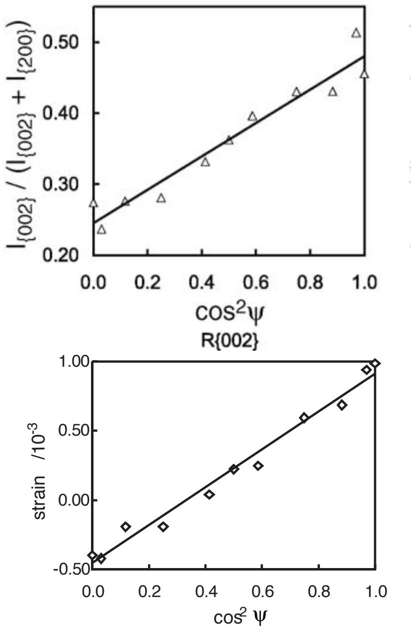

Fig. 1.: The texture variation (top) of the {002} family of planes and the strain variation (bottom) of the {111} family of planes vs $\cos^2\psi$ *inclination show a linear dependance*

References

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