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MODELLING OF THE PIEZO-EFFECT BASED ON THE GROWTH THEORY

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Summary: *The general growth and remodeling theory of DiCarlo is applied on the modeling of piezoelectric effect. This model is verified on the 1D stack comparing the numerical results with the published experimental data. The further possibility of this model to take in account the change of stiffness is outlined.*

1. Introduction

The aim of this contribution is to apply the growth and remodelling theory developed e.g. in DiCarlo & Quiligotti (2002) and further applied for 1D problems in Rosenberg & Hyncik (2007) for the modeling of the piezo-effect. The change of size and form of the piezo-continuum is very similar to the growth of living tissues for which the relevant growth and remodeling theory was developed. In following as an example the behaviour of the 1D piezoelectric stack will be analyzed.

2. Description of the algorithm

This theory of growth and remodeling is deeply introduced in above mentioned papers. Here we use this results to extend it for piezoelectric continuum. Considering the velocity of continuum $\mathbf{v} = \nabla \dot{\mathbf{p}}$ ($\mathbf{p}$ is the placement mapping the initial configuration into the current configuration) and the velocity of growth $\mathbf{V} = \dot{\mathbf{P}}\,\mathbf{P}^{-1}$ ($\mathbf{P}$ is the deformation gradient between the initial and relaxed configuration) and introducing further the Cauchy stress tensor $\boldsymbol{\tau}$, the generalized external remodeling force $\mathbf{C}$, vector of electric flux density $\mathbf{D}$, the electric field vector $\mathbf{E}$, the electric field potential Φ, the generalized virtual working can be expressed as

$$\int_{B_0} \left(-\boldsymbol{\tau} : \nabla \mathbf{v} + \mathbf{b} \cdot \mathbf{v} + \mathbf{z} \cdot \mathbf{v} + \mathbf{C} \cdot \mathbf{V} + \mathbf{B} \cdot \mathbf{V} - \mathbf{D}.\dot{\mathbf{E}} \right) dC + \\ + \int_{\partial B_0} \left(\hat{\tau}\, \mathbf{n} \cdot \mathbf{v} - \hat{\mathbf{D}}.\mathbf{n} \dot{\Phi} \right) dS = 0 \qquad \forall \left(\mathbf{v}, \mathbf{V}, \dot{\Phi} \right) \tag{1}$$

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where $\hat{\boldsymbol{\tau}}\mathbf{n}$ and **D.n** are prescribed stress and electric flux on boundary and **n** is the vector of outer normal. From the principle of objectivity follows $z = \mathbf{0}$, $\boldsymbol{\tau}$ is symmetric, see DiCarlo & Quiligotti (2002). Applying the Green's theorem and further arranging, from (1) the equilibrium and boundary conditions can be obtained in form

$$Div\ \boldsymbol{\tau} + \mathbf{b} = 0 \quad \text{on} \quad B_0\ ,$$

$$\mathbf{B} + \mathbf{C} = \mathbf{0} \quad \text{on} \quad B_0\ ,$$

$$\hat{\boldsymbol{\tau}}\ \mathbf{n} = \boldsymbol{\tau}\ \mathbf{n} \quad \text{on} \quad \partial B_0\ , \tag{2}$$

$$divD = 0 \ \text{on} \quad B_0$$

$$Dn = \hat{D}n \ \text{on} \quad \partial B_0$$

The second law of thermodynamics can be written after some procedure described in Rosenberg & Hyncik (2007) in form

$$\left(\boldsymbol{\tau}_{el} + \boldsymbol{\tau}_{dis} - \frac{\partial \psi}{\partial \mathbf{F}}\right)\dot{\mathbf{F}} + \left(\mathbf{C} + \mathbf{F}\,\boldsymbol{\tau} - \psi\,\mathbf{I}\right)\mathbf{V} + \left(\mathbf{R} - \frac{\partial \psi}{\partial \mathbf{K}}\right)\dot{\mathbf{K}} - \left(D + \frac{\partial \psi}{\partial E}\right)\dot{E} \geq 0 \tag{3}$$

where $\psi(\mathbf{F},\mathbf{E},\mathbf{K}) = \psi_{el}(\mathbf{F},\mathbf{K}) + \psi_{piezo}(\mathbf{F},\mathbf{K},\mathbf{E})$ is the free energy density related to the relaxed volume decomposed into elastic and piezoelectric part. **K** represents the parameters, which can be changing during the material remodelling and on which the material parameters are depending -$\dot{\mathbf{K}}$ is the corresponding velocity. We assume here that the stress $\boldsymbol{\tau}$ can be decomposed into the elastic part $\boldsymbol{\tau}_{el}$ and the dissipative part $\boldsymbol{\tau}_{dis}$. From this inequality we can obtain the constitutive equations

$$\boldsymbol{\tau}_{el} = \frac{\partial \psi}{\partial \mathbf{F}}\ ;\ \boldsymbol{\tau}_{dis} = \mathbf{H}\dot{\mathbf{F}}\ ;\ \mathbf{C} - \psi_{piezo} - \mathbf{E_s} = \mathbf{G}\ \mathbf{V}\ ;\ \ \mathbf{E_s} = \psi_{el}\ \mathbf{I} - \mathbf{F}\,\boldsymbol{\tau}\ ;\ \mathbf{R} - \frac{\partial \psi}{\partial \mathbf{K}} = \mathbf{M}\cdot\dot{\mathbf{K}}\ , \tag{4}$$

$$\mathbf{D} = -\frac{\partial \psi}{\partial \mathbf{E}}$$

where $\mathbf{E}_s$ is the tensor of the Eshelby's type (further shortly Eshelby tensor), **M** ,**H** and **G** are positively definite matrices.

2.1. Example: 1D – piezoelectric continuum

Let the free energy density has the form

$$\psi_{el} = \frac{1}{2}k\left(\frac{l}{l_r}-1\right)^2 ; \psi_{piezo} = -eE\left(\frac{l}{l_r}-1\right)-\frac{1}{2}\kappa E^2 \quad (5)$$

that corresponds to the linear model of piezoelectrical continuum (see e.g. Zemcik et al. (2007)). Here l_0, l_r, l are the lengths of the stack in initial, relaxed and current configuration respectively and k, e, κ the material parameters (k-stiffness, e-piezoelectric coupling coefficient, κ-dielectric permittivity). From the first and last equations in (4) we can obtain the usuall strain-charge form - see e.g. Zemcik et al. (2007).

$$\tau = k\left(\frac{l}{l_r}-1\right)-eE$$

$$D = e\left(\frac{l}{l_r}-1\right)+\kappa E \quad (6)$$

Further we will assume, that the elements of **K** are directly the material parameters k,e and κ.

Putting from (5) into (4) and using the equilibrium equations we can obtain the equations of the following dynamical system describing the behaviour of the piezoelectric stack during time:

a) l is given ("relaxation")

$$m_1\dot{k} = r_1 - \frac{1}{2}\left(\frac{l}{l_r}-1\right)^2 \quad (7)$$

$$m_2\dot{e} = r_2 + E\left(\frac{l}{l_r}-1\right) \quad (8)$$

$$m_3\dot{\kappa} = r_3 + \frac{E^2}{2} \quad (9)$$

$$\dot{l}_r = l_r \frac{\frac{k}{2}l^2 + \left(C - \frac{k}{2} - eE + \frac{1}{2}\kappa E^2\right)l_r^2}{g\,l_r^2 + h\,l^2} \quad (10)$$

where

$$\tau = k\left(\frac{l}{l_r} - 1\right) - eE - h\frac{l}{l_r}\dot{l}_r \tag{11}$$

b) τ **is given ("creep")**

$$m_1\dot{k} = r_1 - \frac{1}{2}\left(\frac{l}{l_r} - 1\right)^2 \tag{12}$$

$$m_2\dot{e} = r_2 + E\left(\frac{l}{l_r} - 1\right) \tag{13}$$

$$m_3\dot{\kappa} = r_3 + \frac{E^2}{2} \tag{14}$$

$$g\,\dot{l}_r = \left[\frac{l}{l_r}\tau - \frac{1}{2}k\left(\frac{l}{l_r} - 1\right)^2 + eE\left(\frac{l}{l_r} - 1\right) + \frac{1}{2}\kappa E^2 + C\right] l_r \tag{15}$$

$$\dot{l} = \frac{l_r}{h}\left\{\tau - k\left(\frac{l}{l_r} - 1\right) + eE + h\frac{l}{gl_r}\left[\frac{l}{l_r}\tau - \frac{1}{2}k\left(\frac{l}{l_r} - 1\right)^2 + eE\left(\frac{l}{l_r} - 1\right) + \frac{1}{2}\kappa E^2 + C\right]\right\} \tag{16}$$

where (16) is obtained from

$$\tau = k\left(\frac{l}{l_r} - 1\right) - eE + h\left(\frac{l}{l_r}\right)^{\bullet} \tag{17}$$

Here $r_i, m_i;\quad i = 1,2,3$ are the components of **R** and **M** and g and h corresponds with **G** and **H**. They can be in general functions of the variables.

We concentrate our attention to the case b) when the external loading is given. The remaining equations can be rearanged into the form

$$\dot{x} = \frac{1}{h}\left[\tau - k(x - 1) + eE\right] \tag{18}$$

$$\dot{k} = \frac{1}{m_1}\left[r_1 - \frac{1}{2}(x-1)^2\right] \tag{19}$$

$$\dot{e} = \frac{1}{m_2}\left[r_2 + E(x-1)\right] \tag{20}$$

where $x = {l}/{l_r}$. Last variable l_r can be obtained from (15) in form

$$\dot{l}_r = \frac{1}{g}\left[x\tau - \frac{1}{2}k(x-1)^2 + eE(x-1) + \kappa E^2 + C\right] l_r$$

resp. (21)

$$(\ln l_r)^{\bullet} = \frac{1}{g}\left[x\tau - \frac{1}{2}k(x-1)^2 + eE(x-1) + \kappa E^2 + C\right]$$

2.1.1. k, e are constant, κ=0

The most simple case we obtain, when we will assume that all the material parameters are constant. Then we can work only with the equations (18) and (21). Equation (18) can be solved analytically

$$x = \frac{1}{k}\left[\tau + eE + k - (\tau + eE)e^{-\frac{k}{h}t}\right] \tag{22}$$

Putting this result into (21) we obtain after integration for $l_r \in (l_0, l_r)$

$$l_r = l_0 \exp\left\{\frac{1}{g}\left[\tau + \frac{(\tau+eE)^2}{2k} + \frac{1}{2}\kappa E^2 + C\right]t + \frac{1}{g}\frac{(\tau+eE)^2 h}{4k^2}\left(e^{-\frac{2k}{h}t} - 1\right)\right\} \tag{23}$$

The limit values for $t \to \infty$ are

$$x_e = 1 + \frac{\tau + eE}{k}$$

$$l_{re} = l_0 e^{\frac{(\tau+eE)^2 h}{4gk^2}} \tag{24}$$

$$l_e = l_0\left(\frac{\tau + eE}{k} + 1\right)e^{\frac{(\tau+eE)^2 h}{4gk^2}}$$

under condition

$$\tau + \frac{(\tau + eE)^2}{2k} + \frac{1}{2}\kappa E^2 + C = 0 \tag{25}$$

To analyze the stability of this equilibrium point we will write the equations in variation for the system (18), (21). After inserting from (24) we obtain

$$\begin{aligned} \dot{\xi}_1 &= -\frac{k}{h}\xi_1 + 0\cdot\xi_2 \\ \dot{\xi}_2 &= 0\cdot\xi_1 + \frac{1}{g}\left[\tau + \frac{(\tau + eE)^2}{2k} + \frac{1}{2}\kappa E^2 + C\right]\cdot\xi_2 \end{aligned} \tag{26}$$

where the coefficient by ξ_2 in the second equation is according (25) equel zero. The corresponding characteristic equation is

$$\begin{vmatrix} -\frac{k}{h} - \lambda; & 0 \\ 0; & -\lambda \end{vmatrix} = 0 \tag{27}$$

The eigenvalues are then $\lambda_1 = 0, \lambda_2 = -k/h$. Because $k > 0, h > 0$ the equilibrium point is stable.

Now we try to verify the above mentioned theory with the experimental results published in Mitrovic & al.(2001). Here we could find the basic material properties of different stacks. As an example we have choosen materiál PZT-5H

$$k = 22\cdot 10^9\ Pa, \quad e = 17\ C/m^2, \quad \kappa = 8\cdot 10^{-9}\ F/m$$

Maximum electric field E applied in experiments was $1.38\ MV/m$ and maximum stress τ applied was $68.9 MPa$. The model (24) corresponds quite good with the published results (Mitrovic & al. (2001), p. 4363 Fig. 4).

To evaluate the hysteresis we will assume the following time dependace of E (see Fig. 1):

$$E=\frac{2E_0}{T}t \quad for \quad t\in\left(0,{T}/{2}\right)$$
$$E=2E_0\left(1-\frac{t}{T}\right) \quad for \quad t\in\left({T}/{2},T\right) \tag{28}$$

Putting it into (24) we obtain following result

$$x-1=\varepsilon=\frac{2eE_0}{kT}t+\frac{1}{k}\left(\tau-\frac{2eE_0}{kT}h\right) \quad for \quad t\in\left(0,{T}/{2}\right) \tag{29}$$

$$x-1=\varepsilon=-\frac{2eE_0}{kT}t+\frac{1}{k}\left(\tau+2eE_0+\frac{2eE_0}{kT}h\right) \quad for \quad t\in\left({T}/{2},T\right) \tag{30}$$

When we replace t with E using (28), we obtain finally the dependence ε on E:

$$\varepsilon=\frac{e}{k}E+\frac{1}{k}\left(\tau-\frac{2eE_0}{kT}h\right) \quad for \quad t\in\left(0,{T}/{2}\right) \tag{31}$$

$$\varepsilon=\frac{e}{k}E+\frac{1}{k}\left(\tau+\frac{2eE_0}{kT}h\right) \quad for \quad t\in\left({T}/{2},T\right) \tag{32}$$

The graph for $\tau=0$ is shown on Fig. 2. The hysteresis depends on h and on the velocity $v={E_0}/{\frac{T}{2}}={2E_0}/{T}$. For h=0.0001 we obtain $\frac{4eE_0}{kT}h=0.0001$ what corresponds roughly with Fig. 4 in Mitrovic & al. (2001).

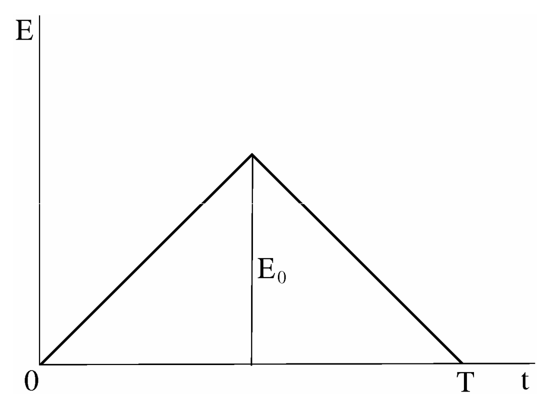

Fig.1: E-t dependance

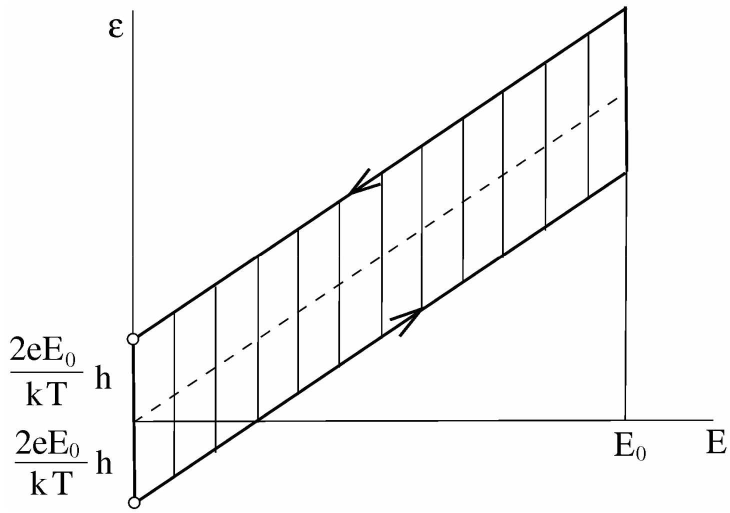

Fig. 2: $\varepsilon - E$ dependence corresponding to Fig. .1 for $\tau = 0$.

For $\tau \neq 0$ we need to solve the above given dynamical system numericaly. The result for the maximum load 55 MPa is shown on the Fig. 3.

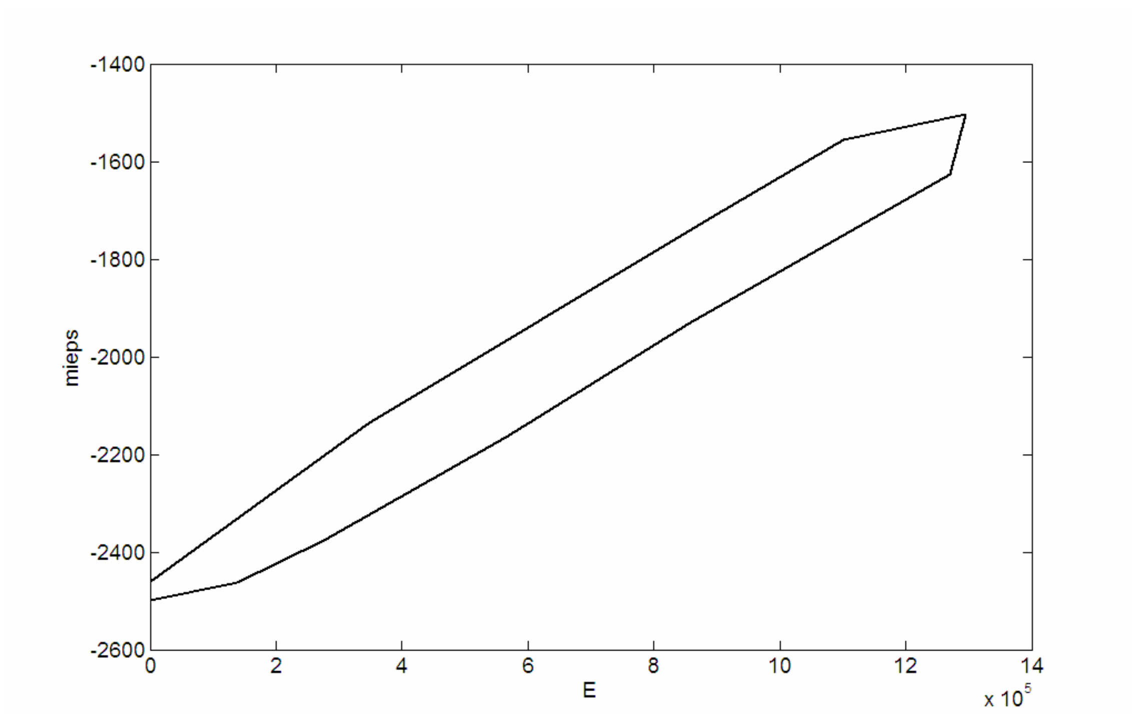

Fig. 3: $\varepsilon - E$ dependence corresponding to Fig. 1 for $\tau = 55\ MPa$.

2.1.2. e is constant, κ =0, k is changing:

Better correspondence must take in account the change of other material parameters during loading and application of electrical field according to the experimental results in above mentioned publication Mitrovic (2001).

Further will be assumed, that only stiffness k is changing during the loading process. In this case it´s necessary to take into account either the dependance of r_1 on the variables or to change the form of ψ . In the last case we can e.g. add the term $\frac{1}{2}\alpha k^2$ into the RHS of (5). Then the new form of (19) will be

$$\dot{k} = \frac{1}{m_1}\left[r_1 - \frac{1}{2}(x-1)^2 + \alpha k\right] \tag{33}$$

and the new form of (21) is

$$\begin{gathered} \dot{l}_r = \frac{1}{g}\left[x\tau - \frac{1}{2}k(x-1)^2 + eE(x-1) + \frac{1}{2}\kappa E^2 + \frac{1}{2}\alpha k^2 + C\right] l_r \\ resp. \\ (\ln l_r)^{\bullet} = \frac{1}{g}\left[x\tau - \frac{1}{2}k(x-1)^2 + eE(x-1) + \frac{1}{2}\kappa E^2 + \frac{1}{2}\alpha k^2 + C\right] \end{gathered} \tag{34}$$

The new dynamical system is given by (18) and (33).

When we put $\varepsilon = x - 1$ then the fix point coordinates (ε_0, k_0) can be obtained solving the following system of equations

$$\begin{gathered} r_1 - \frac{1}{2}\varepsilon_0^2 + \alpha k = 0 \\ \tau - k_0\varepsilon_0 + eE = 0 \end{gathered} \tag{35}$$

For ε_0 we obtain the cubic equation

$$\varepsilon_0^{\ 3} - 2r_1\varepsilon_0 - 2\alpha(\tau + eE) = 0 \tag{36}$$

and for k_0

$$k_0 = \frac{\tau + eE}{\varepsilon_0} \tag{37}$$

From (36) is clear, why it´s necessary that $\alpha \neq 0$. For $\alpha = 0$ we obtain nontrivial solution of (36) $\varepsilon_0 = \sqrt{2r_1}$ which is unrealistic.

Using this model we can obtain the stiffness increase during the activation described in Mitrovic (2001). The stability analysis of this dynamical system under investigation now-a-day.

3. Conclusions

The described model was formulated on both basic situations – loading with isolated ends of stack and with given electric field potential. The deeper analysis was done for the second case. The necessary condition for **C** was developed. The results agree with the published experimental results. The suggested approach can be generalized to take in account the change of the stiffness of the piezoelectric stack according the experimental results. It allows also the simple generalization for nonlinear case and of course for the 3D-continuum.

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