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Modelling of the electromechanical behaviour of PZT

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Abstract. The aim of this paper is to model the one-dimensional behaviour of a soft PZT tested in compression. Thanks to a viscoplastic formulation, the effects of cyclical loading and loading rates are also taken into account. The coupling between remnant strain and polarisation is achieved through a mechanically induced depolarisation function.

1. INTRODUCTION

Some applications of ferroelectric materials develop large displacements or large forces under both electrical and mechanical loadings, in static or dynamic conditions. Irreversible strain and depolarisation thus occur [1]. To improve reliability and life time of these components, it is important to measure and model the effect of cyclical loadings on the response of the material. Non linear constitutive laws are then required to design complex geometries and to estimate device performance.

From thermodynamical considerations, Bassiouny and Maugin proposed an interesting formulation using the theory of plasticity, where remnant strain and polarisation are chosen as internal variables [2, 3]. This scheme was also used by Kamlah and Tsakmakis who presented a phenomenological model of the non-linear electromechanical coupling in ferroelectrics [4]. This model was recently implemented in a FEM-code [5]. Besides, McMeeking and Landis presented a simplified formulation by rigidly linking the remnant strain to the remnant polarisation [6].

In this paper, another non-linear electromechanical model is presented. To take into account time effects, the evolution laws of the internal variables are given in a viscoplastic formulation. It describes the characteristic phenomena of ferroelectricity: the dielectric hysteresis, the butterfly loop and the ferroelastic hysteresis of a unit volume. Nevertheless, experimental measurements are needed to identify the model parameters. A soft PZT obtained from a commercial source is tested cyclically in compression. This one-dimensional formulation of the model is successfully validated using the experimental data.

2. MATERIAL AND EXPERIMENTAL PROCEDURES

A commercial bulk soft ceramic is used in this study, which non-linear behaviour is known to be more pronounced than for hard PZT. It is furthermore easy to depole under stress by ferroelastic effect. PIC 255 is produced by PI Ceramic, Germany, and is indicated for actuators and high sensitive receivers applications (Table 1). It is available in form of poled cylinders (15 mm height, 10 mm diameter).

A special device has been designed to carry out compressive experiments and to allow electrical measurements. To offer a better stress state in the sample, compliant layers made of glass/epoxy isotropic composite are used. Longitudinal strain is measured by means of an extensometric gauge. For poled ceramics, stress is parallel to polarisation. Electrodes are short-circuited and electric charges are recorded

with a Kistler 5015 charge amplifier. Some samples are deposed by heating treatment above Curie temperature.

Table 1. Properties of soft PIC 255

Density (g.cm ⁻³)	7.8
Curie temperature (°C)	350
Relative permittivity ϵ_{33}	1800
Coupling factor k_p	0.62
Mechanical Q_m	80
Charge constant d_{333} (pC/N)	400

3. DESCRIPTION OF THE MODEL

Our goal is not to go into details of the model, which is fully explained in [7]. To shorten the body of the present article, only its one-dimensional formulation is given (according to direction 3).

The thermodynamical state of a system at a given instant is defined by two types of variables: the observable variables (related to the reversible phenomena) on one hand, and the internal variables (which keep track of the material history) on the other hand.

To describe the irreversible electromechanical behaviour, two independent variables are needed: the internal or remnant strain S_{33}^r and the internal or remnant polarisation P_3^r (electrical polarization P_3 has been chosen instead of electrical displacement D_3 , as they are directly related). Physically, the macroscopic internal variables must be viewed as averages of the corresponding microscopic quantities. The total strain and polarisation can thus be split into:

$$\begin{aligned} S_{33} &= S_{33}^{\text{rev}} + S_{33}^{\text{ir}}, \\ P_3 &= P_3^{\text{rev}} + P_3^{\text{ir}}, \end{aligned} \quad (1)$$

where the reversible components are given by the classical linear equations of piezoelectricity:

$$\begin{aligned} S_{33}^{\text{rev}} &= s_{3333} T_{33} + d_{333} E_3, \\ P_3^{\text{rev}} &= d_{333} T_{33} + \epsilon_{33} E_3. \end{aligned} \quad (2)$$

where T_{33} is the stress and E_3 the electric field, d_{333} a piezoelectric coefficient and s_{3333} the elastic compliance which equals $1/Y_{33}^E$.

It is known that applying an electric field can generate a remnant strain due to ferroelectric domain switching. On the other hand, a compressive stress can cause an irreversible ferroelastic strain because of domain switching in random directions. Therefore, the irreversible strain has to be split up in two components, a remnant strain S_{33}^{rem} and a depolarisation (or ferroelastic) strain S_{33}^{dp} :

$$S_{33}^{\text{ir}} = S_{33}^{\text{rem}} + S_{33}^{\text{dp}}. \quad (3)$$

S_{33}^{rem} is directly connected to the remnant polarization by:

$$S_{33}^{\text{rem}} = S_{\text{max}}^{\text{rem}} \frac{|P_3^{\text{ir}}|}{P_{\text{max}}}. \quad (4)$$

P_{max} represents the maximum value of the polarization in a material subjected to a high electric field and $S_{\text{max}}^{\text{rem}}$ is the maximum value of the strain reached for $|P_3^{\text{ir}}| = P_{\text{max}}$.

The evolution laws of the two internal variables are chosen to be time-dependent:

$$\dot{S}_{33}^{\text{dp}} = \dot{S}_0^{\text{dp}} \left\langle \frac{|T_{33} - \alpha_{33}^m| - T_0}{N^m} \right\rangle^{n^m} \frac{T_{33} - \alpha_{33}^m}{|T_{33} - \alpha_{33}^m|} \quad (5a)$$

$$\dot{P}_3^{\text{ir}} = \dot{P}_0^{\text{ir}} \left\langle \frac{|E_3 - \alpha_3^e| - E_0}{N^e} \right\rangle^{n^e} \frac{E_3 - \alpha_3^e}{|E_3 - \alpha_3^e|} \quad (5b)$$

The superscripts m and e indicate respectively the parameters associated with the mechanical and the electrical variables. The internal variables α_{33}^m and α_3^e are kinematic hardening variables and E_0 and T_0 are constant parameters corresponding to the activation thresholds of the irreversible variables from which one may understand the use of the Mac Cauley brackets ($\langle x \rangle = x$ if $x > 0$ and $\langle x \rangle = 0$ otherwise). The other terms introduced in (5) are some constants of the model. The time-independent formulation (i.e. plasticity) is the asymptotic case of this approach for high n^m and n^e exponents.

Due to similarities between ferroelectric hysteresis and ferroelastic curves, the same expression of the evolution laws is chosen for the kinematic variables α_{33}^m and α_3^e . The shape of the polarisation cycles is composed of a part tending towards reversibility in the neighbourhood of the saturation polarisation and another part, irreversible, leading to a steep evolution in the vicinity of the coercive field. Thus, each of the non-linear kinematic variables is split up in two terms, a reversible component α^r and an irreversible component α^{ir} :

$$\begin{aligned} \alpha_{33}^m &= \alpha_{33}^{\text{rm}} + \alpha_{33}^{\text{irm}} \text{ with } \alpha_{33}^{\text{rm}}(0) = \alpha_{33}^{\text{irm}}(0) = 0, \\ \alpha_3^e &= \alpha_3^{\text{re}} + \alpha_3^{\text{ire}} \text{ with } \alpha_3^{\text{re}}(0) = \alpha_3^{\text{ire}}(0) = 0, \end{aligned} \quad (6)$$

and their evolution laws are given by:

$$\begin{aligned} \dot{\alpha}_{33}^{\text{rm}} &= b^{\text{rm}} (a^{\text{rm}} + |\alpha_{33}^{\text{rm}}|) \dot{S}_{33}^{\text{dp}}, \\ \dot{\alpha}_{33}^{\text{irm}} &= b^{\text{irm}} \left(a^{\text{irm}} \dot{S}_{33}^{\text{dp}} - \alpha_{33}^{\text{irm}} \left| \dot{S}_{33}^{\text{dp}} \right| \right), \end{aligned} \quad (7a)$$

$$\begin{aligned} \dot{\alpha}_3^{\text{re}} &= b^{\text{re}} (a^{\text{re}} + |\alpha_3^{\text{re}}|) \dot{P}_3^{\text{ir}}, \\ \dot{\alpha}_3^{\text{ire}} &= b^{\text{ire}} \left(a^{\text{ire}} \dot{P}_3^{\text{ir}} - \alpha_3^{\text{ire}} \left| \dot{P}_3^{\text{ir}} \right| \right). \end{aligned} \quad (7b)$$

with the terms b and a constants of the model. The irreversible components have the formulation initially proposed by Armstrong and Frederick [8] and widely used later [9][10] and are extended here to the electrical variables. The laws used for the reversible components are much less classical.

Furthermore, it is widely brought up in the literature [5][11] that the piezoelectric coefficients d_{ij} depend on the initial polarization. As a consequence, the coefficient d_{333} is written as a function of the irreversible polarization P_3^{ir} :

$$d_{333} = d_{333_0} + d_{333_{\text{max}}} \frac{P_3^{\text{ir}}}{P_{\text{max}}}. \quad (8)$$

d_{333_0} (being possibly equal to zero) is the spontaneous piezoelectric coefficient in the absence of an induced polarisation. $d_{333_{\text{max}}}$ is the maximum value of the piezoelectric coefficient induced when the polarisation is saturated to the value $|P_k^{\text{ir}}| = P_{\text{max}}$.

Finally, the material can loose its polarisation in an irreversible way when a compressive stress is increased beyond a threshold value. It means that the variables S_{33}^{dp} and P_3^{ir} are not completely independent as it has been assumed in the thermodynamical approach. Considering this, we introduce a

depolarisation function f_{dp} :

$$f_{dp} = 1 - \beta \langle -S^{dp_c} - S_0^{dp_c} \rangle \frac{\langle -T_{33} \rangle}{|T_{33}|} \quad \text{with } \dot{S}^{dp_c} = \dot{S}_{33}^{dp} \quad (9)$$

where β is a constant of the model and S^{dp_c} represents the strain associated to the compressive stress causing depolarisation beyond the threshold value $S_0^{dp_c}$. Below this value, f_{dp} is equal to 1. This function is used for all terms depending on P_3^{ir} . Besides, in order to simulate the effect of stress on dielectric hysteresis [12], α_3^{ire} is multiplied by f_{dp} :

$$\alpha_3^{ire} = b^{ire} f_{dp} (a^{ire} P_3^{ir} - \alpha_3^{ire} |P_3^{ir}|) \quad (10)$$

as well as the piezoelectric part and the remnant part of the strain, so that total strain and polarisation can be written as:

$$S_{33} = \frac{T_{33}}{Y_{33}^E} + \left(\left(d_{333_0} + d_{333_{max}} \frac{P_3^{ir}}{P_{max}^{ir}} \right) E_3 + S_{max}^{rem} \frac{|P_3^{ir}|}{P_{max}^{ir}} \right) f_{dp} + S_{33}^{dp} \quad (11)$$

$$P_3 = \varepsilon_{33} E_3 + \left[\left(d_{333_0} + d_{333_{max}} \frac{P_3^{ir}}{P_{max}^{ir}} \right) T_{33} + P_3^{ir} \right] f_{dp} \quad (12)$$

This formalism, applied to the one-dimensional case, will be used for all the simulations presented in the next section.

4. VALIDATION OF THE MODEL

When possible, parameters are determined either with manufacturer's data, or graphically on experimental curves. In other cases, identification is processed by means of a local method. The Levenberg-Marquardt algorithm is an effective way to solve non-linear least squares problems. The values of the mechanical and electrical parameters used in the model are given in Table 2.

Table 2. Parameters used for the simulations

Parameters	Unit	Value	Parameters	Unit	Value
Y_{33}^E	GPa	110	b^{rm}	-	2.65×10^3
N^m	MPa	11.9	b^{irm}	-	750
n^m	-	15.8	a^{rm}	MPa	3.2×10^{-3}
T_0	MPa	13	a^{irm}	MPa	45
β	-	180	\dot{S}_0^{dp}	s^{-1}	10^{-4}
S_{max}^{rem}	-	6.2×10^{-3}	$S_0^{dp_c}$	-	1×10^{-4}
ε_{33}	C/m.V	1.59×10^{-8}	b^{re}	m^2/C	42
N^e	V/m	10^6	b^{ire}	m^2/C	5.7
n^e	-	1	a^{re}	V/m	9.1×10^{-4}
E_0	V/m	0	a^{ire}	V/m	1.6×10^6
P_{max}	C/m ²	0.6	$d_{333_{max}}$	pC/N	500
P_0^{ir}	C/m ² /s	5	d_{333_0}	pC/N	0

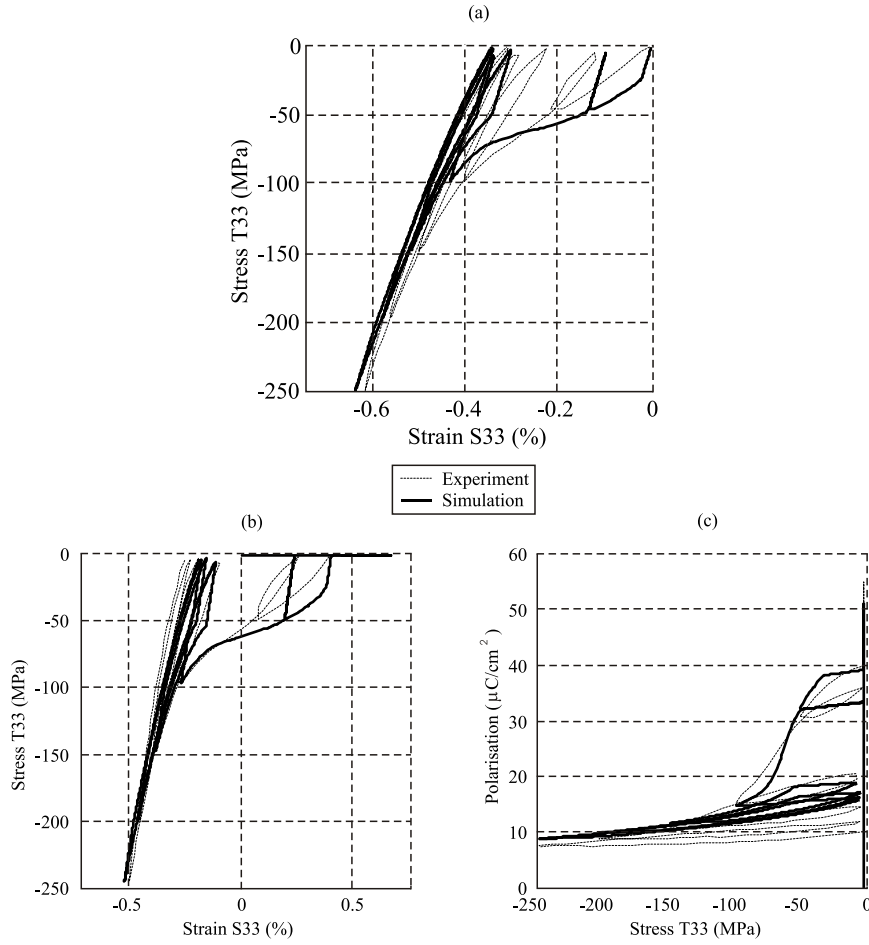


Figure 1. Experimental and model curves: mechanical behaviour for an unpoled specimen (a) and a poled one (b), depolarisation according to stress (c)

As the specimens are poled by the manufacturer, the poling process has to be simulated. A typical dielectric hysteresis for soft PZT found in the literature [13] is fitted using manufacturer's information such as the value of the coercive field (1.5 kV/mm), so that remnant polarisation reaches $40 \mu\text{C}/\text{cm}^2$ and remnant strain 0.4%.

4.1. Compressive loadings

Unpoled and poled PZT are loaded by repeated compressive growing cycles (Figure 1). As more domains are available to switching for the poled ceramic, strain levels are higher than for the unpoled one [14] [15]. In spite of experimental observations, the threshold stress T_0 has to be different than 0 in order to model the looping of the stress/strain curve, so that under low stress levels model does not completely describe the real behaviour of the PZT. Poled specimen is affected by the ferroelastic effect: f_{dp} is activated by the compressive stress and depolarization occurs.

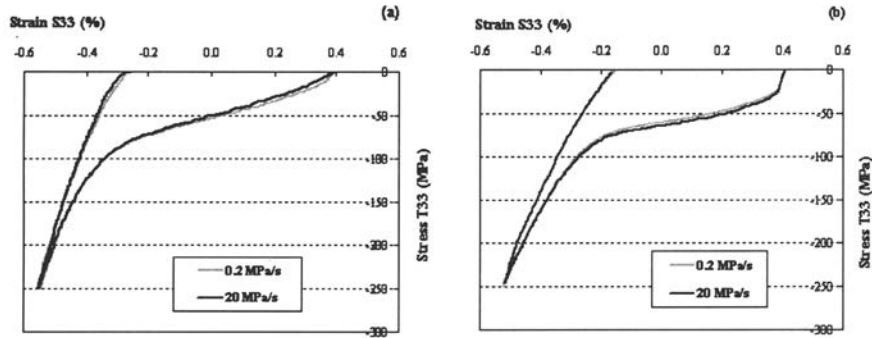


Figure 2. Effect of loading rate on experimental (a) and model (b) curves

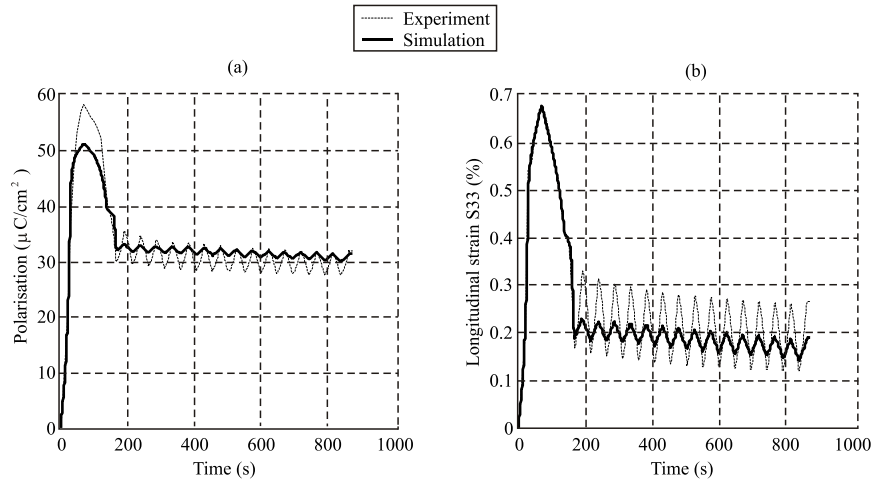


Figure 3. Response of a poled ceramic to a cyclical loading (a-depolarisation and b-strain)

4.2. Influence of loading rate

For poled specimens, the influence of the loading rate is explored by carrying out a -250 MPa loading/unloading cycle. A ratio 100 is chosen between both loading speeds (set to 0.2 MPa/s and 20 MPa/s). No major influence of the loading rate is highlighted on depolarisation and stress strain curves and maximal strain and depolarisation levels are comparable (Figure 2). As a conclusion, mechanically induced switching processes for soft PZT do not seem to be highly influenced by stress rate.

4.3. Response to cyclic loadings

Fifteen 50 MPa compressive cycles are performed on poled samples. Material evolution is maximal during the first cycle and after 10 cycles, responses of the material can be superimposed while strain and polarisation levels stagnate (Figure 3). Thus the material accommodates to the cyclic loading and no so-called ratchetting effect is observed. This signifies that the degradation of the material properties may stabilise independently from long-term ageing phenomena.

Experimentally, polarisation and strain are related in a linear manner together. As they depend both on domain configuration these variables are coupled, which is taken into account by f_{dp} in the present

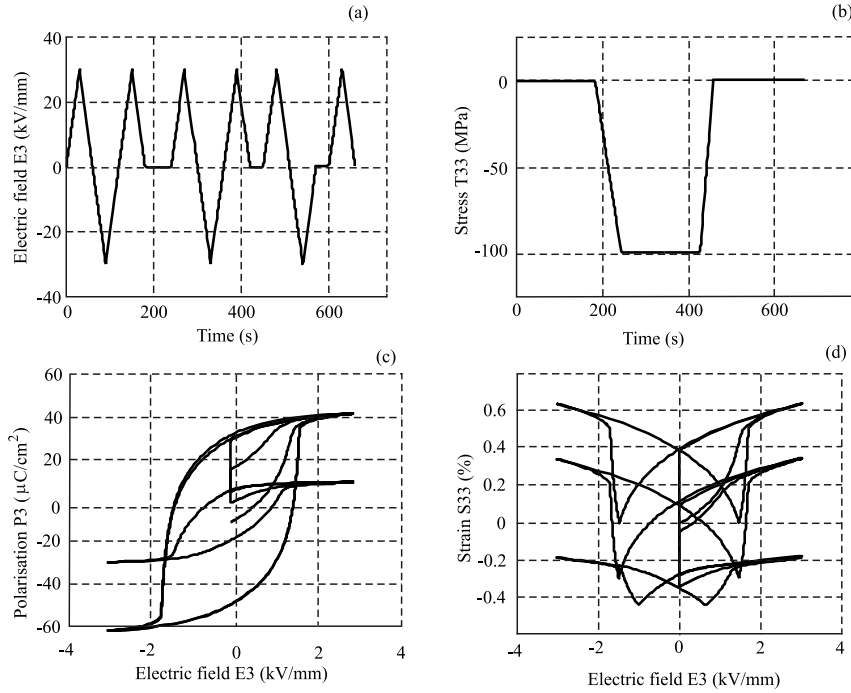


Figure 4. Simulation of the effect of an applied stress on poling process: applied electric field (a) and stress (b) according to time; polarisation hysteresis (c) and butterfly loops (d).

definition of the model. The simulation reproduces well this tendency, although the amplitude of the cycles is less pronounced than actually.

4.4. Poling under stress

Under a compressive stress, the polarisation curve is contracted and tilted. The strain versus electric field curve is also translated along the strain axis and in the direction of lower values of the strain [12]. However the remnant strain and polarisation can be reset by application of electric field at zero stress. This is the so-called “memory effect”. The mechanical load prevents from domain switching when electric fields are applied in a PZT actuator component. The model describes this phenomenon as f_{dp} is reset to 1 during the last electric loading at 0 stress, although T_0 remains constant (Figure 4).

5. CONCLUSION

This electromechanical model is promising to fit the non-linear coupling of the PZT ceramics in its one-dimensional formulation. The experimental results for one type of soft bulk PZT are simulated qualitatively and more or less quantitatively. Other viscoplastic phenomena such as creep under constant stress can be grasped with this model.

Nevertheless, in some cases the initially independent internal variables are found to be coupled. In fact, the remnant polarization does not directly keep track of the microstructural changes in the material. Indeed different configurations of the mass fractions of ferroelectric domains may lead to the same polarization state (remember for example the case of a totally stress depoled ceramic and an unpoled ceramic, which response are different under the same mechanical loading). The approach

based on phenomenological theory is however well adapted for loadings close to uniaxial including cyclic ones [16]. On the other hand, two-dimensional tests on convenient structures should permit to propose and validate a multidirectional formalism of the model chosen among the possible formulations.

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