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# Multiscale finite element modeling of nonlinear behavior of polycrystalline piezoceramics with account of tetragonal and rhombohedral phases

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## Abstract

The nonlinear behavior of a polycrystalline piezoceramic materials based on the two-level finite element homogenization method was investigated. Numerical experiments were carried out for rhombohedral and mixed (tetragonal-rhombohedral) variants within a single crystal using a micromechanical model of the material. Based on the results of numerical experiments, the remanent part of the free energy accounting dependence of the saturation strain on the type of the multiaxial deformed state was constructed.

*Keywords:* ferroelectrisity/ferroelasticity; piezoceramic; strain saturation;finite element homogenization; constitutive behavior; phenomenological model

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**Nomenclature**

| | |
|---|---|
| $\boldsymbol{\varepsilon}$ | strain tensor |
| $\boldsymbol{D}$ | electric displacement vector |
| ${}^4\boldsymbol{S}$ | tensor of elastic modulus |
| ${}^3\boldsymbol{d}$ | tensor of piezoelectric modulus |
| $\boldsymbol{k}$ | tensor of dielectric permittivity |
| $\boldsymbol{\sigma}$ | stress tensor |
| $\boldsymbol{E}$ | electric field intensity vector |
| $\boldsymbol{\varepsilon}_r$ | remanent part of strain tensor |
| $\boldsymbol{P}_r$ | remanent part of electric displacement vector |
| $\boldsymbol{\mu}_\alpha$ | Schmid orientation tensor |
| $\boldsymbol{s}_\alpha$ | unit vector in the direction of the change in remanent polarization |
| $\Psi^r$ | remanent part of the free energy associated only with the internal state of material |
| $\Psi^s$ | stored elastic energy |
| $H_0^m$ , $\varepsilon_c$ | parameters of the material |
| $\bar{\boldsymbol{\sigma}}$ | external stress tensor |
| $\bar{\boldsymbol{D}}$ | external electric displacement vector |
| $\bar{\boldsymbol{E}}$ | external electric field intensity vector |
| $\bar{\boldsymbol{\varepsilon}}$ | external strain tensor |

## 1. Introduction

Ferroelectroelastic materials are widely used in modern engineering and research investigations as shown in Zhukov (2009) and Ivashov (2014). One of such materials is polycrystalline piezoelectric ceramics. Ferroelastic materials are used as elements of sensors and actuators (fuel injection valves, vibration dampers, micromotors, nanopositioners, sensors for monitoring the integrity of structures, etc.).

The main purpose of this work is to simulate the nonlinear behavior of the polycrystalline ferroelectroelastic materials by means of homogenization using a finite element method with the tetragonal and rhombohedral phases. A new phenomenological model of ferroelectroelastic materials, which is based on determination of the effective properties of polycrystals is also presented in the paper.

The constitutive response of the ferroelectroelastic solid can be written as

$$\begin{Bmatrix} \varepsilon \\ D \end{Bmatrix} = \begin{bmatrix} {}^4\boldsymbol{S} & {}^3\boldsymbol{d}^{\mathrm{T}} \\ {}^3\boldsymbol{d} & \boldsymbol{k} \end{bmatrix} \begin{Bmatrix} \sigma \\ E \end{Bmatrix} + \begin{Bmatrix} \boldsymbol{\varepsilon}_r \\ \boldsymbol{P}_r \end{Bmatrix}, \tag{1}$$

where $\boldsymbol{\varepsilon}$ is the strain tensor, $\boldsymbol{D}$ is the electric displacement vector, ${}^4\boldsymbol{S}$ is the tensor of elastic modulus, ${}^3\boldsymbol{d}$ is the tensor of piezoelectric modulus, $\boldsymbol{k}$ is the dielectric permittivity, $\boldsymbol{\sigma}$ is the stress field, $\boldsymbol{E}$ is the electric field intensity vector, $\boldsymbol{\varepsilon}_r$ and $\boldsymbol{P}_r$ are the remanent parts of strain and electric displacement, respectively. Domains with different orientations and different values of ${}^4\boldsymbol{S}$ , ${}^3\boldsymbol{d}$ , $\boldsymbol{k}$ exist inside the single crystal.

## 2. Ferroelectric/ferroelastic switching

Two differently oriented domains can be combined into a ferroelectroelastic switching system. In a tetragonal variant within the single crystal $M = 6$ orientations of the spontaneous polarization are realized (along the positive and negative directions of the three crystallographic axes) corresponding to the $N = M\,(M\text{-}1) = 30$ switching systems. In a rhombohedral single crystal, $M = 8$ spontaneous polarization orientations are realized along the directions of the four main diagonals of the crystal cell corresponding to $N = 56$ switching systems. Ferroelectric switching occurs as a result of the movement of the walls of domains, which leads to a change in the concentration of domains in the crystal.