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Theoretical saturated domain-orientation states in ferroelectric ceramics

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Abstract

Theoretical saturated domain-orientation states in tetragonal, rhombohedral and orthorhombic ferroelectric ceramics under electrical or arbitrary mechanical loading were accurately calculated using a simple statistical method. A pure shear stressing cannot induce a pure shear strain state but rather a strain state very close to axisymmetric elongation.
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Keywords: Ferroelectric ceramics; Domain orientation; Shear stressing; Crystal symmetry

1. Introduction

Ferroelectric ceramics have been widely used in a variety of fields [1]. A ferroelectric ceramic is an agglomeration of numerous small crystals, fitted together in a random way. When a ferroelectric ceramic is cooled from the paraelectric to the ferroelectric state, the unit cell deforms and domains will form to minimize the strain energy. Domain switching may occur in a ferroelectric ceramic subjected to high electric field or high stress [2]. When a ferroelectric ceramic subjected to an electric field reaches a state of ideally saturated polarization, its remnant strain also saturates. Under a large enough uni-axial tension, a ferroelectric ceramic will reach a state of positive saturated remnant strain despite the fact that no net polarization can form. Theoretically, the value of the ideally saturated remnant strain which can be achieved by tensioning, equals that of the saturated strain obtained by applying an electric field. But in a real ceramic, due to the low fracture strength, the maximum remnant strain achievable under tensile loading is much lower than that under a strong electric field [3]. If a ferroelectric ceramic is subjected to a high compressive stress, it will deform with all its domains switching as close as possible to the plane perpendicular to the compressive direction. Thus, a negative saturated strain is obtained. But, what are the saturated domain-orientation states in a ferroelectric ceramic subjected to arbitrary mechanical loading, such as a pure shear stress? This question will be addressed in the present study.

Since the original crystallographic directions of the grains in a ferroelectric ceramic are oriented at random, the line-up of polar axes cannot be as perfect as that in the case of single crystal. Thus, the magnitude of the ideally saturated polarization and strain will be smaller than those in a single crystal. Baerwald [4] has provided the values of ideally saturated polarization, which can be materialized in pseudo-cubic ceramics of various symmetries. The corresponding saturated strains for the tetragonal and rhombohedral ceramics were given by Rosenthal [5], but the value for the orthorhombic is absent. Meanwhile, it must be noted that in the book by Jaffe et al. [5], the expression the "fraction of single crystal distortion that can be realized ideally in ceramics" is likely to cause some confusion. In such an expression, for example, the corresponding value for the tetragonal should not be 0.368 but $3/2 \times 0.368 = 0.552$ [2,6,7], i.e., $\varepsilon_{33}^{*}/\varepsilon_{33}^{S} = 0.552$, where ε_{33}^{*} and ε_{33}^{S} are the saturated longitudinal strains in the tetragonal ceramics and single crystals, respectively. The value 0.368 comes from the equations $\varepsilon_{33}^{*} =$

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$0.368(c/a-1)$ [8], and $(c/a-1)=3/2\times(c/a_0-1)=3/2\times\varepsilon_{33}^{S}$, where c, a and a_0 are lattice constants for the tetragonal phase and the cubic phase, respectively.

Recently, Landis studied the strain saturation conditions in ferroelectric ceramics [9]. It was found that a pure shear strain state cannot be obtained by a pure shear stressing. Due to the computational complexity of the self-consistent model employed, only the tetragonal crystals are considered and the saturated strain state under arbitrary mechanical loading is lacking. In this paper, the ideally saturated domain-orientation states in ferroelectric ceramics of three crystal-symmetries (tetragonal, rhombohedral and orthorhombic), which can be materialized by applying an electric field or arbitrary mechanical load, will be obtained accurately by a simple statistical method. Some universal values of saturated domain-orientation states are presented for the first time. For ferroelectric ceramics of complicated crystal symmetries, a simple and effective method will be proposed to estimate the ideal values of saturated polarization and strain after a perfect poling treatment.

2. Material initialization

To calculate the saturated domain-orientation states of a ferroelectric ceramic accurately, it is crucial to initialize the material with random oriented crystallographic directions. The state of a cubic grain, which may contain several types of domains, can be described by three Euler angles (θ,φ,ψ) in a fixed global Cartesian coordinate system. This global system and the local Cartesian coordinate system of grains as well as the three Euler angles (θ,φ,ψ) are illustrated in Fig. 1. The following transformation relations exist between the global and the local coordinate systems:

$$x_i = R_{ij}X_j \tag{1}$$

where x_i, X_j are the components of vectors in the local and global coordinate systems, respectively, R_{ij} are components of the unit rotating tensor between the two coordinate systems [6,10], i.e.,

$$[R_{ij}]=\begin{bmatrix}\cos\theta\cos\varphi\cos\psi-\sin\varphi\sin\psi & \cos\theta\sin\varphi\cos\psi+\cos\varphi\sin\psi & -\sin\theta\cos\psi\\ -\cos\theta\cos\varphi\sin\psi-\sin\varphi\cos\psi & -\cos\theta\sin\varphi\sin\psi+\cos\varphi\cos\psi & \sin\theta\sin\psi\\ \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta\end{bmatrix} \tag{2}$$

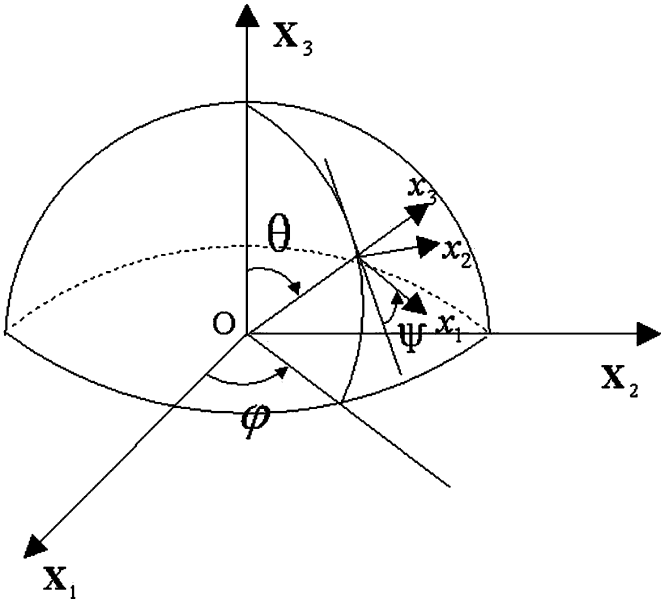

Fig. 1. Illustration of the global Cartesian coordinate system $\mathbf{X}_1$–$\mathbf{X}_2$–$\mathbf{X}_3$, the local Cartesian coordinate system x_1–x_2–x_3 and the three Euler angles (θ,φ,ψ).

The relation between the global and local strain tensors is as follows:

$$\boldsymbol{\varepsilon}(\theta,\varphi,\psi)=\mathbf{R}^{\mathbf{T}}(\theta,\varphi,\psi)\cdot\boldsymbol{\varepsilon}_s\cdot\mathbf{R}(\theta,\varphi,\psi) \tag{3}$$

where $\boldsymbol{\varepsilon}(\theta,\varphi,\psi)$ and $\boldsymbol{\varepsilon}_s$ are the strain tensors in the global and local coordinate systems, respectively.

The local spontaneous polarization vector and strain tensor of the possible oriented domains in the tetragonal, rhombohedral and orthorhombic ferroelectric ceramics have been given in Appendix A, where P_0 and γ_0 are magnitudes of the spontaneous polarization and strain, respectively.

For the generation of randomly distributed crystallographic directions, it is convenient to arrange things in such a manner that the end points of the unit vectors, which start from the origin and are parallel to the x_3 axis, described by θ and φ, distribute uniformly on the spherical surface, as shown in Fig. 1, and that the positive x_1 direction , described by ψ, distributes uniformly on the plane perpendicular to the x_3 axis. In other words, both φ and ψ distribute uniformly in the region $[0,2\pi]$, while the probability of θ complies with the following distribution function:

$$f(\theta)=\frac{1}{2}\sin\theta\quad\theta\in[0,\pi] \tag{4}$$

The normalization condition of the distribution function is then written as

$$\int_0^{\pi}\frac{1}{2}\sin\theta\,\mathrm{d}\theta\int_0^{2\pi}\frac{1}{2\pi}\mathrm{d}\varphi\int_0^{2\pi}\frac{1}{2\pi}\mathrm{d}\psi=\int_0^{\pi}\int_0^{2\pi}\int_0^{2\pi}\frac{1}{8\pi^2}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi\,\mathrm{d}\psi=1 \tag{5}$$

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