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Efficient Modeling of Ferroelectric Behavior for the Analysis of Piezoceramic Actuators

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ABSTRACT: This work proposes a method of efficiently modeling the hysteresis of ferroelectric materials. Our approach includes the additive combination of a reversible and an irreversible portion of the polarization and strain, respectively. Whereas the reversible parts correspond to the common piezoelectric linear equations, the irreversible parts are modeled by hysteresis operators. These operators are based on Preisach and Jiles-Atherton hysteresis models which are well-established tools in ferromagnetic modeling. In contrast to micro-mechanical approaches, a Preisach or a Jiles-Atherton hysteresis operator can be efficiently numerically evaluated. A comparison of the resulting simulations to measured data concludes the article.

Key Words: piezoceramic actuator, ferroelectric behavior, hysteresis, butterfly curve, Jiles-Atherton Model, Preisach model.

INTRODUCTION

PIEZOELECTRIC devices do not only serve as sensors in a broad spectrum of applications: actuators based on piezoelectric material are becoming more and more common. Their application field includes, but is not limited to, automation technology (high precision positioning devices), office equipment (piezoelectric inject printers), medical technology (ultrasound transducers), and automotive technology (injection valves with multi-layer actuators). Extremely large forces paired with practically no static energy losses, as well as excellent dynamic properties, make piezoelectric actuators very interesting for many application areas.

The majority of today's piezoelectric actuators are based on ceramic materials, mainly lead zirconium titanate (PZT) due to its strong inverse piezoelectric effect. Unfortunately, these ceramic materials exhibit increasingly nonlinear behavior directly related to the high driving levels necessary for actuators. This characteristic, which includes a hysteresis loop for the electric polarization and a so-called butterfly loop for the mechanical strain, is usually referred to as ferroelectric behavior. Figure 1 depicts the two hysteresis loops.

Modeling these actuators has presented a challenge to many researchers for quite some time and different

approaches have been considered. One approach considers just the actuator working range and models the hysteresis of the mechanical strain phenomenologically. Early attempts, e.g., Harper (1981), used differential equations or polynomials to model the rising and falling branches of the strain within the actuator working range separately. Very soon the Preisach model, developed for modeling of magnetic hysteresis curves (Preisach, 1935), was adopted for piezoceramic materials. The model averages the states of a large number of switching operators. Sreeram et al. (1993) use this model to predict the behavior of a piezoelectric bending actuator. Jendritza (1995) also describes the modeling of the voltage-displacement relations with Preisach models. He takes the problem one step further and inverts the attained model to linearize a control path. Other applications of the Preisach model can be found in, e.g., Hughes and Wen (1995).

A different phenomenological approach is introduced by Goldfarb and Celanovic (1997). They use a number of superimposed generalized Maxwell resistive capacitor elements with different parameters to form a smooth hysteresis curve. Reiländer (2003) revives these ideas again and puts them into the context of other rheological models. He also investigates Preisach models and concludes that the computational effort for Preisach models is greater than for rheological models. On the other hand, he notes, rheological models are not rate independent and therefore not suitable for general

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Figures 1–8 and 10 appear in color online: <http://jim.sagepub.com>

hysteresis modeling for piezoelectric actuators. Besides the hysteresis effects, Reiländer also looks at creep effects and presents a model integrating both creep and hysteresis to predict the deflection of a piezoelectric actuator.

Kuhnen (2001) superimposes different operators for modeling the mechanical strain of piezoceramic actuators. The hysteresis is described by a Prandtl-Ishlinskii hysteresis operator, a special case of the general Preisach operator. Creep phenomena are included through the superposition of a Prandtl-Ishlinskii creep operator. He points out that the advantage of Prandtl-Ishlinskii operators for the controller/compensator design is that, in contrast to general Preisach operators, the inverse Prandtl-Ishlinskii operator is again a Prandtl-Ishlinskii operator. Compared to general Preisach operators, the complexity is reduced too. Using an inverted Prandtl-Ishlinskii operator, Kuhnen is able to design a compensator, which alters the input voltage signal such that the reference trajectory for the mechanical strain is closely followed.

While many authors concentrate on modeling the mechanical strain behavior of piezoelectric actuators, Simkovics et al. (2000) are interested in the dielectric polarization. They succeed in modeling the electrical behavior using a Preisach model within a nonlinear finite element analysis. Smith and Hom (1999) also focus on the dielectric behavior. In contrast to the previous authors, where phenomenological modeling is performed, Smith and Hom try to base their model on the physical understanding of domain wall movements and internal energy losses in the material. They follow a similar theory presented by Jiles and Atherton (1984) for ferromagnetic hysteresis.

While most of the models above perform well for their given task, they fail to predict the complete ferroelectric behavior (Figure 1). This is where micromechanical models come into play. Micromechanical models are

inspired by the typical granular structure of ferroelectric materials. Within one grain (Weiss domain) the polarizations of all dipoles point in the same direction. Micromechanical models usually approach this with the finite element method (FEM). One finite element represents one domain of the material. Certain criteria cause the direction of the polarization to rotate. Chen and Lynch (1998) use internal energy levels to reorient the polarization of each cell. Each cell's behavior is governed by the piezoelectric constitutive equations supplemented with nonlinear ferroelectric and ferroelastic relations. The macroscopic behavior of the ceramic is obtained by averaging over all cells in the volume. Chen and Lynch simulate the complete polarization cycle and present hysteresis and butterfly curves, which, however, differ quantitatively from measured curves.

Seemann et al. (2004) also introduce a micromechanical model containing 1000 three-dimensional cells. The polarization switching of each cell is controlled by a probability function dependent on the internal energy levels, which smoothes the resulting polarization curves to a more realistic shape. Arockiarajan et al. (2005) and Delibas et al. (2005) develop this model further and also show strain butterfly curves. Their simulation results are not compared to measured data. Fröhlich (2001) also presents a micromechanical model focused on verifying linear electromechanical material parameters. His work gives interesting insight to the strain and electric field strength distribution, especially at the grain boundaries.

The major drawback of the micromechanical approaches is the computational effort required. Due to the consideration of the microscopic grains, the simulation of complete macroscopic actuator devices is not feasible. This is where thermodynamically consistent models become useful. In contrast to the micromechanical models, the material is not discretized down to grain level. The fundamentals thereof were outlined in the late 1980s in a series of articles by Bassiouny et al. (1988a, b) and Bassiouny and Ghaleb (1989a, b). However, to the authors' knowledge, their ideas have only recently been applied by various researchers.

Kamlah and Tsakmakis (1999), Kamlah and Jiang (1999) and Kamlah and Böhle (2001) developed a constitutive framework based on thermodynamic fundamentals. The core of the framework is the decomposition of the dielectric polarization and the mechanical strain into a reversible and an irreversible part analogous to Bassiouny and Ghaleb. A set of internal variables motivated by the microscopic structure of the material is also introduced. In detail, the internal variables describe the relative polarization and the ratio of domains where the polarization is aligned in certain directions. The model incorporates the dependence of the irreversible polarization and strain on the mechanical stress. The reversible parts of strain and polarization are defined by the linear piezoelectric equations in d-form

Figure 1. Hysteresis of dielectric polarization and mechanical strain on a piezoceramic actuator.

with the anisotropy of the d-tensor depending on the load history. Using the finite element analysis, Kamlah et al. succeed in predicting the behavior of a stack actuator qualitatively. The obtained hysteresis and butterfly curves are not smooth on some spots.

Huber et al. (1999) also use the decomposition of polarization and strain. Landis et al. (2004), enhance this model further and embed it into a thermodynamically consistent frame. The internal variables are defined in compliance to the plasticity theory. The calculated strain and polarization curves seem to be closer to the real behavior of piezoceramic materials than Kamlah's, but are not compared directly to measured data.

Schröder and Romanowski (2004) also published a thermodynamically consistent model. The shape of their hysteresis curves is defined by a superposition of parameterized *artanh* and *ln* functions. Therefore, the resulting curves are, except in the return points, continuous and look very realistic. Only the initial polarization curve seems too flat.

In conclusion, three different trends for modeling ferroelectric behavior can be observed. Firstly, there are the thermodynamically consistent models, which use a macroscopic technique to describe microscopically caused phenomena. Secondly, the micromechanical models, which are sometimes also based on thermodynamic fundamentals, approach the problem by breaking the material down to the size of single grains. And thirdly there are the models containing some kind of hysteresis operator, modeling either the strain or the polarization hysteresis in the actuator working range.

All of the modeling approaches above perform well in their designated environments or give new insight to internal working mechanisms, respectively. However, the full dynamic analysis of complex structures containing nonlinear piezoelectric actuators using the finite element method (FEM) has not yet been feasible. Therefore, we try to combine certain advantages of the previous techniques to obtain a model that can efficiently be evaluated with FEM. First results have been published in Hegewald et al. (2006). The present paper describes our method in detail and shows more results.

METHODS

This section describes the core ideas behind our model. Firstly, we introduce the superposition of reversible and irreversible parts of the mechanical strain and the dielectric displacement, respectively. Secondly, the utilized hysteresis models are introduced followed by a short overview of the measurement setup. Lastly, the parameter identification procedure is discussed.

Model Fundamentals

The behavior of piezoelectric ceramics is governed by the ferroelectric properties of the ceramic and by the piezoelectric properties which strongly depend on the material's state of polarization. Therefore, the dielectric displacement $\vec{D}$ is broken down into a reversible part $\vec{D}^r$ and into an irreversible part $\vec{D}^i$

$$\vec{D} = \vec{D}^r + \vec{D}^i. \quad (1)$$

The formulation with the dielectric displacement $\vec{D}$ corresponds to the approach originally suggested by Bassiouny et al. (1988a) for the polarization $\vec{P}$. Many researchers revived their ideas (e.g., Landis, 2003; Kamlah and Tsakmakis, 1999). In our case, using the general relation between dielectric displacement $\vec{D}$, electric field strength $\vec{E}$, and polarization $\vec{P}$, and setting $\vec{D}^i = \vec{P}^i$, Equation (1) can directly be converted in the original formulation

$$\begin{aligned} \vec{D} &= \vec{D}^r + \vec{D}^i \\ &= \epsilon_0 \vec{E} + \vec{P}^r + \vec{P}^i. \end{aligned} \quad (2)$$

Analogously to Equation (1), the mechanical strain $\vec{S}$ (strain tensor in vector notation according to Voigt) is also broken up into a reversible part $\vec{S}^r$ and an irreversible part $\vec{S}^i$

$$\vec{S} = \vec{S}^r + \vec{S}^i. \quad (3)$$

The decomposition of the strain $\vec{S}$ is done in compliance with the theory of elastic-plastic solids assuming very small deformations (Bassiouny and Ghaleb, 1989b). This assumption is generally true for piezoceramic materials with maximum strains not more than 0.2 %.

The reversible parts of mechanical strain $\vec{S}^r$ and dielectric displacement $\vec{D}^r$ are described by either set of the following equations

$$\vec{D}^r = e \vec{S}^r + \epsilon^S \vec{E} \quad (4)$$

$$\vec{T} = c^E \vec{S}^r - e^T \vec{E}, \quad (5)$$

or

$$\vec{D}^r = d \vec{T} + \epsilon^T \vec{E} \quad (6)$$

$$\vec{S}^r = s^E \vec{T} + d^T \vec{E} \quad (7)$$

with the vector of mechanical stresses $\vec{T}$ (stress tensor in Voigt notation), the vector of the electric field strength $\vec{E}$, the tensors of the mechanical stiffness and compliance c^E and s^E (measured at constant electric field), the tensors of the piezoelectric moduli e and d , and the tensors of the dielectric permittivity ϵ^S (obtained at constant strain) and ϵ^T (obtained under constant stress conditions).

Equations (4) and (5) essentially represent the linear piezoelectric constitutive equations in e-form.

Equations (6) and (7) correspond to the d-form thereof (IEEE, 1987). Both forms are equally valid descriptions and can be converted into each other, but have different application areas. Whereas the e-form is the first choice for finite element analyses because of the straight forward substitution into Navier's equation, the d-form is mostly established in controls because its parameters are easier to measure.

In contrast to the thermodynamically motivated approaches, the irreversible polarization shall be computed from the history of the driving electric field $\vec{E}$ by a hysteresis operator $\mathcal{H}$. Two possible realizations of this operator will be discussed in the section 'Hysteresis Models'. For now $\vec{P}^i$ is generally defined as

$$\vec{P}^i = \mathcal{H}[\vec{E}] \vec{e}_P \quad (8)$$

with the unit vector of the polarization $\vec{e}_P$ set equal to the direction of the applied electric field. This simplification can be made for uni-axial loaded – especially prepoled thickness and longitudinal mode – actuators. A more general approach would need to consider the load history for the direction of the polarization $\vec{e}_P$, as suggested in some micromechanical and thermodynamic consistent constitutive models.

The butterfly curve for the mechanical strain cannot easily be modeled with a simple hysteresis operator. Nevertheless, as it can be seen in Figure 2, the mechanical strain S_{33} seems to be proportional to the squared dielectric polarization P_3^2 ($S \propto P^2$). The relation $S^i = \beta \cdot (\mathcal{H}[\vec{E}])^2$, with a model parameter β , seems obvious. However, to keep the model more general, the setup

$$S^i = \beta_1 \cdot \mathcal{H}[\vec{E}] + \beta_2 \cdot (\mathcal{H}[\vec{E}])^2 + \dots + \beta_n \cdot (\mathcal{H}[\vec{E}])^n \quad (9)$$

Figure 2. Measured mechanical strain and squared dielectric polarization on a piezoceramic actuator on different axes.

is chosen. Here the influence of the mechanical load on the irreversible strain is neglected (see also the discussion section and conclusion). Using the volume preserving properties of the domain switching process, the symmetric tensor of the irreversible strain S^i can be defined from Equation (9) (see also Kamlah and Tsakmakis, 1999)

$$S^i = \frac{3}{2} \left(\beta_1 \cdot \mathcal{H}[\vec{E}] + \beta_2 \cdot (\mathcal{H}[\vec{E}])^2 + \dots + \beta_n \cdot (\mathcal{H}[\vec{E}])^n \right) \left(\vec{e}_P \vec{e}_P^T - \frac{1}{3} \mathbf{I} \right). \quad (10)$$

The parameters $\beta_1 \dots \beta_n$ need to be fitted to measured data (see section 'Parameter Identification'). In practice, a fourth degree polynomial has been sufficient.

Furthermore, the entries of the tensor of the piezoelectric moduli are now assumed to be a function of the irreversible dielectric polarization. Here the underlying idea is that the piezoelectric properties of the material only appear once the material is poled. Without any polarization the domains in the material are not aligned and, therefore, coupling between the electrical side and the mechanical side does not occur. If the polarization is increased, the coupling increases too. Hence, the following relations are defined

$$e(\vec{P}^i) = \frac{P_P^i}{P_s} \cdot e \quad (11)$$

$$d(\vec{P}^i) = \frac{P_P^i}{P_s} \cdot d. \quad (12)$$

Herein, P_P^i stands for the element in polarization direction of the vector $\vec{P}^i$ (in many cases $P_P^i = P_3^i$), P_s for the saturation polarization, e and d for the tensors of the constant piezoelectric moduli, and $e(\vec{P}^i)$ and $d(\vec{P}^i)$ for the tensors of the variable piezoelectric moduli. Equations (11) and (12) imply a uni-axial electric loading along the fixed polarization axis (usually the 3-direction) which is a normal working condition for many actuator applications.

Finally, the following system of coupled equations using the e-form can be established

$$\vec{D} = e(\vec{P}^i) \vec{S}^r + \varepsilon^S \vec{E} + \mathcal{H}[\vec{E}] \vec{e}_P \quad (13)$$

$$\vec{S} = \vec{S}^r + \vec{S}^i \quad (14)$$

$$\vec{T} = c^E \vec{S}^r - e'(\vec{P}^i) \vec{E}. \quad (15)$$

Analogously, the system of coupled equations using the d-form is established as

$$\vec{D} = d(\vec{P}^i) \vec{T} + \varepsilon^T \vec{E} + \mathcal{H}[\vec{E}] \vec{e}_P \quad (16)$$

$$\vec{S} = s^E \vec{T} + d'(\vec{P}^i) \vec{E} + \vec{S}^i. \quad (17)$$

In Equations (14) and (17), $\vec{S}^i$ denotes the six-component vector of the irreversible strain in Voigt notation corresponding to the strain tensor $\mathbf{S}^i$ from Equation (10).

HYSTERESIS MODELS

This section briefly describes two possible realizations of the hysteresis operator $\mathcal{H}[\circ]$. The two hysteresis models to be discussed here are the Jiles-Atherton hysteresis model and the Preisach model. Hereby, only the scalar forms of the models are considered. A comparison of the two with respect to finite element modeling of piezoelectric actuators can be found in Hegewald et al. (2005).

JILES-ATHERTON MODEL

The Jiles-Atherton hysteresis model was developed by Jiles and Atherton (1984) for modeling ferromagnetic hysteresis. Smith and Hom (1999) used an analogous theory for ferroelectric materials considering domain wall movement and bending. Due to the underlying physics, the original models use the notation M (magnetization) or P (polarization), respectively. To better represent a general hysteresis operator, the notation is switched to H (hysteresis). The model starts with the weighted superposition of an anhysteretic part H_{an} and a hysteretic (or irreversible) part H_{irr} . The value of the hysteresis operator $\mathcal{H}[\circ]$ can then be expressed as

$$\mathcal{H}[E](t) = cH_{an}(t) + (1 - c)H_{irr}(t). \quad (18)$$

Both internal variables, $H_{an}(t)$ and $H_{irr}(t)$, and the input quantity $E(t)$, are functions of time.

Domain interactions define the general shape of the curve. The anhysteretic part $H_{an}(t)$ is defined by the electric field strength $E(t)$ and the saturation quantity H_s as¹

$$H_{an}(t) = H_s \left[\coth \left(\frac{E(t) + \alpha H_{irr}(t)}{a} \right) - \frac{a}{E(t) + \alpha H_{irr}(t)} \right]. \quad (19)$$

Here it is assumed that the material is originally isotropic and the dipole orientation can be in any direction (Langevin model) Smith and Hom (1999).

Finally, by considering domain wall dynamics, hysteresis is incorporated in the model with the irreversible part $H_{irr}(t)$ defined implicitly through

$$\frac{dH_{irr}}{dt}(t) = \frac{dE}{dt}(t) \cdot \frac{\tilde{\delta}(H_{an}(t) - H_{irr}(t))}{k\delta - \alpha(H_{an}(t) - H_{irr}(t))}. \quad (20)$$

The operator $\delta = \text{sign}(dE/dt)$ incorporates the changing direction of the electric field. Another operator, $\tilde{\delta}$, prevents the physically not justified increase in $\mathcal{H}$, just after the applied electric field switched changing direction, with the definition

$$\tilde{\delta} = \begin{cases} 1, & \text{for } (dE > 0 \text{ and } \mathcal{H} < H_{an}) \text{ or } (dE < 0 \text{ and } \mathcal{H} > H_{an}) \\ 0, & \text{else} \end{cases}. \quad (21)$$

The variables c , a , α , and k are parameters for the Jiles-Atherton model and need to be identified for a certain material. Solving this set of nonlinear algebraic and ordinary differential equations for each time step of the simulation results in the hysteresis $\mathcal{H}$, dependent on the input electric field $E(t)$ and the initial conditions.

The main advantage of the Jiles-Atherton model is that only five model parameters (c , a , α , k , and H_s) need to be identified. Furthermore, due to the contained differential equation, different initial conditions, i.e. prepolarizations, can be considered. A major drawback of the simple Jiles-Atherton model is the disability to follow minor loops in the hysteresis curve (Hegewald et al., 2005).

PREISACH HYSTERESIS MODEL

Preisach developed this hysteresis model for ferromagnetic materials in the early 1930s (Preisach, 1935). The Preisach model uses an infinite number of relay operators $\gamma(\alpha, \beta)$ with up and down switching thresholds α, β , which are combined with weight functions $\wp(\alpha, \beta)$ and then integrated over all values of α and β within the definition range $S = \{(\alpha, \beta) \in \mathbb{R}^2 | \alpha \geq \beta\}$ (the Preisach plane)

$$\mathcal{H}[\circ] = \int_S \wp(\alpha, \beta) \gamma(\alpha, \beta) d\alpha d\beta \quad (22)$$

to obtain a smooth hysteresis curve. As detailed in the literature (Mayergoyz, 2003), the hysteresis can also be computed from a set of extremal values e_m by a simple summation

$$\mathcal{H}[E] = \mathcal{E}(-e_1, e_1) + 2 \sum_{i=1}^{m-1} \mathcal{E}(e_i, e_{i+1}) \quad (23)$$

with the Everett function $\mathcal{E}(e_1, e_2)$ defined on the Preisach plane as

$$\mathcal{E}(e_1, e_2) = \text{sign}(e_2 - e_1) \int_{T(e_1, e_2)} \wp(\alpha, \beta) d\alpha d\beta \quad (24)$$

¹For the numerical evaluation, the Langevin function $\coth z - 1/z$ is replaced with the first element of the series expansion $z/3$ for values $z < 0.1$.

Figure 3. Measurement setup.

with $T(e_1, e_2) = \{(\alpha, \beta) \in \mathbb{R}^2 \mid \min\{e_1, e_2\} \leq \beta \leq \alpha \leq \max\{e_1, e_2\}\}$. It is interesting to note that the hysteresis can be calculated from a finite set of dominant extreme input values $e_1 \dots e_m$ by a simple summation. This set, $e_1 \dots e_m$, is determined from the input $E(t)$ according to certain deletion rules (Mayergoyz, 2003). The deletion rules ensure that only the dominant extrema remain stored, making the model very attractive for numerical implementation, particularly within the finite element method.

Compared to the Jiles-Atherton model, the Preisach model requires more effort to fit the hysteresis loop to measured data. In particular the identification of the weight functions $\varphi(\alpha, \beta)$ is relatively complex. Section 'Parameter Identification' describes the method we use for this purpose. The advantage of the Preisach model is its ability to follow minor loops within the main hysteresis loop. This makes the Preisach model our first choice for simulating piezoceramic actuator behavior within the actuator working range.

Measurement Setup

The necessary measurements were performed with a fairly simple setup (Figure 3). The setup includes a signal generator and a power amplifier to generate the necessary input voltage. The electric current $I(t)$ to the actuator and the voltage $U(t)$ at the actuator electrodes were recorded for each input signal sequence. The mechanical displacement $x(t)$ was observed by a laser vibrometer and recorded as well. Depending on the actuator type, the actuator was mechanically preloaded, but not clamped. Hence, constant stress conditions can be assumed. Although we used stack actuators for our tests here, the setup is not restricted to these actuator types. Measurements on bulk material actuators are also possible. However, the measurements taken for either type of actuator cannot be generalized for the other type made of the same ceramic material since the different manufacturing process and the distinct system design change the parameters significantly. Hence, the measurements should be performed for every actuator system to be analyzed.

A typical driving scheme for the identification procedure is shown in Figure 4. As described in the literature (Mayergoyz, 2003), a triangular waveform

Figure 4. Entire driving sequence: input electric field strength over time.

with increasing amplitude has been advantageous for the identification of the Preisach weight functions. We added an extra triangle with maximum amplitude at the beginning of the driving cycle to guarantee the same initial polarization for every measurement. A short pause between each voltage triangle ensures that the transient creep phenomena are completed before a new triangle starts.

Using the geometrical properties of the actuator, stress $T_{33 \text{ meas}}(t)$ (usually constant), strain $S_{33 \text{ meas}}(t)$, and electric field strength $E_{3 \text{ meas}}(t)$ could be computed from the measured quantities. The dielectric displacement $D_{3 \text{ meas}}(t)$ was obtained by a numerical integration of the measured current. Here, in the case of the stack actuator, the number of layers was also taken into account.

As Figure 4 shows, measurements on piezoelectric stack actuators were typically only performed with positive input voltages. That means instead of a full polarization hysteresis loop, only a small area in the electric field – polarization plane is covered. An analogous observation can be made for the electric field – strain plane. Figure 5 depicts the small areas, also known as actuator working range, within the complete hysteresis and butterfly curves. Since the primary goal of this work here is to model piezoceramic actuators under typical working conditions, most of the analyses here are restricted to the positive input voltage range. To account for the fact that the polarization does not return to zero for a zero electric field (remanent polarization), which cannot directly be detected through the current measurements, the remanent polarization P_{rem} is added to the integral $D_{3 \text{ meas}}(t) = P_{\text{rem}} + \int I(t)dt$ for unipolar measurements (Figure 5a).

For the analysis of the full polarization cycle, the excitation scheme looks similar to Figure 4, except the minimum field strength is reduced from $E_{3 \text{ min}} = 0$ to $E_{3 \text{ min}} = -E_{3 \text{ max}}$. A symmetric excitation scheme is also possible.

Figure 5. The actuator working range compared to the complete cycle: (a) dielectric polarization, and (b) mechanical strain measured on a piezoceramic actuator for unipolar and bipolar input voltages.

Parameter Identification

To obtain the necessary parameters for the model, an identification procedure was developed. An initial guess for the irreversible polarization P_3^i is obtained from Equation (16) with the known linear material parameters d_{33} and ε_{33}^T

$$P_3^i(t) = D_3 \text{ meas}(t) - d_{33} T_{33}(t) - \varepsilon_{33}^T E_3(t). \quad (25)$$

A simple iterative scheme determines the parameter $d_{33}(\vec{P}^i)$ and the final values of $P_3^i(t)$ for each point in time

$$d_{33}(\vec{P}^i) = \frac{P_3^i(t)}{P_s} d_{33} \quad (26)$$

$$P_3^i(t) = D_3 \text{ meas}(t) - d_{33}(\vec{P}^i) T_{33}(t) - \varepsilon_{33}^T E_3(t). \quad (27)$$

The rearrangement of Equation (7) inserted in (3) gives the irreversible strain

$$S_{33}^i(t) = S_{33} \text{ meas}(t) - s_{33}^E T_{33}(t) - d_{33}(\vec{P}^i) E_3(t). \quad (28)$$

Therewith, the polynomial coefficients β_i ($i = 1 \dots 4$) for the irreversible strain are calculated using a linear regression least squares algorithm

$$\beta_1 \cdot P_3^i(t) + \dots + \beta_4 \cdot (P_3^i(t))^4 = S_{33}^i(t). \quad (29)$$

Finally, the parameters of the hysteresis operator $\mathcal{H}[E_3(t)]$ are fitted to the measured data

$$\mathcal{H}[E_3(t)] = P_3^i(t). \quad (30)$$

Figure 6. Differential susceptibilities χ on the hysteresis vs. electric field plane.

The fitting procedure itself depends on the hysteresis operator (Preisach or Jiles-Atherton) and is explained in detail in the following subsections.

JILES-ATHERTON PARAMETER FIT

This section briefly describes the procedure used to fit the five parameters of the Jiles-Atherton hysteresis operator to measured data. The procedure follows the approach presented by Smith and Ounaies (1999) very closely.

The differential susceptibilities $\chi = \frac{dH}{dE}$ at certain loop points are important for the determination of model parameters from experimental data (Figure 6).

Due to their interdependence, the five parameters cannot be computed directly from measured data. Only an iterative calculation scheme leads to results. Start-up values are defined as

- (1) $k = E_c$
 - (2) $c = \frac{\chi_m^-}{\chi_m^+}$
 - (3) $a = \frac{H_s}{3\chi_{an}}$
 - (4) α solve implicit equation for α
- $$H_r = H_{an}(H_r) + \frac{k}{\alpha + ((1+c)\chi_r - c(dH_{an}(H_r)/dE))^{-1}}$$
- with $H_{an}(H_r) = H_s \left(\coth \frac{\alpha H_r}{a} - \frac{a}{\alpha H_r} \right)$.

H_s , the saturation hysteresis, which corresponds to the saturation polarization P_s for ferroelectric materials, needs to be chosen carefully. Ideally, the value for $P_s (= H_s)$ is reported by the manufacturer of the material. In practice, an ‘educated guess’ is often necessary. Furthermore, the anhysteretic susceptibility χ_{an} , as well as the initial susceptibility χ_{in} , are not usually available from measurements. Therefore, the approximations from Smith and Ounaies (1999) are used.

The four parameters, a , α , c , and k are combined into $q = [a, \alpha, c, k]$. Finally, the algorithm for the determination of the parameters finishes with a simultaneous minimization

$$\min_{[a, \alpha, c, k]_{H_s}} (F_a(q)^2 + F_\alpha(q)^2 + F_c(q)^2 + F_k(q)^2) \quad (31)$$

of the four functions specified by the equations

$$\begin{aligned} F_a(q) &= H_m - H_s \left(\coth \frac{E_m + \alpha H_m}{a} - \frac{a}{E_m + \alpha H_r} \right) \\ &\quad - \frac{\chi_m^+ k}{1 - a - \chi_m^+} \\ F_\alpha(q) &= H_r - H_s \left(\coth \frac{\alpha H_r}{a} - \frac{a}{\alpha H_r} \right) \\ &\quad - \frac{k}{\alpha + \left((1+c)\chi_r - c \frac{dH_{an}(H_r)}{dE} \right)^{-1}} \\ F_c(q) &= \frac{c}{c+1} \frac{H_s}{3a} - \chi_{in} \\ F_k(q) &= H_s \left(\coth \frac{E_c}{a} - \frac{a}{E_c} \right) \\ &\quad \times \left(\alpha + \left((1+c)\chi_c - c \frac{dH_{an}(H_c)}{dE} \right)^{-1} \right) - k. \end{aligned}$$

The fifth parameter, H_s , is usually not known exactly *a priori*. Therefore, the simultaneous minimization is repeated for slightly varied values of H_s . At the end, the parameter tuple leading to the best results is selected for the Jiles-Atherton operator.

Even further improvement of the behavior can be achieved through a least squares fit of the operator’s output to measured data.

PREISACH PARAMETER FIT

This section briefly describes the method to identify the Preisach weight functions $\wp(\alpha, \beta)$. Once the input E and the output P of the Preisach operator $\mathcal{H}$ are directly available, the problem of identifying the weight function $\wp$ amounts to a linear integral equation of the first kind

$$\int_S \wp(\alpha, \beta) \gamma(\alpha, \beta) [E](t) d\alpha d\beta = P^i(t) \quad t \in [0, \bar{t}]. \quad (32)$$

Note, in contrast to standard integral equations, the dimensions of the integration domains in the preimage and in the image space differ.

Using a discretization of the Preisach operator as a linear combination of elementary hysteresis operators $\mathcal{H}_\lambda$

$$\mathcal{H} = \sum_{\lambda \in \Lambda} a_\lambda \mathcal{H}_\lambda \quad (33)$$

and evaluating the output at n_T discrete time instances $0 \leq t_1 < t_2 < \dots < t_{n_T} \leq \bar{t}$, we approximate the solution of (32) by solving a linear least squares problem for the coefficients $\mathbf{a} = (a_\lambda)_{\lambda \in \Lambda}$

$$\min_{\mathbf{a}} \sum_{i=1}^{n_T} \left(\sum_{\lambda \in \Lambda} a_\lambda \mathcal{H}_\lambda [E](t_i) - P^i(t_i) \right)^2. \quad (34)$$

In (33), $\mathcal{H}_\lambda$ may be chosen as simple relays,

$$\mathcal{H}_\lambda = \gamma(\alpha_i, \beta_j)$$

with $(\alpha_j, \beta_i) \in, i = 1, \dots, n_\alpha, j = 1, \dots, n_\beta$, which corresponds to a piecewise constant approximation of the weight function. In that case, the set Λ obviously consists of index pairs $\lambda = (i, j)$ corresponding to different up- and down-switching thresholds α_i, β_j , and the array λ is supposed to be reordered in a column vector to yield a reformulation of (34) in standard matrix form. Possible smoother basis functions for the discretization of $\wp$ lead to smoothly shaped elementary hysteresis operators $\mathcal{H}_\lambda$ in place of $\gamma(\alpha_i, \beta_j)$.

Since the data E, P^i are given only on a one-dimensional time interval $[0, \bar{t}]$ and the sought function $\wp$ depends on two variables, it cannot be expected to be uniquely determined. However, using an incremental triangle excitation as input (Figure 10), one can make use of the deletion rules defining the Preisach memory to conclude identifiability along certain lines in the Preisach plane S . By refining the incremental triangle excitation in such a way that its peaks form a larger subset of possible

Figure 7. Results of the Jiles-Atherton fitting algorithm compared to the measurements of the complete bipolar driving cycle: (a) dielectric polarization and (b) mechanical strain.

Figure 8. Results of the Preisach fitting algorithm compared to the measurements within the actuator working range: (a) dielectric polarization and (b) mechanical strain.

threshold values (α, β) for the elementary relays $\gamma(\alpha, \beta)$, the set of identified weight function values $\wp(\alpha, \beta)$ can be enlarged. For more details, we refer to Hoffmann et al. (1988), Kaltenbacher and Kaltenbacher (2005), and especially to Hoffmann and Meyer (1989) for a convergence analysis of the least squares approach described above.

RESULTS

This section presents some of the results obtained with the model. Firstly, results of the parameter identification procedure (section ‘Parameter Identification’) are shown. Secondly, the model is exposed to different driving cycles and the obtained output is compared to measured data.

Fitting Results

Figure 7 shows the results of the fitting procedure for the model with the Jiles-Atherton operator compared to measured data of the full bipolar polarization cycle. The parameters for the Jiles-Atherton hysteresis operator were obtained using the procedure from section ‘Jiles-Atherton Parameter Fit’ including the refinement through a least squares algorithm. Table 1 lists the model parameters for this set of measured data.

The model fit to measured data in the actuator working range is shown in Figure 8. Here, the Preisach operator was employed for modeling the hysteresis, since the Jiles-Atherton operator does not perform well for unipolar input signals with varying amplitude. The Preisach operator, however, is able to follow the so-called first order return curves and minor loops in the

Table 1. Parameters of the model using the Jiles-Atherton hysteresis operator.

Polynomial coefficients			Jiles-Atherton operator parameters		
β_1	5.35×10^{-5}	m^2/C	a	1.57×10^6	C/m^2
β_2	2.25×10^{-2}	m^4/C^2	α	9.96×10^6	Vm/C
β_3	1.50×10^{-3}	m^6/C^3	k	1.17×10^6	V/m
β_4	8.41×10^{-2}	m^8/C^4	c	0.774	
			P_s	0.49	C/m^2

Table 2. Parameters of the model using the Preisach hysteresis operator.

Polynomial coefficients		Preisach operator parameters	
β_1		1.72×10^{-2}	m^2/C
β_2		4.48×10^{-2}	m^4/C^2
β_3		3.62×10^{-1}	m^6/C^3
β_4		-5.6×10^{-0}	m^8/C^4

hysteresis curve in great detail. Table 2 specifies the parameters obtained with the procedure from section ‘Parameter Identification’. The Preisach weight functions $\wp(\alpha, \beta)$, determined according to ‘Preisach Parameters Fit’, are shown in Figure 9 as grey values in the upper left triangle of the α - β plane (or Preisach plane).² Due to the limited number of triangles in the input sequence and the unipolar magnitude, only few weight functions are allocated with influential values.

Simulation Results

Whereas figures in the previous section only show how well our model can be adapted to fit a certain set of measured data, this section will give some results showing how well the model will predict the behavior of piezoelectric actuators for altered driving schemes. Due to our main goal to model piezoceramic actuators under normal operating conditions, and due to the poor performance of the Jiles-Atherton hysteresis operator for unipolar input signals, we concentrate in this section on the model with the Preisach hysteresis operator.

Firstly, an input scheme according to Figure 10 is applied. Figure 11 presents a selection of the simulated response of the model with the Preisach hysteresis operator compared to measured data for the same input signal. To underline the necessity of the hysteresis simulation, the results of a linear simulation with typical linear material parameters are also included in the figure.

The simulated strain plotted versus time is compared to measured data and linear simulation results for one period of the input signal in Figure 12. Shortcomings of the linear simulation are clearly visible. The amplitude, and particularly, the shape of the linear simulation strain

Figure 9. Identified Preisach weight functions $\wp(\alpha, \beta)$ in the α - β plane (Preisach plane) for $M = 35$. Values of $\wp(\alpha, \beta)$ are gray coded as shown by the gray value bar on the right. **Figure 10.** Input scheme of the electric field for the comparison of measurement and simulation.

results do not match the measured curves, whereas the nonlinear simulation reflects the measurement well.

Figure 13 shows the strain output of the model with the same parameters as above for a sinusoidal input signal. Although not as significant as for the triangular input signal, the improvement of the simulated strain through the nonlinear simulation with hysteresis can be observed.

DISCUSSION AND CONCLUSION

The need for a nonlinear simulation model for ferroelectric materials is indisputable. The model presented here combines the ability to efficiently simulate the dielectric polarization and the mechanical strain at the same time.

Based on the physically motivated decomposition of the mechanical strain and the dielectric displacement into

² M , the size of the α - β plane, defines the number n of Preisach weight functions $\wp(\alpha, \beta)$ according to $n = M(M + 1)0.5$.

Figure 11. Simulation of the model response using the Preisach hysteresis operator compared to the linear simulation and to measurements: (a) dielectric polarization and (b) mechanical strain.

Figure 12. Simulated strain for a triangular input signal, using the Preisach hysteresis operator in the model, compared to the linear simulation and to measurements.

Figure 13. Simulated strain for a sinusoidal input signal, using the Preisach hysteresis operator, compared to the linear simulation and to measurements.

reversible and irreversible components, the model incorporates the well-known linear piezoelectric equations and a phenomenological approach for modeling the nonlinear hysteresis with mathematical hysteresis operators. In this work, we have shown two possible realizations, the Jiles-Atherton hysteresis operator and the Preisach hysteresis operator. Whereas the Jiles-Atherton operator is distinguished by its small number of parameters (five) and therefore simpler parameter identification procedure, the Preisach operator is characterized by its high flexibility. Usage of the Jiles-Atherton operator quickly leads to satisfactory behavior of the model for a bipolar large signal driving scheme (full polarization cycle). The complete polarization hysteresis curve and the strain butterfly curve are reproduced by the model very successfully.

However, if a unipolar driving signal is used, which corresponds to normal working conditions for piezoceramic actuators, the Jiles-Atherton operator performs poorly. In those cases the Preisach operator needs to be employed. Due to the larger number of parameters the fitting procedure is more complex and time-consuming.

Nevertheless, the effort pays off, since the model with the Preisach operator performs excellently in the actuator working range for all levels of input signals. In our experience, the larger the number n of weight functions $\wp(\alpha, \beta)$ (and therefore relay operators $\gamma(\alpha, \beta)$) in the hysteresis operator, the better the model output can be fitted to measured data. For our data, a Preisach plane size of $M = 30 \dots 40$, resulting in $n = 465 \dots 820$, has been sufficient. Enlarging the α - β plane any further did not result in any visible improvement of the model output but only in significantly increased calculation times for the identification routine.

Despite the satisfying results, we realize some shortcomings of our current model. Firstly, the model is rate independent. Several publications (e.g., Kuhnén, 2001; Reiländer, 2003) point out that the behavior of ferroelectric ceramics has a rate dependency, mostly displayed by the creep effects which can be observed in Figure 12 as a small drift in the measured strain when the input signal is back to zero. The simulation also predicts this behavior for the used set of data (due to similar behavior in the training data). However, in

contrast to the measurements, the effect in the simulation is rate independent. A driving signal with a different frequency would reveal the problem. The necessary rate dependence could be included through a creep operator in combination with the hysteresis operator. It is also possible to ignore the rate dependence for applications with nearly constant driving frequencies. Then, the measurements for the parameter identification need to be performed in exactly that frequency range.

Secondly, the direction of the polarization is pre-defined in the model. Equations (8), (11), and (12) define the direction of the polarization and of the piezoelectric effect to coincide with the direction of the electric field. This is, in our opinion, a valid simplification for many applications encountered (thickness extensional and longitudinal length mode transducers). The shown full hysteresis and butterfly curves for bipolar input (Figure 7) has to be understood in that context. For the modeling of the full load history dependence, including a change in direction of the polarization, considerably more effort is needed (as demonstrated by the constitutive models of Kamlah and Böhle (2001) and Landis et al. (2004)).

Thirdly, the model presented here does not account for strongly varying stress conditions. Increased stress usually leads to compressed polarization and strain curves (Zhou, 2003; Pertsch, 2003). In the extreme case, high compressive stresses in the direction of the polarization can completely depolarize the material, resulting in the loss of the piezoelectric properties of the ceramic. We can neglect this case for our actuator model, since this is not a desirable operating condition for actuators. Moreover, the intended use of the model is restricted to actuator applications where the relative change of stress compared to the pre-stress of the piezoceramic actuator is very small. In that case, the stress independent irreversible polarization and strain formulation is justified. Doubtlessly, applications where these conditions do not hold will require more advanced models which incorporate the stress dependence of the irreversible polarization and strain (e.g., Kamlah and Böhle (2001) or Landis et al. (2004)).

In conclusion, the model presented here predicts the response of a piezoceramic actuator with an *a priori* known poling direction and nearly constant stress conditions for different driving schemes satisfactorily. In our opinion, the combination of the physically motivated decomposition of strain and polarization with the mathematical hysteresis operator entails an efficient model for ferroelectric devices while maintaining a very realistic model output. Therefore, the model adequately facilitates simulation of ferroelectric behavior, and promises to be a valuable tool for designing complex structures containing piezoceramic actuators.

Currently we are implementing the proposed model in our FE software in order to perform simulations of complex structures containing piezoceramic actuators. In addition, we plan to extend the scalar Preisach hysteresis model to be vector valued, to fully take any rotation of the polarization into account. Results hereof will be shown in a following publication.

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