Available online at www.sciencedirect.com

ScienceDirect

Procedia Structural Integrity 6 (2017) 90–94

Structural Integrity Procedia

www.elsevier.com/locate/procedia

XXVII International Conference "Mathematical and Computer Simulations in Mechanics of Solids and Structures". Fundamentals of Static and Dynamic Fracture (MCM 2017)

Modeling of nonlinear behavior of polyrcystalline lead-free piezoceramics with a content of tetragonal, rhombohedral and orthorhombic phases under cyclic loading

Sviatoslav M. Lobanov[a], Artem S. Semenov[a]*

[a] *Peter the Great St.Petersburg Polytecnic University, Polytechnicheskaya, 29, St.Petersburg, 195251, Russia*

Abstract

The micromechanical model proposed by analogy with crystal visco-plasticity and taking into account the volume fraction of tetragonal, rhombohedral and orthorhombic ferroelectric phases is used for the simulation of hysteresis behavior of lead-free piezoceramics. The model parameters identification is considered and discussed. The results of simulation demonstrate a good agreement with the experimental data for a wide range of cyclic electrical loading amplitudes.

Keywords: ferroelectics, lead-free, nonlinear, hysteresis, tetragonal, rhombohedral, orthorhombic, BNT, BKT, KNN

1. Introduciton

Ferroelectric and ferroelastic materials are used in wide range of technical applications such as piezo-actuators, nanopositioners, controllers, sensors etc. Nowadays the most common ferroelectrics are lead zirconate-titanate and its solid solutions (PZT). Even though, usage of it should be decreased in the nearest future due to the EU government directives which restrict the usage of lead consisting materials. Consequently, an interest in lead-free ferroelectric/ferroelastic materials rises as is shown by Rödel et al. (2009). Recently it was found that at the morphotropic phase boundary (MPB), when there coexist two or three phases, $BaTiO_3$ and its solid solutions can

---

* Corresponding author. Tel.: +7-921-974-24-68.
E-mail address: slobanov92@yandex.ru

10.1016/j.prostr.2017.11.014

depict remanent strain and polarization at a level close to PZT. Thereby a strong need in numerical and finite element (FE) modeling of nonlinear behavior of lead-free piezoceramics close to MPB exists, which is the main goal of the present research.

The BNT-BKT-KNN compositions, consisting of tetragonal $(Bi_{0.5}K_{0.5})TiO_3$ (BKT), rhombohedral $(Bi_{0.5}Na_{0.5})TiO_3$ (BNT) and orthorhombic $(K_{0.5}Na_{0.5})NbO_3$ (KNN), were examined closely to MPB by Seifert (2010) with a lot of experimental data presented. The composition is described as:

$$\left(1-\frac{y}{100}\right)\left[\left(1-\frac{x}{100}\right)BNT+\frac{x}{100}BKT\right]+\frac{y}{100}\left[97KNN+3BKT\right] \qquad (1)$$

and can be named by a pair of numbers *x;y*. The diagram of possible solutions around the MPB at 80BNT-20BKT is shown in fig. 1.

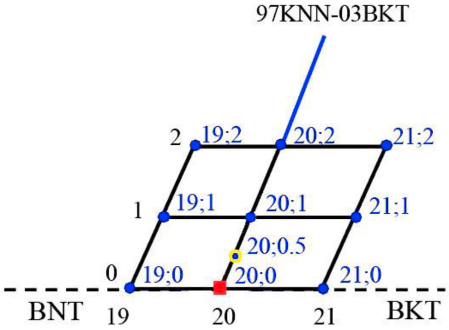

Fig. 1. The diagram of possible solutions closely to the MPB 80BNT-20BKT marked in red (after Seifert (2010)).

Great interest in the ferroelectrics behaviour close to MPB is due to the fact that in the vicinity of the MPB, the crystal structure changes abruptly, and the dielectric and electromechanical properties of piezoelectric materials reach the maximum magnitude. The aim of this work is to study hysteresis behavior of polyrcystalline lead-free piezoceramics closely to MPB by means of numerical simulations taking into account simultaneous presence of tetragonal, rhombohedral and orthorhombic phases.

2. Hysteresis behavior modeling

2.1. Micromechanical model

The proposed modified micromechanical ferroelectric/ferroelastic model is based on the ideas of Huber et al. 1999, Huber J.E. et al 2001, Liskowsky A.C. et al. 2005, Pathak and McMeeking 2008, Neumeister and Balke 2011, Semenov et al. 2011. The contribution of each domain is described by a volume fraction c_I ($I = 1 \dots N$, where N is number of a domain). The constitutive equations are based on the Voigt homogenization under the assumption of constant electric field and mechanical stress:

$$\begin{Bmatrix}\boldsymbol{\varepsilon}\\ \mathbf{D}\end{Bmatrix}=\sum_{I=1}^{N}c_I\left(\begin{bmatrix}{}^4\mathbf{S}_I^E & {}^3\mathbf{d}_I^T\\ {}^3\mathbf{d}_I & \boldsymbol{\kappa}_I^\sigma\end{bmatrix}\circ\begin{Bmatrix}\boldsymbol{\sigma}\\ \mathbf{E}\end{Bmatrix}+\begin{Bmatrix}\boldsymbol{\varepsilon}_I^r\\ \mathbf{P}_I^r\end{Bmatrix}\right)=\left(\sum_{I=1}^{N}c_I\begin{bmatrix}{}^4\mathbf{S}_I^E & {}^3\mathbf{d}_I^T\\ {}^3\mathbf{d}_I & \boldsymbol{\kappa}_I^\sigma\end{bmatrix}\right)\circ\begin{Bmatrix}\boldsymbol{\sigma}\\ \mathbf{E}\end{Bmatrix}+\begin{Bmatrix}\boldsymbol{\varepsilon}^r\\ \mathbf{P}^r\end{Bmatrix}, \qquad (2)$$

where **ε, D, σ, E** are the averaged strain tensor, the dielectric displacement vector, the stress tensor and the electric field intensity vector, $^4\mathbf{S}^E_I$, $^3\mathbf{d}^E_I$, $\mathbf{k}^\sigma_I$ are the elastic compliance, piezoelectric coefficient and dielectric permittivity tensors, which correspond to I^{th} domain.

Evolution equations for averaged remanent (inelastic) strain and polarization $\boldsymbol{\varepsilon}^r$ and $\mathbf{P}^r$ are following: