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MODELLING COUPLED DYNAMICS: PIEZOELECTRIC ELEMENTS UNDER CHANGING TEMPERATURE CONDITIONS

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ABSTRACT

In this paper the dynamics of piezoelectric solids is studied as a coupled thermo-electromechanical problem using tools of mathematical and computer modelling. The mathematical model is based on three coupled partial differential equations, the equation of motion, the Maxwell equation for electric field and the energy balance equation. The coupling effect is amplified by the constitutive equations and boundary conditions. We provide modelling results demonstrating that thermal fields can influence significantly on the characteristic (electromechanical) properties and the performance of piezoelectric elements and structures. Examples of computer modelling are given for lead zirconate-titanate (PZT) piezoceramic materials widely used in many applications of acoustic wave generation, piezo-transducers/transformers design, as well as in piezo-sensors/actuators for the vibration control of flexible structures.

Introduction

The manufacture of more accurate and cheaper devices based on different types of energy transformations (e.g., electromechanical, magnetomechanical, thermomechanical) is essential in many technological processes and products. It becomes apparent that further progress in this field, driven on a commercial scale by an increasing integration of mechanical components of devices with electronics and information processing, will rely substantially on a better understanding of the dynamics of adaptive materials subjected to different inputs and environmental conditions. In particular, an increasing interest in the smart material and structure technology generated by many industrial applications has put a special emphasis on a better understanding of the dynamic behaviour of piezoelectrics as an integral part of this technology. Due to the ability to generate a charge in response to a mechanical deformation (the direct piezoelectric effect) and to provide mechanical strains when an electric field is applied (the converse piezoelectric effect), piezoelectric materials are employed both as sensors and actuators in the development of smart structures. In many industrial applications piezoelectric sensors and actuators are used as embedded control elements in advanced composites and smart structures that are subjected to severe mechanical and thermal environments. The influence of thermal effects on the dynamic behaviour of piezoelectrics and the coupling between thermal, mechanical, and electric fields are key issues in the analysis of such structures (e.g. [1,2,3] and references therein). Although these issues are also important in many traditional applications of piezo-transformers, acoustic wave generators, transducers, and other devices with an active piezoelectric element [4,5], they have not been studied in the literature with the vigour they deserve. Since mathematical and computer modelling provide a powerful tool in the study of the coupled dynamics of thermoelectromechanical fields, this paper is devoted to this study with exemplification based on cylindrical piezoelectric elements.

Mathematical Models in Dynamic Thermoelectroelasticity

Following earlier work in this direction (see [6,7,8,9,10,11] and references therein) we consider a coupled system for piezoelectrics that includes the equation of motion and the Maxwell equation for electric field

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \sigma_{ji,i} + F_i, \quad D_{i,i} = f_2, \quad i,j = 1,2,3, \tag{1}$$

where u_i are components of the mechanical displacement vector, ρ is the density of the material, σ_{ij} is the stress tensor, D_i are electric displacements, F_i are components of the vector of mass forces, f_2 is the electric charge density. An important new element of this work is that we consider in detail aspects of mathematical and computer modelling of the full thermo-electromechanical coupling by employing the following state equations

$$\sigma_{ij} = c_{ijkl}\epsilon_{kl} - e_{ijm}E_m - \gamma_{ij}\theta, \quad D_i = \varepsilon_{ik}E_k + e_{ikl}\epsilon_{kl} + p_i\theta, \tag{2}$$

where ϵ_{ij} are strains, E_i are components of the electric field with the potential φ ($\mathbf{E} = -\nabla\varphi$), θ is the difference between the current, T, and the reference temperature, T_0, c_{ijkl} are elements of the matrix of elastic moduli, e_{ikl} are piezoelectric constants, γ_{ij} are elements of the matrix product $\Lambda \cdot \Xi$ (Λ is the matrix of elastic moduli, Ξ is the thermal expansion matrix), ε_{ik} are dielectric permittivities, and p_i are pyroelectric (thermoelectric coupling) constants. The Cauchy formula is assumed for the strain-displacement relation. The energy balance equation is expressed in the form of the continuity equation for the amount of heat and supplemented by the constitutive equation for the entropy (per unit volume), S,

$$T\frac{\partial S}{\partial t} = -q_{i,i} + Q, \quad S = \gamma_{ij}\epsilon_{ij} + c_\epsilon^V \theta / T_0 + p_i E_i, \tag{3}$$

where c_ϵ^V is the (volumetric) heat capacity, $\mathbf{q} = (q_1, q_2, q_3)$ is the heat influx through the body surface and Q is the energy due to heat generation inside of the body.

In the general case the complete set of equations is nonlinear. The heat capacity, thermal conductivity, and electric resistance are all functions of temperature. Even assuming that these functions are constants within the range of temperatures under consideration, the nonlinearity of system (1)–(3) comes from the factor $T = T_0(1 + \theta/T_0)$ in the energy balance equation. Formally, the assumption $|\theta/T_0| \ll 1$ will reduce the system (1)–(3) to a linear one.

Note that in consideration of piezoelectric materials for practical purposes it has been accepted for a long time that the effects of the magnetic field can be ignored [6] and we follow this assumption in this paper. The analysis of the influence of these effects on the electromechanical characteristics of piezoelectrics will be analysed in a separate paper.

Modelling Dynamics of Cylindrical Piezoelectric Elements

In many applications where piezoelectric elements are used as part of engineering devices, the cylindrical topology has a number of advantages compared to other topological designs. In what follows we consider nonstationary axisymmetric oscillations of hollow thin-walled piezoceramic cylinder. If the thickness of this cylinder (i.e. the difference between its external, R_1, and internal, R_0, radii) is considerably smaller than its length (mathematical speaking we call such cylinders "infinitely long"), one dimensional models are sufficient to describe adequately the most important characteristics of piezoelectric-based devices. All such characteristics are functions of the dynamics of coupled thermoelectromechanical fields. Therefore, for the analysis of thermoelectroelastic fields and determination of device characteristics the solution of a general time-dependent (rather than steady-state) problem is required. This leads to quite challenging mathematical problems which, in such a generality, have not been addressed in the literature for the cases other than the axial preliminary polarisation. We note that in the constitutive equations typically used in this area one assumes that the field of preliminary polarization is homogeneous and directed along the axial axis (then the constitutive equations coincide with the material dependencies for the class 6mm piezoelectric crystals with the Oz symmetry axis of the sixth order). If the field of preliminary polarisation changes, all coefficients in the constitutive equations become functions of coordinates of the interior part of the element. If, however, the external field of preliminary polarisation has some properties of symmetry, constitutive equations can still be written with constant coefficients in the appropriate system of coordinates. In what follows we deal with a hollow piezoceramic cylinder with radial preliminary polarisation where the constitutive equations can be written with constant coefficients for the cylindrical system of coordinates [9,10].

Our main interest in this paper lies with the coupled system of mixed partial differential equations written in the cylindrical system of coordinates

$$\rho\frac{\partial^2 u}{\partial t^2} = \frac{1}{r}\frac{\partial}{\partial r}(r\sigma_r) - \frac{\sigma_\theta}{r} + f_1(r,t), \quad \frac{1}{r}\frac{\partial}{\partial r}(rD_r) = f_2(r,t), \tag{4}$$

$$T_0\left(1+\frac{\theta}{T_0}\right)\frac{\partial S}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}(kr\nabla\theta) + f_3(r,t), \tag{5}$$

where f_i, $i = 1,2,3$ are given functions. Following [12] the constitutive equations of the polarised piezoceramics are equivalent to the equations of piezocrystal of *hexagonal 6mm* symmetry (in our

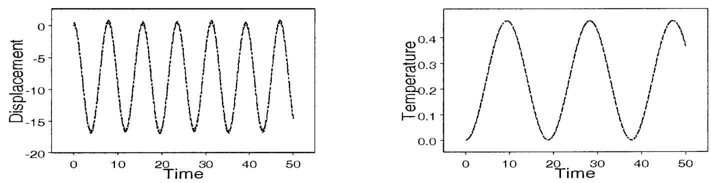

FIG. 1
A negligible effect of temperature on mechanical characteristics of devices.

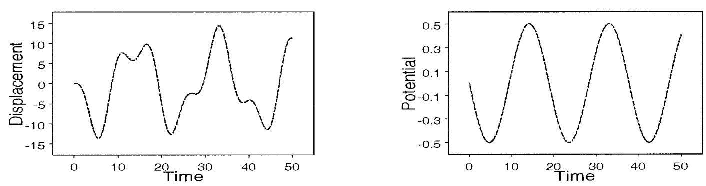

FIG. 2
Voltage as a control variable of thermomechanical characteristics of devices.

case preliminary polarised radially). As in the general case, we choose strain, electric field and temperature as independent variables in our constitutive equations.

Denoting by $\boldsymbol{\sigma} = (\sigma_r, \sigma_\theta)^T$, $\boldsymbol{\epsilon} = (\epsilon_r, \epsilon_\theta)^T$, and $\mathbf{E} = (E_r, E_\theta)^T$ vectors of stress, strain, and electric field, respectively, the constitutive equation (2) for stress can then be written in the generalised Duhamel-Neumann form and in a similar manner we rewrite the constitutive equation (2) for electric displacement

$$\boldsymbol{\sigma} = \mathbf{c}\boldsymbol{\epsilon} - \mathbf{e}^T\mathbf{E} - \boldsymbol{\gamma}\theta, \quad \mathbf{D} = \mathbf{e}\boldsymbol{\epsilon} + \varepsilon\mathbf{E} + \mathbf{p}\theta. \tag{6}$$

The entropy of the thermoelectroelastic system under consideration is

$$S = \boldsymbol{\gamma}^T\boldsymbol{\epsilon} + \mathbf{p}^T\mathbf{E} + c_\epsilon^V\theta/T_0, \tag{7}$$

where vectors $\boldsymbol{\gamma}$ and $\mathbf{p}$ have specific forms discussed below, and $c_\epsilon^V = \rho c_\epsilon^S$ (c_ϵ^S is the specific heat capacity). The Cauchy relationship between deformations (strains) and (radial) displacements, and the electrostatic form for the electric field (via the electrostatic potential, φ) are

$$\epsilon_r = \frac{\partial u}{\partial r}, \quad \epsilon_\theta = \frac{u}{r}, \quad E_r = -\frac{\partial \varphi}{\partial r}. \tag{8}$$

Other things to note about (6)–(7) is the specific forms of the vector of pyroelectric coefficients, $\mathbf{p} = (p_3, 0)^T$, and the elastic (stiffness) and electric constant matrices

$$\mathbf{c} = \begin{pmatrix} c_{33} & c_{13} \\ c_{13} & c_{11} \end{pmatrix} \quad \mathbf{e} = \begin{pmatrix} e_{33} & e_{13} \\ 0 & 0 \end{pmatrix}. \tag{9}$$

Finally, the thermoelastic pressure vector $\boldsymbol{\gamma} = (\gamma_{33}, \gamma_{11})^T$ in (6) and (7) is defined as

$$\boldsymbol{\gamma} = \mathbf{c}\boldsymbol{\alpha}, \tag{10}$$

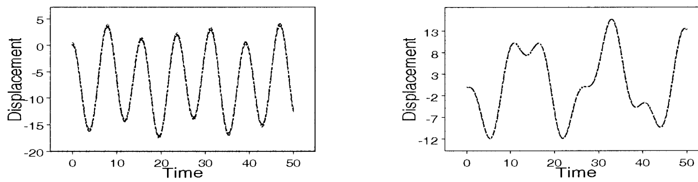

FIG. 3
The effect of temperature on mechanical characteristics of devices.

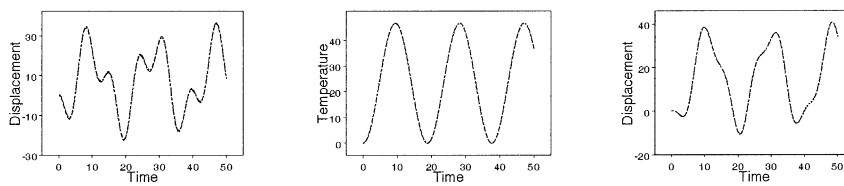

FIG. 4
Thermally induced nonlinear effects in piezoelectric devices.

where $\boldsymbol{\alpha} = (\alpha_{33}, \alpha_{11})^T$ is the vector of thermal expansion coefficients (taken as in [13]). The system (4)–(8) has been supplemented by the initial

$$u = u_0(r), \quad \frac{\partial u}{\partial t} = u_1(r), \quad \theta = \theta_0(r), \tag{11}$$

and boundary conditions

$$\sigma_r = p_i(t), \quad \varphi = \pm V(t), \quad \frac{\partial \theta}{\partial r} = 0, \quad r = R_0, R_1 \tag{12}$$

with given functions $p_i(t), i = 1, 2$, $V(t)$, $u_0(r)$, $u_1(r)$, and θ_0.

Material Properties and Scaling Procedures

In many applications of acoustic wave generation, piezo-transducers/transformers design, and piezo-sensors/actuators in the vibration control of flexible structures, piezoceramics such as lead zirconate titanates (PZT) are known to be excellent materials to use. In this paper all computations were performed for piezoceramic PZT-5. Characteristics of this material are presented in Table 1.

TABLE 1
Characteristics of PZT-5 Piezoceramics

c_{11}	12.1×10^{10}	N/m^2	e_{33}	15.8	C/m^2	α_{11}	$5. \times 10^{-6}$	$1/°C$
c_{13}	7.52×10^{10}	N/m^2	e_{13}	-5.4	C/m^2	c_ϵ^S	420	$J/(kg°C$
c_{33}	11.1×10^{10}	N/m^2	ϵ_0	8.85×10^{-12}	F/m	ρ	7.5×10^3	kg/m^3
α_{33}	$5. \times 10^{-6}$	$1/°C$	p_3	$4. \times 10^{-4}$	$C/(m^2K)$	k	1.25	$W/(kgK)$

All constants required for computation are given in Table 1 along with their units (consult [13] on pyroelectric and thermal expansion coefficients, and [6] for other characteristics). It is easy to find that $c_\epsilon^V = 3.255 \times 10^6 \mathrm{J}/(\mathrm{m}^3\mathrm{K})$, and that $\boldsymbol{\gamma} = (9.31, 9.81)^T \times 10^5 \mathrm{N}/(\mathrm{m}^2\mathrm{K})$ (the latter follows from (10)). In all computations we assumed $T_0 = 300^\circ K$ and $\epsilon_{33} = 830\epsilon_0$. Note also that coefficients in the matrix $\mathbf{c}$ were taken at constant electric field $\mathbf{E}$ (for alternative considerations the reader should consult [6] e.g., where constants measured at constant electric displacement are also given).

A substantial difference in parameter magnitudes requires paying due attention to scaling procedures performed with respect to system (4)–(12) prior to its numerical solution. By introducing dimensionless variables as follows

$$\tilde{t} = t/t_*, \tilde{r} = r/R_*, \tilde{u} = u/u_*, \tilde{\theta} = \theta/\theta_*, \tilde{\varphi} = \varphi/\varphi_*, \tilde{D}_r = D_r/D_*, \tilde{\boldsymbol{\sigma}} = \boldsymbol{\sigma}/\sigma_*, \tag{13}$$

we re-write the equation of motion and the Maxwell equation in the following form

$$\left[\rho\frac{u_*}{t_*^2}\right]\frac{\partial^2 u'}{\partial t'^2} = \frac{1}{r'(R_*)^2}\frac{\partial}{\partial r'}(rR_*\sigma_r'\sigma_r^*) - \frac{\sigma_\theta'\sigma_\theta^*}{R_*r'} + f_1, \quad \frac{1}{r'R_*^2}\frac{\partial}{\partial r'}(r'R_*D_r'D_r^*) = f_2, \tag{14}$$

with the state equations

$$\sigma_r'\sigma_* = \left[c_{33}\frac{u_*}{R_*}\right]\frac{\partial u'}{\partial r'} + C_{13}\frac{u_*}{R_*}\frac{u'}{R'} + e_{33}\frac{\varphi_*}{R_*}\frac{\partial\varphi'}{\partial r'} - \gamma_{33}\theta_*\theta', \tag{15}$$

$$\sigma_\theta'\sigma_* = \left[c_{13}\frac{u_*}{R_*}\right]\frac{\partial u'}{\partial r'} + C_{11}\frac{u_*}{R_*}\frac{u'}{R'} + e_{13}\frac{\varphi_*}{R_*}\frac{\partial\varphi'}{\partial r'} - \gamma_{11}\theta_*\theta', \tag{16}$$

$$D_r'D_* = \epsilon_{33}\frac{\varphi_*}{R_*}\frac{\partial\varphi'}{\partial r'} + e_{33}\frac{u_*}{R_*}\frac{\partial u'}{\partial r'} + e_{13}\frac{u_*}{R_*}\frac{u_*}{R_*}\frac{u'}{r'} + p_3\theta_*\theta'. \tag{17}$$

Now if we set

$$\rho u_*R_*/(t_*^2\sigma_*) = 1, \quad c_{11}u_*/(R_*\sigma_*) = 1, \quad \epsilon_{33}\varphi_*/(D_*R_*) = 1, \quad \text{and} \quad \gamma_{33}\theta_*/\sigma_* = 1, \tag{18}$$

we reduce the original system (4)–(12) to a dimensionless form

$$\rho\frac{\partial^2 u}{\partial t^2} = \frac{1}{r}\frac{\partial}{\partial r}(r\sigma_r) - \frac{\sigma_\theta}{r} + f_1(r,t), \quad \frac{1}{r}\frac{\partial}{\partial r}(rD_r) = f_2(r,t), \tag{19}$$

where new coefficients take computationally convenient values and can be computed from the original values presented in Table 1, using appropriate scaling laws. Note that by using the first two equalities in (18) it is straightforward to deduce (by equating u_*/σ_* expressed from both these equalities) that the time-space scale for this problem is determined by $t_* = R_*\sqrt{\rho/c_{11}}$. Also note that scaling laws for elastic and piezoelectric constants $\tilde{c}_{ij} = c_{ij}/c_{11}$, $\tilde{e}_{kl} = e_{kl}/\sqrt{\epsilon_{33}c_{11}}$ lead to the following matrices of coefficients

$$\tilde{\mathbf{c}} = \begin{pmatrix} 0.917 & 0.621 \\ 0.621 & 1. \end{pmatrix} \quad \mathbf{e} = \begin{pmatrix} 0.530 & -0.181 \\ 0 & 0 \end{pmatrix}.$$

As follows from the above discussion, the original system is reduced to a system that describes the dynamics of a piezoelectric material with the normalised density $\tilde{\rho} = 1$, in which pure elastic waves propagate with the velocity $c = R_*/t_* = \sqrt{c_{11}/\rho}$. In what follows we take $R_* = 1$.

As for the energy balance equation, we reduce it to the following form

$$\frac{\partial \tilde{\theta}}{\partial \tilde{t}} = \frac{\kappa}{\omega c_\epsilon^V}\left[\frac{1}{\tilde{r}}\frac{\partial}{\partial \tilde{r}}(k\tilde{r}\nabla\tilde{\theta}) + \tilde{f}_3\right] - \frac{\partial}{\partial \tilde{t}}\left(\tilde{\gamma}_{33}\tilde{\epsilon}_r + \tilde{\gamma}_{11}\tilde{\epsilon}_\theta + \tilde{p}_3\tilde{E}_r\right), \tag{20}$$

where $\tilde{f}_3 = R_*^2 f_3/\theta_*$, $\kappa = t_*/R_*^2$, $\omega = 1 + \theta_*\tilde{\theta}/T_0$. This form allows us to extend numerical procedures described and analysed in detail in [9,10] to problem (4)–(8).

Computational Experiments

Up to now, many efforts have been devoted to vibration suppression of piezoelectric-based structures subjected to mechanical loading. Since many such structures work under fairly large variations in temperature in the presence of electric fields, our experiments concern the influence of thermal and electrical loading patterns on mechanical characteristics of piezoelectric-based devices. Therefore, in all experiments we assume stress-free boundary conditions and neglect any mass forces (that is $p_i = 0$, $i = 1, 2$, $f_1 = 0$), while imposing special regimes for thermal excitations of piezoelectric-based elements.

Experiment 1. Figure 1 (left) presents the result of computation of radial displacements on the external surface of the cylinder. The thickness of the cylinder is 0.1 in the dimensionless units. The temperature distribution in time is given in Fig 1 (right). The result was obtained for periodic thermal excitations induced by $\tilde{f}_3 = 1.e9\sin(t/3)$. In this case the potential difference was kept constant, equal to 1 in the dimensionless units, i.e. V=0.5 in (3.11). By comparing left part of Fig. 1 with the values of displacements obtained in the framework of electroelasticity theory [9], we conclude that the effect of thermal field on the mechanical field is practically negligible in this case.

Experiment 2. If observed oscillations are to be controlled (as is the case in many piezo-sensor/actuator applications), this can be achieved by using the voltage (supplied to the actuators) as a control variable. This, however, is a nontrivial task because the input voltage depends on the effective surface electrodes and the electrical displacement [13]. For the modelling purposes we take $V = 0.5\sin(t/3)$. Under the same temperature conditions as in the previous example, the effect of variable voltage (Fig. 2 (right)) on the displacements is demonstrated by Fig. 2 (left).

Experiment 3. In this experiment we increase the amplitude of thermal excitations in 10 times by setting $\tilde{f}_3 = 1.e10\sin(t/3)$. The effect of the increasing temperature on the mechanical characteristics of the device is demonstrated in Fig. 3, obtained under the constant (Fig. 3(left)) and variable (Fig. 3 (right)) potential difference.

Experiment 4. Further increase in temperature (simulated by another increase of the amplitude of thermal excitations in 10 times), leads to the situation where nonlinear effects become increasingly important due to violation of the condition $|\theta/T_0| \ll 1$ (see Fig. 4).

We conclude this section with two remarks on nonlinear models for studying coupled dynamics of piezoelectric structures and devices.

Remark 1. In many traditional applications of piezoelectrics (e.g. applications of ultrasonic transducers) the linear models are sufficient to predict effectively most characteristics of the device that are of primary importance to industry. Nonlinear effects become significant in many new technological applications where we often have to deal with (i) high electric fields, (ii) significant temperature gradients, (iii) large deformation and/or (iv) increased heterogeneity of the material (e.g. [14]). It would be fair to say that the interest in the study of nonlinear effects has increased dramatically due to the new applications of piezoelectric materials as sensors/actuators, rotor systems, robots, high-precision systems, and space structures, to name just a few [15]. Since such structures should often be flexible under dynamic excitations, in the most general formulation nonlinear effects should be incorporated into the model describing the *dynamic* behaviour of such structures. These applications (see also [12,16,17,18]) require further development of coupled thermopiezoelectricity models discussed in the previous sections. Some such models have been recently considered in [19,20]. A detailed computational study of such models for the analysis of coupled dynamic thermo-piezoelectric-mechanical fields is outside the scope of this paper.

Remark 2. While models of piezoelectricity for homogeneous materials have been put on a rigorous mathematical basis and their well-posedness has first been established more than a decade ago [21], the situation is different for dynamic models of thermopiezoelectricity applied for heterogeneous media. At the same time, the development of such models become increasingly important due to technological advances in piezocomposites, e.g. for electro- and hydroacoustic applications. For example, in many hydroacoustic applications, the low value of the hydrostatic strain coefficient limits the applicability of piezoelectric ceramics, and the main material parameters of a piezoelectric composite used in piezoelectric transducers are often significantly superior than a single phase monolithic material. Although the problem of determining the overall properties of piezoelectric composites has been addressed by a number of authors in the context of uncoupled behaviour of composites, only a few papers have been devoted to the *coupled* behaviour of piezoelectric composites [22,23]. Even obtaining estimates (or bounds) on global homogenised properties of piezocomposite materials is a challenging and important problem in homogenisation theory and practice, and bounds on the overall properties of such composites, even in the linear case, has been obtained only recently via a Hasin-Shtrikman type variational principle with a reduction of the original problem to two nested *stationary* problems [24]. Furthermore, it should be noted that classical (static) homogenisation techniques lead to reasonable estimates only for static properties without dispersive behaviour. A technique for the investigation of dynamic behaviour of piezocomposites in the linear case has been proposed in [22] using the Bloch expansion. However, in the context of piezocomposite-based sensors/actuators applications, this technique cannot be applied without modifications due to the necessity to account for thermal effects as a result of (a) the direct influence of temperature on properties of the device; (b) the effect of temperature on the properties of the material of the structure (i.e. substrate, whose response the sensor monitors), and (c) thermally induced stresses in the sensor/actuator and in the substrate. In these applications temperature could be responsible for drastic variations of in piezoelectric material properties such as a decrease in sensor resistivity. Since composites are often designed for structures working at elevated temperatures and applications of heterogeneous piezoelectric materials in many "thermo-sensitive" areas of applications (e.g., underwater acoustics, flow meters, smart material and system technology, biophysics), interest in the determination of macroscopic properties of piezoelectric composites subject to thermal fields has grown rapidly [25,26,27,23,28]. Applications of homogenisation procedures to mathematical models for heterogeneous piezoelectric elements lead to new dynamic models which have typically discontinuous coefficients. An efficient numerical algorithm capable of dealing with such dynamic models has recently been described and tested in [29].

Conclusions and Future Directions

In this paper the influence of coupled thermal and electric fields on mechanical characteristics of piezoceramic-based devices has been analysed on the example of axisymmetric oscillations of hollow thin-walled piezoceramic cylinders. It was shown that the thermal field can contribute substantially to such important characteristics of devices as radial displacements. The observed effects become increasingly important in such cases where a piezoelectric has to be considered as a part of smart structure (especially when such a structure/substrate made a polymeric composite material) whose response piezoelectric sensors should monitor, or where the piezoelectric-based device is imbedded into an acoustic interacting media. Although technically non-trivial, mathematically it is relatively straightforward to generalise our numerical schemes to these cases.

In this paper the main source of nonlinearities in the model came from the energy balance equation. Other forms of nonlinearities may prove be more important in some existing and developing areas of piezoelectric applications in smart materials and structures. In particular, nonlinear effects become significant in most applications of piezoelectric materials involving high electric fields, large temperature gradients, and/or increased heterogeneity of the material.

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