ECCOMAS MSF 2019

4th International Conference on Multi-scale Computational Methods for Solids and Fluids

PROCEEDINGS

September 18-20, 2019
Sarajevo, Bosnia and Herzegovina

Editors:
A. Ibrahimbegovic, S. Dolarević, E. Džaferović,
M. Hrasnica, I. Bjelonja, M. Zlatar, K. Hanjalić

Organized by:

Faculty of Civil Engineering, University of Sarajevo,
Faculty of Mechanical Engineering, University of Sarajevo,
University of Technology of Compiègne, Alliance Sorbonne University, Paris

Supported by:

Academy of Sciences and Arts of Bosnia and Herzegovina, ANU BIH

Editors:

Adnan Ibrahimbegovic, Samir Dolarević, Ejub Džaferović,
Mustafa Hrasnica, Izet Bjelonja, Muhamed Zlatar, Kemal Hanjalić

Publisher: Faculty of Civil Engineering, University of Sarajevo,
Patriotske lige 30, 71000 Sarajevo, Bosnia and Herzegovina

Printed by: Štamparija Fojnica d.o.o.

Number of printed copies: 160

Date: September, 2019

ISBN: 978-9958-638-57-2

CIP - Katalogizacija u publikaciji
Nacionalna i univerzitetska biblioteka
Bosne i Hercegovine, Sarajevo

624:004(063)(082)

INTERNATIONAL Conference on Multi-scale Computational Methods for Solids and Fluids (4 ; 2019 ; Sarajevo)
Proceedings / 4th International Conference on Multi-scale Computational Methods for Solids and Fluids, Sarajevo, September 18-20, 2019 ; editors Adnan Ibrahimbegovic ... [et al.]. - Sarajevo : Faculty of Civil Engineering = Građevinski fakultet, 2019. - 417 str. : ilustr. ; 30 cm

Bibliografija uz svaki rad. - Registar.

ISBN 978-9958-638-57-2

COBISS.BH-ID 27453702

NUMERICAL IMPLEMENTATION OF DEBYE MEMORY FOR PIEZOELECTRIC MATERIALS

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1. Introduction

Piezoelectric materials are used in a wide range of applications such as sensors/actuators in civil and aeronautic engineering, medical devices, energy harvesters, and many other operations. In the last decades, there exist a tendency to miniaturize electro-mechanic devices, for instance for the Micro-Electro-Mechanics (MEMs) technology. These materials are characterized by a set of two coupled constitutive equations including mechanical, electrical variables and also thermal. The continuous reduction of scale in many applications results in the significance of second-order effects such as the *Debye* memory, that can be understood as an electric viscosity-like interaction due to the momentary delay in the spontaneous orientation of the electric dipoles. The classical constitutive equations must then be enriched with time-dependent electrical variables and with an additional empirical relaxation time to take into account the delay.

The main aim of the present work is to develop a numerical formulation based on the Finite Element Method (FEM) to study the no-linear piezoelectric behavior with *Debye* memory. Despite the fact that small strains and rotations are assumed, the complexity of the present work emerges from: i) non-linearities due to the *Maxwell* stress tensor, which quadratically depends on the electric field [1], and ii) time-dependent constitutive equations due to this *Debye* memory.

To undertake these objectives, a thermodynamical formulation based on the Extended Non-Equilibrium Thermodynamic [1], [2] is conducted to obtain a set of two time-dependent constitutive equations. Numerically, the non-linearities are solved by the *Newton-Raphson* algorithm and the time integration by the *Newmark*–β technique; as a new contribution, also by convolution integrals for the time-dependent constitutive equations, as typically done in the classical theory of visco-elasticity for uncoupled materials.

Finally, the numerical formulation is implemented in the research FEM code `FEAP` [3] and several tests are executed to validate this implementation and to extract conclusions on the importance of the *Debye* effect on the piezoelectric response.

2. Outline of governing equations

The piezoelectric governing equations are composed of linear and angular momentum balances, *Gauss* law, constitutive equations and boundary conditions. The first is stated by:

$$\rho_m \, \ddot{u} = \nabla \cdot (T + T^M) + \mathbf{f}. \tag{1}$$

where u, T, T^M and $\mathbf{f}$ denote displacement field, *Cauchy* stress tensor, *Maxwell* tensor and body force vector, respectively. The symbols $(\cdot)$ and $(\ddot{\,})$ represent inner product and double time derivative. According to [1], T^M is symmetric and given by:

$$T^M = \frac{1}{2}\Big(D \otimes E + E \otimes D - \varepsilon_0 E \cdot E\, I\Big), \tag{2}$$

where D, E and ε_0 denote electric displacement, electric field and vacuum permitivity, respectively. Furthermore, I is the identity second order tensor and $(\otimes)$ the outer product. Assuming that T^M is symmetric, the angular momentum balance is automatically stated since:

$$T + T^M = (T + T^M)^\top, \tag{3}$$

where $(\ )^\top$ denotes transposition.

The electric *Gauss* law states the electric field equilibrium, in the absence of free electric charge this equation is extracted from the *Maxwell* laws:

$$\nabla \cdot D = 0. \tag{4}$$

In addition, assuming small strain and rotations, with S the small strain tensor, the compatibility equations are given by:

$$S = \frac{1}{2}\left(\nabla \otimes u + u \otimes \nabla\right)\ ; \qquad E = -\nabla V, \tag{5}$$

Classically, the piezoelectric constitutive equations are a set of two coupled relationships that relate electric and mechanical fields:

$$\begin{aligned} T &= \mathbf{C} : S - (e^V)^\top \cdot E, \\ D &= e^V : S + \varepsilon \cdot E, \end{aligned} \tag{6}$$

where $\mathbf{C}$, e^V and ε denote elastic, piezoelectric and permitivity tensors, respectively.

As commented, due to the presence of momentary delay in the spontaneous polarization of the electric dipoles, the *Debye* memory appears. This effect is mathematically represented by rewriting the second equation (6) as:

$$D + \tau_p \dot{D} = e^V : S + \varepsilon \cdot E, \tag{7}$$

where τ_p is the relaxation time, also called equilibration time in Extended Non-equilibrium Thermodynamics terminology and $(\dot{\ })$ first derivative with respect to time.

Finally, the set of governing equations is completed with the boundary conditions:

Dirichlet type	Neumann type	
$u = \bar{u}$	$(T + T^M) \cdot \mathbf{n} = \bar{\mathbf{t}},$	(8)
$V = \bar{V}$	$D \cdot \mathbf{n} = \bar{\mathbf{q}}_\Gamma,$	

where $\bar{u}$, $\bar{V}$, $\bar{\mathbf{t}}$ and $\bar{\mathbf{q}}_\Gamma$ denote prescribed displacements, prescribed voltage, traction vector, and electric charges on the boundary Γ, respectively. The initial conditions for $u(0)$, $\dot{u}(0)$, $D(0)$ are all taken to zero.

3. Finite element formulation

The piezoelectric equations including *Debye* memory are now expressed in a weak form on the volume Ω and boundary:

$$\begin{aligned} \int_\Omega \Big[\delta u \cdot (\mathbf{t} - \rho_m \ddot{u}) - \delta S : T\Big]\, \mathrm{d}\Omega + \oint_\Gamma \delta u \cdot \bar{\mathbf{t}}\, \mathrm{d}\Gamma &= 0, \\ \int_\Omega \Big[(\nabla \delta V) \cdot D\Big]\, \mathrm{d}\Omega - \oint_\Gamma \delta V\, \bar{\mathbf{q}}_\Gamma\, \mathrm{d}\Gamma &= 0. \end{aligned} \tag{9}$$

Standard three-dimensional shape functions of *Lagrangian* type are used to discretize the spacial coordinates and the degrees of freedom: displacements a^u and voltage a^V. In addition, a formulation based on residuals (mechanical $\mathcal{R}^u$ and electrical $\mathcal{R}^V$) is developed since the *Maxwell* stress tensor introduces non-linearities.

Assuming constant coefficients, the time-dependent constitutive (7) is rewritten in convolution integral form:

$$D(t) = \frac{1}{\tau_p} \int_0^t \left[e^v : S(t') + \varepsilon \cdot E(t') \right] \mathrm{e}^{-(t-t')/\tau_p} \, \mathrm{d}t', \tag{10}$$

This Ordinary Deferential Equation has exact solution (see [4]) if the constitutive coefficients are constant, a reasonable hypothesis in the functioning range of the piezoelectric of following section. In the previous equation, the time evolution of the strains $S(t')$ and electric field $E(t')$ can be approximated at each time increment with the finite-difference θ-method and $\theta_1 = \theta_2 = 0.5$ (Crank-Nicholson).

The tangent matrices are calculated and the final system of algebraical equations is given by:

$$\begin{bmatrix} c_1 \mathcal{K}^{uu} + c_3 \mathcal{M}^{uu} & c_1 \mathcal{K}^{uV} \\ c_1 \mathcal{K}^{Vu} & c_1 \mathcal{K}^{VV} \end{bmatrix}^k \begin{Bmatrix} \mathrm{d}a^u \\ \mathrm{d}a^V \end{Bmatrix}^k = \begin{Bmatrix} \mathcal{R}^u \\ \mathcal{R}^V \end{Bmatrix}^k, \tag{11}$$

where $\mathcal{K}$, M denote stiffness and mass matrices, k is the number of iteration of the *Newton-Raphson* algorithm and c_i denote the order of the time derivative. The residuals are directly derived by derivation from the weak forms (9) and the and tangent submatrices from derivations of these residuals with respect to the degrees of freedom.

As commented, this numerical formulation is implemented in an user element of the the research code `FEAP`, [3].

4. Results

Two tests are presented to verify the model and its implementation, in particular, the influence of the relaxation time in the piezoelectric response for two different signals.

The geometry corresponds to a piezoelectric plate 7R-34-23-2500 of dimensions $33.3 \times 22.8 \times 0.8$ [mm] and material properties listed in [4]. This piezoelectric is designed in actuator mode (as in the following examples) but can also be used as a sensor. It is clamped and electrically grounded on its base, while the upper surface is free to vibrate, for which it is connected to an electric source of variable voltage.

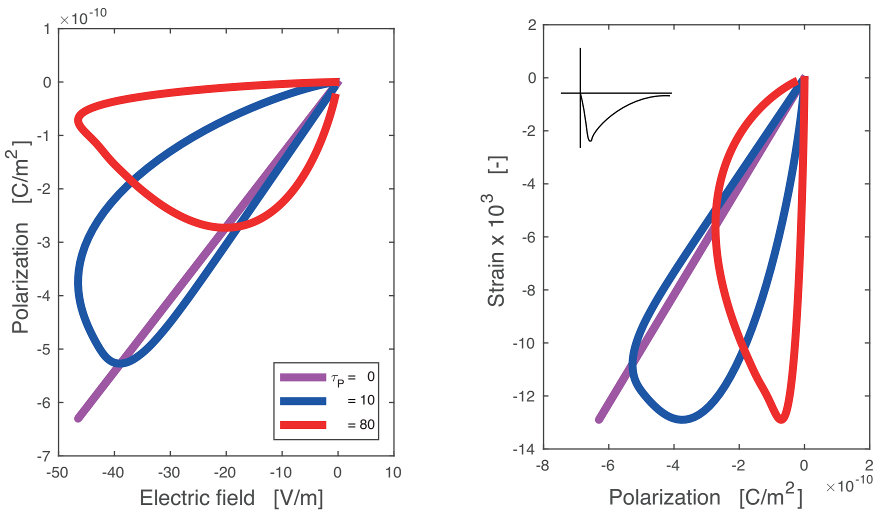

Figure 1: Polarization vs. electric field applied for classical and *Debye* memory models.

Figure 1 left shows the polarization (direct effect) $P = D - \varepsilon_0 E$ (ε_0 is the vacuum permittivity) through the thickness versus an spike with maximum E = -4.7$\times10^5$ [V/m] (cause); this spike is a frequency-dependent function $\exp(-\omega t)$. The distributions are for the classical $\tau_p = 0$ (no dissipation, thermodynamically reversible process) and *Debye* $\tau_p \neq 0$ (medium and high dissipations). As observed, the relaxation time produces a hysteresis-like response that must be considered for fast applications such as ultrasounds. The area of the loop increases with τ_P, which implies that a frequency-dependency appears. Although the values of τ_P have not been directly measured for this material, 10 and 80 have been taken from those of similar ones.

The loops' inclination reduces with the value of τ_P; the explanation can be found in the following equation, used among others for the calculation of the FE tangent matrices. The higher the relaxation time the closer the exponential value to 1 and the derivative of D (proportional to P_z) with respect to the electrical field tends to zero.

$$\frac{\partial D^{n+1}}{\partial \tilde{V}_b^{n+1}} = -\theta_2 \left(1 - \mathrm{e}^{-\Delta t/\tau_P}\right) \varepsilon \, \mathcal{B}_b. \tag{12}$$

In the right figure, the two generated P_z and S_{zz} are related. Both magnitudes are fully coupled through the piezoelectric effect and loops appear, but now due to the product of e^V with the exponential of (10). Because of this loop, a given polarization causes two strain states depending on the time history. This "memory" behavior should be taken into account for the design of actuators, particularly in sophisticated applications that require the monitoring of precise deformations.

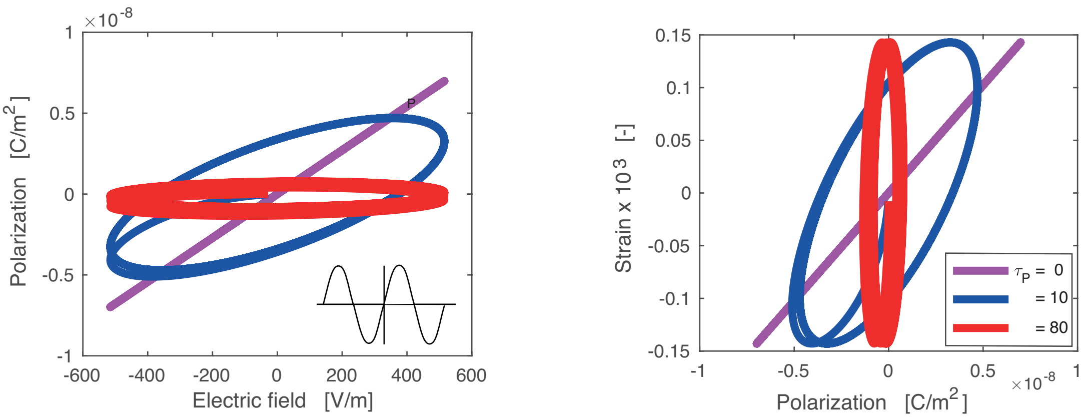

Figure 2: Polarization vs. electric field applied for classical and *Debye* memory models.

The figure 2 plots the same distributions but for a sinusoidal electric signal of $\pm E = 4.5$ [V/m] repeated eight times during approximately 400 [s] (low frequency).

The trends are similar to those of the previous figure, but now it can be observed that when the first sine signal is repeated the paths superimpose themselves, meaning that with this model no energy is dissipated (for instance into heat).

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9 789958 638572

Proceedings:

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