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Simulation of nonlinear properties of ferroelectric and piezoceramic materials

Bülent Delibas*[1], **Arunachalakasi Arockiarajan**[1], and **Wolfgang Seemann**[2]

[1] University of Kaiserslautern, Department of Mechanical and Process Engineering, Germany.
[2] University of Karlsruhe, Department of Mechanical Engineering, Germany.

Ferroelectric and piezoelectric materials are becoming a very significant part of smart materials that are used widely as actuators, sensors and most common applications such as vibration control, precision positioning, precision cutting and microelectromechanical systems (MEMS). Piezoceramic materials show nonlinear characteristics when they are under high electromechanical loading. In this study, nonlinear behaviour of tetragonal perovskite type piezoceramic materials is simulated using micromechanical model. In the simulations uni-axial loading is applied. The calculations which are based on a linear constitutive model, nonlinear domain switching model and a model of probability to switch are performed at each grain. The different domain switching effects (90^0 or 180^0 domain switching for tetragonal perovskite structure) due to energy differences, different probability functions, different statistical random generators and material parameters are analyzed. Finally, simulation results are compared with the data of experiments are giving in literature.

1 Introduction

Piezoelectricity is a phenomenon that a material generates an electric displacement if a mechanical loading is applied or has displacement when it is subjected to an electric field. Most piezoceramic materials such as BaTiO3, PZT and PLZT have a perovskite tetragonal microstructure. The basics of piezoelectric and ferroelectric materials are explained by Jaffe et al. [1]. Ferroelectric materials behave strongly nonlinear when they are under high electromechanical loads. The nonlinearity is mainly coming from domain switching which is the change of direction of the spontaneous polarization at the microstructure level. In literature there have been various approaches in order to simulate nonlinear characteristics of piezoelectric materials either using phenomenological or micromechanical models. [2-4]. In this paper a new micromechanical modeling of ferroelectric and piezoelectric materials is proposed. The main difference of the model is using probability functions in the energy equations for domain switching. The results of the simulations are shown in curves for the electric displacement versus electric field hysteresis and strain versus electric field butterfly curves under a uniformly loaded cyclic electric field.

2 Model and simulations

Constitutive equations are used for calculating the electric displacement or macroscopic polarization and the mechanical strain of the piezoelectric material. Electric displacement(D_k) and mechanical strain (S_{ij}) are calculated by $D_k = \epsilon_{kn} E_n + d_{klm}\sigma_{lm} + P_0$ and $S_{ij} = s_{ijlm}\sigma_{lm} + d_{ijn}E_n + S_0$ respectively, where E_n is the electric field tensor, σ_{lm} is the mechanical stress tensor, S_0 is the spontaneous strain, P_0 the spontaneous polarization, d_{klm} is the piezoelectric constant, ϵ_{kn} is the dielectric constant and s_{ijlm} is the elastic constant. Spontaneous polarization and spontaneous strain terms are changing nonlinearly due to the domain switching in the lattice. For perovskite type tetragonal elements, only two types of domain switching are possible. These are 90^0 and 180^0 switching, the names of which are related to the angle of rotation which the position vector to the central atom undergoes during switching relative to its previous direction. It is assumed that the bulk piezoceramic material consists of 1000 elements each of which stands for the characteristics of an individual grain of the material. Orientations of grains are given statistically which is achieved by using a random generator. Euler angles are used to describe the orientations. Each grain has random orientation in properties of polarization and strain. Euler angles are chosen between 0 to 2Π. In the simulation, local coordinate systems are assigned to every grain and a global coordinate system is introduced. The relation between the global coordinate (x_g, y_g, z_g) and local coordinates (x_l, y_l, z_l) is given by $(x_g, y_g, z_g)^T = R(\alpha, \beta, \gamma)(x_l, y_l, z_l)^T$ using the transformation matrix $\mathrm{R}(\alpha, \beta, \gamma)$. At each grain, in addition to the piezoelectric constitutive equation, a nonlinear switching model is implemented for domain switching. The domain switching at each grain is determined by using the electromechanical energy criteria $\Delta P_i E_i + \Delta S_{ij}\sigma_{ij} = U_i$, where ΔP_i and ΔS_{ij} are the change of polarization and strain during domain switching respectively. U_i is the energy required for the threshold of domain switching. In the model, in order to take into account intergranular effects, a

* Corresponding author: e-mail: delibas@rhrk.uni-kl.de, Phone: +49 631 205 4835, Fax: +49 631 205 2823

probability for domain switching is introduced by $p(E_i) = (\|E_i\| \,/\, \|E_{ci}\|)^n$, where p is the probability for domain switching and E_{ci} is coercitive electric field. This probability is able to explain the nonlinearity of piezoelectric materials even in a small electromechanical loading range. The power (n) is chosen two, three, four and five for getting an optimum matching to experimental results. Figure 1(left) shows a polarization versus electric field hysteresis curve without considering a probability function in the simulation. Figure 1(right) shows the model in which fifth order polynomials ($n = 5$) for the probability function is implemented, and comparison with experimental curve is given. The simulated results obtained with a probability function fit better with experimental results than those curves which were simulated without using a probability criteria.

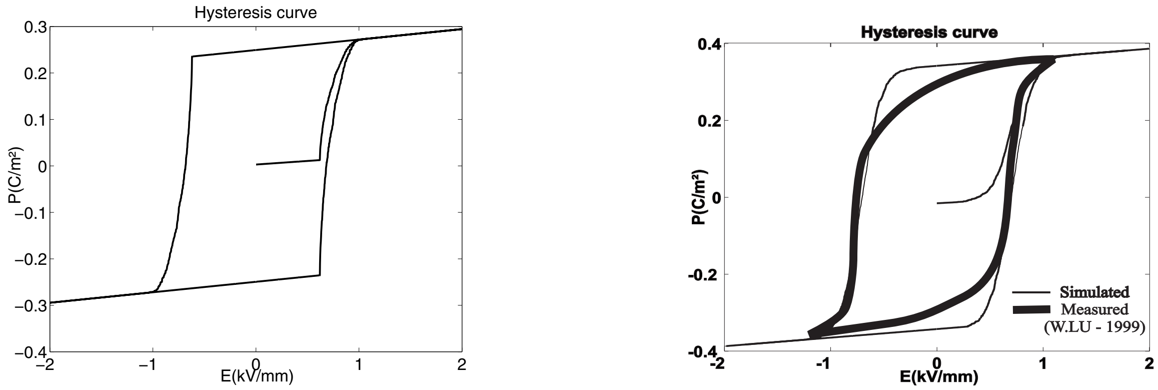

Fig. 1 **Left**: (Hysteresis curve without taking probability); **Right**: (Hysteresis curve with probability (n=5))

Figure 2 shows the strain versus electric field butterfly curves with and without covering probability functions. Smoothness of the curves near the coercive electric field levels can be observed easily from figure 2 (right).

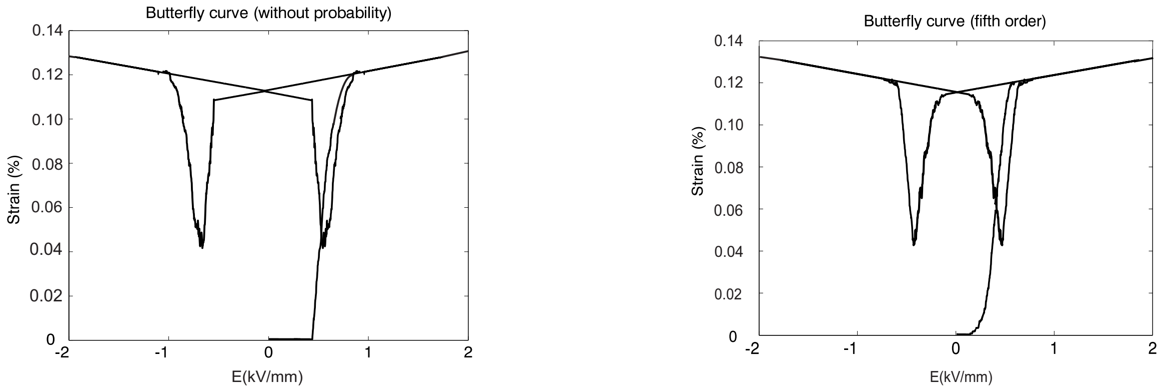

Fig. 2 **Left**: (Butterfly curve without taking probability); **Right**: (Butterfly curve with probability (n=5))

3 Conclusion

A micromechanical model is presented which is able to show nonlinear properties of perovskite type ferroelectric and piezoelectric ceramic material under high cyclic electrical loads. The simulations are based on both a linear constitutive model and on nonlinear domain switching. A probability function is used to describe the model. The hysteresis and butterfly curves which are simulated by this model show better correspondence to the experimental hysteresis curves than simulation results which are only based on an energy criterion.

References

[1] B. Jaffe, W. R. Cook and H. Jaffe: Piezoelectric Ceramics, Academic Press, London and New York, 1971.
[2] M. Kamlah and Q. Jiang: A model for PZT ceramics under uni-axial loading, *Wissenschaftliche berichte, Forschungszentrum Karlsruhe*, Institut für Materialforschung, 1997.
[3] W. Chen and C. S. Lynch: A micro-electro-mechanical model for polarization switching of ferroelectric materials, *Acta Mater.*, **46**, 5303-5311(1998).
[4] W. Lu, D.N. Fang, C. Q. Li,and K.C. Hwang: Nonlinear electric-mechanical behaviour and micromechanics modeling of ferroelectric domain evolution, *Acta Mater.*, **47**, 2913-2926(1999).