# Relaxation model of piezoelectric materials

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Polarization switching inside grains is time dependent. When external applied loading is not quasi-static, macroscopic properties of piezoelectric materials changes with the rate of loading. In this paper, a 2-D micromechanical model is proposed in order to simulate the rate dependent properties of certain perovskite type tetragonal piezoelectric materials based on linear constitutive, nonlinear domain switching, intergranular effects and kinetics models. The material is electrically loaded with an alternating voltage of various frequencies. For the onset of domain switching, energy equation is implemented. Propagation of the domain wall during domain switching in grains is modeled by means of exponential kinetics relation after domain nucleation. Mechanical strain butterfly loops under different frequencies (0.01Hz-1Hz) are simulated. The model gives important insights into the rate dependency of the piezoelectric materials that have been observed in some experiments reported in the literature.

## 1 Introduction

Piezoelectric materials became a highly interesting part of smart materials due to their various commercial engineering and scientific applications. Ferroelectric and piezoelectric materials have a spontaneous polarization which can change its direction when they are subjected to high electromechanical loading when the temperature is under the Curie temperature. Polarization switching and kinetics of it in the grains of piezoelectric materials are dependent on the frequency of the cyclic loading. The influences of the loading rate on the electric displacement and mechanical strain are observed by various researches in the literature using either experiments or modeling [1] - [4]. In this paper, the rate dependent properties of PIC151 piezoelectric materials are investigated using a two-dimensional micromechanical model. The simulation results are presented in butterfly curves which are mechanical strain versus electric field.

## 2 Model and simulation and results

Macroscopic polarization and the corresponding mechanical strain of piezoceramic material can be calculated by using constitutive equations. Electric displacement $(D)$ and mechanical strain $(S)$ are calculated by $D = \epsilon E + \sigma d + P_s$ and $S = s\sigma + dE + S_0$ respectively, where $E$ is the electric field, $\sigma$ is the mechanical stress, $S_s$ is the spontaneous strain, $P_s$ is the spontaneous polarization, $d$ is the piezoelectric constant, $\epsilon$ is the dielectric constant and $s$ is the elastic constant. Domain switching in microstructures is the main factor for the nonlinearity. There are only two types of domain switching which are $90^0$ and $180^0$ switching for a perovskite type tetragonal lattice element. In this 2-D micromechanical model a bulk piezoelectric ceramic is considered to consist of 900 (30x30) elements. Randomness of orientations is introduced by means of Euler angles, which are chosen to be equally distributed between 0 and $2\pi$. During the simulation local coordinate systems for every grain and one global coordinate system are defined for transforming the calculated values from the local coordinate systems to global coordinate.

Nonlinearities of piezoelectric materials are also affected by intergranular stresses and non-uniform electrical characteristics of neighboring elements of crystals. The domain switching at each grain is determined by using the electromechanical energy criteria which are written for both type of domain switching respectively; $E_n P_n + \sum [C_p(P_{n+i}E_{n+i}T_{n+i})] + W_{n90} > 0$ ($90^0$ domain switching), $E_n P_n + \sum [C_p(P_{n+i}E_{n+i}T_{n+i})] + W_{n180} > 0$ ($180^0$ domain switching). $E_n$ and $P_n$ is the electric field and polarization value of $n^{th}$ element. The second term stands for the neighboring elements electric field and polarization value that are multiplied by constant $C_p$. In these relations $C_p$ is assumed to be material dependent. $T_{n+i}$ is the transformation matrix from $(n+i)^{th}$ element to $n^{th}$ element. $W_{n90}$ and $W_{n180}$ are mechanical energy requirements for both types of domain switchings. It is geometrically proofed that $180^0$ domain switching requires double energy than $90^0$ domain switching ($W_{n180} = 2W_{n90}$). According to this criterion, domain switching occurs if the electromechanical energy is higher than zero. With this model nonlinearities can be explained even in small electromechanical loading range micromechanically [5]. As explained above, for the rate dependency we have applied cyclic loading with three different frequency values (1 Hz, 0.1 Hz, 0.01 Hz) and 1 kV/mm electric field amplitude. Exponential kinetics theorem is applied for the calculation of rate dependency. In this simulation $W_{n90}$ is assumed to be 80 kJ. $C_p$ value is chosen as 0.65. The other piezoelectric material parameters are

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chosen according to the experimental values of PIC 151. Figure 1 illustrates the mechanical strain versus electric field butterfly curve for such frequency loadings.

It can be concluded from this figure that the coercive electric field is dependent on the frequency of the loading, which can also be achieved from experimental curves. The coercive electric field is increasing when the frequency is increased from 0.01 Hz to 1 Hz. Another important observation for this curve under cyclic loading with a high frequency is that the mechanical strain is increasing even for a decreasing electric field during unloading provided that the actual electric field is larger than the coercive field. For a cyclic loading with a frequency of 1 Hz, the mechanical strain cannot reach the saturation level. Instead, the mechanical strain is increasing for a decreasing electric field as far as the applied electric field is larger than the coercive field
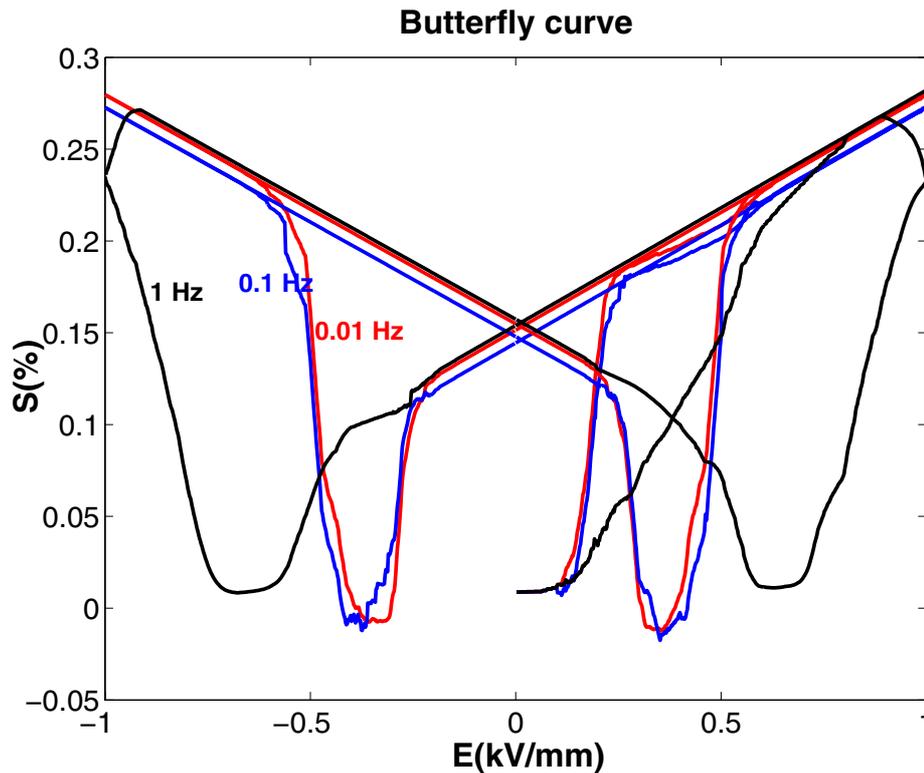


**Fig. 1**   (Butterfly curve with various frequency loadings)

## 3   Conclusion

Relaxation properties of perovskite type tetragonal piezoelectric materials under cyclic electrical loading by using a new micromechanical model is implemented to PIC 151 PZT ceramic. A piezoelectric linear constitutive model and a nonlinear domain switching with intergranular effects have been used in the model. The butterfly curves are simulated with various material parameters values (0.01Hz-1Hz). The simulations have been performed with various frequencies values in order to understand the macroscopic characteristics of such materials.

## References

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