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# Finite-element Modelling of Ferroic Domain Switching in Piezoelectric Ceramics

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## Abstract

*Piezoelectricity in polycrystalline materials like PZT ceramics is a complex phenomenon of both linear and ferroic electromechanical coupling based on the single crystal piezoeffect and on domain switching, respectively. The latter can be caused by mechanical and/or electrical loading and yields to changes of the polarisation texture of the polycrystalline material. The ferroelastic and ferroelectric hystereses can be understood by means of a micromechanical model. In order to include the grain-to-grain interaction finite-element (FE) method is its own recommendation. The micromechanical model has been implemented into the FE code ANSYS © (SOLID 45). Furthermore the 3D piezoelectric element SOLID 5 has been extented to the nonlinear option. On the basis of these elements the mechanical and the electrical hystereses and the strain versus electric field curve have been modelled. Special attention has been directed to the asymmetry of tension and compression by comparing experimental and simulation results.*

*Keywords*: mechanical properties, ferroelectric properties, piezoelectric properties, PZT, micromechanical model.

## 1 Introduction

In order to assess the reliability of piezoelectric devices such as actuators, bimorphs, etc. one must take into consideration both the intrinsic, purely linear piezoelectric effect and the so-called 'domain switching' effect. The latter is the source of the ferroelasticity and ferroelectricity of piezoelectric ceramics. The switching affects the nonlinear strain versus electric field behaviour known as butterfly shaped curve. Other attempts have been made to explain phenomena such as electrical field dependent fracture toughness by means of domain switching.[1,2]

The switching occurs under mechanical and electrical loading and causes the polycrystalline material both to deform and to polarise. It seems to be reasonable to define a 'switching condition' on the basis of the mechanical work plus the electrical work done in switching.[3–5]

In the finite-element model presented here, the ceramic is made up of many randomly oriented grains. Orientation changes of 90° and 180° are allowed as observed in tetragonal PZT ceramic near the morphotropic phase boundary. A constitutive equation taking into account the spontaneous strains and polarisations was derived. In contrast to phenomenological formulations our 3D micromechanical model which is explicitly based on the polarisation texture yields all effects of electromechanical coupling in a natural way. The model has been implemented into the commercial FE code ANSYS©.[6]

## 2 Phenomenological and Micromechanical Modelling

There are two principal ways to describe the material behaviour: phenomenological and micromechanical models. Phenomenological models (e.g. the Rayleigh model[7,8]) confine to reflect the observed behaviour without attempting to explain its physical origin. This type of material laws is favoured about all because of its easy handling. For more complex loading situations like stress triaxiality and electromechanical coupling plausible assumptions are necessary.

In micromechanical models (e.g. the Preisach model[3,9]) a set of physical equations is solved on a small material volume from which the macroscopic behaviour is calculated by averaging. The material behaviour is described by means of physically meaningful variables. The main advantage of these models lies in their predictive capability.

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## 3 Micromechanical Model for Domain Switching

Domain switching occurs at sufficiently high stress, $T$ or field levels, $E$. Switching is connected with changes of both the spontaneous strain, $\Delta S^s$ and the spontaneous polarisation, $\Delta P^s$. Favourably oriented domains grow at the expense of unfavourably oriented domains. Because of crystal symmetry (e.g. tetragonal, rhombohedral) there are more than one possible new direction of spontaneous polarization.

In the 3D micromechanical model used here the work done by switching is assumed to exceed a (positive) critical value:

$$\underline{T}\cdot\Delta\underline{S}^s + \vec{E}\cdot\Delta\vec{P}^s = \Delta w \leq \Delta w^c \qquad (1)$$

which corresponds to critical stress or critical electric field under uncombined uniaxial loading. As a consequence of this combined energy criterion the critical stress value is linearly dependent on the applied electric field.[5]

### 3.1 Micromechanical simulation without grain-to-grain interaction

The behaviour of piezoelectric ceramics simulated by means of the combined energy criterion eqn (1)[3] well corresponds to the experimentally observed behaviour as far as available. In this numerical simulation, inhomogeneities of the electric field and stress have been ignored. Thus each grain was subjected to the applied electric field and/or stress. The simulated stress versus strain behaviour shows a high degree of asymmetry between tension and compression.[3] Own analytical investigations on the basis of a well-defined polarization texture function[10] yield to very similar results (Fig. 1). Both the numerical and analytical results are in contradiction to recent experimental observations on PZT four point bending specimens (H. Weitzing and G. A. Schneider, unpublished results) (Fig. 2) which show a low stress–strain asymmetry only. Probably the high asymmetry in the simulated mechanical behaviour is caused by neglection of the grain-to-grain interaction.

### 3.2 Micromechanical simulations with grain-to-grain interaction

Obviously, in piezoelectric ceramics the changes of both the ferroelastic strain and the ferroelectric polarization of a single domain cannot take place without clamping reactions of neighbouring domains and grains. First of all, the misorientation relations are responsible for the inhomogeneous reaction of polycrystalline materials.

Finite-element (FE) methods are very suitable to investigate the behaviour of such inhomogeneous materials. All FE results shown here are based on calculations by means of the FE software package ANSYS©. The nonlinear material behaviour is described by means of the domain switching model. The macroscopic behaviour of the inhomogeneous material arises from averaging over all sub-elements.

In the first place the uncoupled mechanical and electrical behaviour has been simulated on the basis of the nonlinear 3D finite element SOLID 45. Figures 2 and 3 show the results of FE simulations for both the ferroelastic and the ferroelectric behaviour of polycrystalline samples with randomly oriented grains of tetragonal structure. Initially each grain consists of the six tetragonal domain orientations. Thus the polarisation texture is given by the whole of the volume fractions of all domains which change during domain switching.

The results of the mechanical simulations well correspond to the experimental results concerning the low asymmetry between tension and compression.

From the ferroelectric hysteresis (Fig. 3) a characteristic dependence of the experimentally observable coercive field on the micromechanically defined critical field strength can be seen. The coercive field strength appears as a cooperative switching of 180° domains.

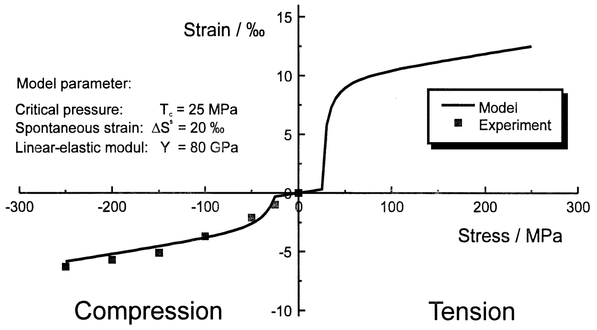

**Fig. 1.** Strain versus stress on the basis of the domain switching modell without grain-to-grain interaction. Experimental results from. Ref. 5.

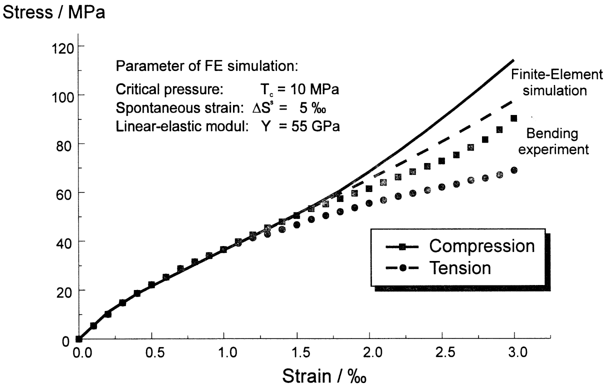

**Fig. 2.** Stress versus strain on the basis of the domain switching model with grain-to-grain interaction. Experimental results from H. Weitzing and G. A. Schneider (unpublished).

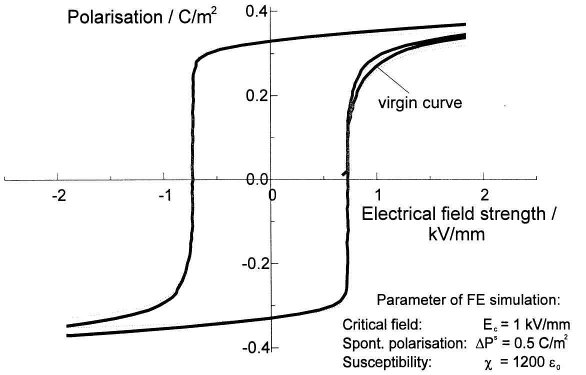

**Fig. 3.** Polarisation versus field on the basis of the domain switching model with grain-to-grain interaction. Dotted lines show the ferroelectric part of polarisation.

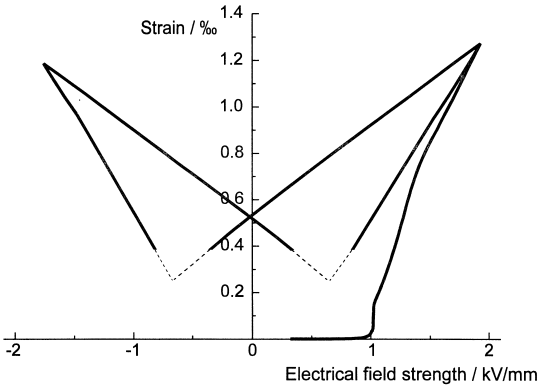

**Fig. 4.** Strain versus field on the basis of the domain switching model with grain-to-grain interaction.

In the second place the full coupled behaviour has been simulated on the basis of the 3D finite element SOLID 5 which has been extented to the nonlinear option for both the mechanical and the electrical behaviour. The domain switching changes the polarisation texture which can result in higher or lower macroscopic piezoelectric activity on the basis of the single crystal piezo coefficients.

Fig. 4 shows a typical butterfly-shaped curve simulated by means of the nonlinear piezoelectric element.

## 4 Conclusions

The domain switching model based on a combined energy criterion is suitable to describe the behaviour of piezoelectric ceramics. The model has been implemented into the Finite-Element code ANSYS© by which the elastic and electrical interaction within the polycrystalline structure is taken into account. The typical behaviour of ferroelastic, ferroelectric, and piezoelectric materials has been simulated. In the case of ferroelastics the FE results show a low degree of mechanical asymmetry like observed in PZT ceramics.

As a next step the influence of combined loading conditions has to be investigated. Such loading conditions are obeserved in piezoelectric devices like multilayer actuators and multimorphs. The micromechanical piezoelement should allow to derive realistic material laws for such complex piezoelectric structures under electromechanical loading conditions. In the field of nonlinear fracture electromechanics the special emphasis is turned to the understanding of ferroelastic fracture toughening.

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