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INFLUENCE OF THE THERMAL LOAD ON PIEZOELECTRIC SOLIDS AT MICRO/NANO SCALE

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Abstract. In recent decades the application of a micro/nano electromechanical system for sophisticated energy harvesting devices have increased in popularity. In order to design such a sophisticated devices, it is necessary to know the mechanical behavior of such a structures at micro/nano scale under various thermal conditions. The thermal conductivity at nano scale can be reduced significantly at nanoscales. If the size of the nanostructure is smaller than the phonon mean free path, they are scattered on interfaces and thermal conductivity is reduced. It is known that piezoelectric materials convert mechanical energy into the electrical energy. This electro mechanical coupling is even more pronounced at nano scale where the flexoelectric effect is present. Flexoelectricity is size dependent and requires strain gradients in order convert mechanical energy in to electrical. The micro/nano electromechanical systems work in a different multiphysical environment, therefore, in order to ensure the structural integrity of these sophisticated devices it is necessary to have numerical models that take into account size dependency and electro-thermo-mechanical interaction. The nonlocal higher order heat conduction equation with incorporated size effects will be considered. The new mathematical model will be established based on the generalized heat conduction model and strain gradient elasticity theory with one microstructural length scale parameter. The interaction of thermal mechanical and electrical fields and the influence of the size effect will be numerically modeled.

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1. Introduction

Due to the higher demand of sophisticated energy harvesting devices in the last decades, the development of microelectromechanical systems (MEMS) and nano-electromechanical systems (NEMS) has played a significant role and are now integral to a vast array of applications, including advanced medical diagnostics, consumer electronics, automotive systems, and are used as energy harvesters for autonomous systems [1]. Among the various energy harvesting modalities, the piezoelectric effect has emerged as one of the most promising and efficient mechanisms, especially at the micro and nano scales. Piezoelectric materials possess the unique electromechanical coupling property of generating an electric potential in response to applied mechanical stress.

However, the transition from macroscopic design principles to the micro and nano scales has introduced a new physical phenomena and constraints that are typically negligible at larger scales but become dominant at smaller dimensions. The foundational principles of classical continuum mechanics, which underpin most conventional engineering models, begin to lose their predictive accuracy when the characteristic dimensions of a component become comparable to the material's intrinsic length scales, such as inter-atomic distances or crystalline grain sizes [2].

A particularly important size-dependent phenomenon is the flexoelectric effect. Flexoelectricity refers to the coupling between polarization and a *strain gradient*. Crucially, flexoelectricity is a property inherent to all dielectric materials, irrespective of their crystal symmetry. At the nanoscale, however, strain gradients can become exceptionally large – for instance, near crack tips, sharp corners, or in highly bent nanostructures [3, 4]. Consequently, neglecting the flexoelectric effect in the modeling of NEMS can lead to substantial inaccuracies in predicting their electromechanical performance and reliability, therefore, flexolectricity has attracted many researchers [5-7] .

Another critical factor governing the performance and structural integrity of MEMS/NEMS is the thermal load. These devices frequently operate in environments with fluctuating temperatures. Furthermore, the nature of heat transport changes at the nanoscale. The classical Fourier's law of heat conduction, which assumes a diffusive process, breaks down when a system's characteristic length is smaller than or comparable to the mean free path of the primary heat carriers – phonons in dielectric solids. To accurately capture these non-local thermal effects, it is necessary to employ generalized heat conduction models, often incorporating finite relaxation times for heat flux [8, 9]

To this end, there is a clear need for advanced multiphysics models for the accurate design and optimization of sophisticated piezoelectric energy harvesters. Such models must be capable of simultaneously describing the fully coupled electro-thermo-mechanical fields while rigorously incorporating size-dependent phenomena, namely flexoelectricity and non-local heat transport [10]. While numerous studies have addressed certain aspects of this complex problem in isolation, a comprehensive and unified theoretical framework that integrates all these critical effects remains an open challenge [11]. Developing such a framework is essential for advancing the design and application of next-generation nano-scale electromechanical systems.

Therefore, the objective of this work is to develop and establish a new, generalized continuum model for the analysis of thermo-piezoelectric solids at the micro/nano scale. This model will be based on a generalized elasticity theory that incorporates a microstructural length scale parameter to capture size dependency. It will be fully coupled with a generalized heat conduction equation to accurately describe thermal transport and will also include the influence of the flexoelectric effect. The interaction between the thermal, mechanical, and electrical fields under the influence of these size effects will be investigated through numerical modeling.

2. Governing equations for piezoelectric solids at micro/nano scale

2.1. Constitutive relations

Higher order gradient effects can play an important role in the diffusion of atoms and heat in nano-sized structures. To include these effects, the classical partial differential equation needs to be augmented by higher order spatial gradients of concentration or higher order time derivatives. Similar extensions hold for the heat equation, as advocated by Cattaneo [8], who introduced the heat flux rate in a double temperature mixture type theory. Cattaneo's first generalization of the heat equation has the form:

$$c\rho\dot{\theta}(\mathbf{x},\tau) = k_{ij}\theta_{,ij}(\mathbf{x},\tau) - \theta_0 A_{ij}\dot{\theta}_{,ij}(\mathbf{x},\tau) \tag{1}$$

where k_{ij}, ρ, and c are the thermal conductivity tensor, mass density, and specific heat, respectively. The additional material parameter A_{ij} represents a higher order effect in an anisotropic heat-conducting solid. The reference temperature is denoted by θ_0. It deviates from the classical heat equation by an additional contribution which is proportional to the Laplacian of the temperature rate of change in an isotropic case. The derivation of the above equation is based on a modification of Fourier's heat conduction.
The constitutive equations for thermo-electro-mechanical coupling in piezolectric solids with pyrolectric effect at micro/nano scale are described as follows:

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} - e_{kij}E_k - \gamma_{ij}\theta \tag{2}$$

$$\tau_{jkl} = -f_{ijkl}E_i + g_{jklmni}\eta^e_{nmi} \tag{3}$$

$$D_k = a_{kl}E_l + e_{kij}\varepsilon_{ij} + f_{klmn}\eta_{lmn} + p_k\theta \tag{4}$$

Where the stress-temperature modulus can be expressed through the stiffness coefficients and the coefficients of linear thermal expansion β_{kl}

$$\gamma_{ij} = c_{ijkl}\beta_{kl} \tag{5}$$

Coefficients **a**, **c**, **e**, **f**, and **g** in equations (2)-(4) are the material property tensors. Symbols **a** and **c** denote the second-order permittivity and the fourth-order elastic constant tensors, respectively. The symbol **e** denotes the piezoelectric coefficient, while **f** is the flexoelectric coefficient representing the higher-order electromechanical coupling induced by the strain gradient. The symbol **p** denotes the vector of pyroelectric coefficients. The tensor **g** denotes the higher-order elastic coefficient. The symbols τ_{ijk} and D_i represent the higher-order stress and electric displacement components, respectively.

Kinematic equations relate the strain tensor ε_{ij} and the electric field vector E_j with the displacements u_i and the electric potential ϕ, respectively

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right), \;\; E_j = -\phi_{,j} \tag{6}$$

The strain-gradient tensor $\boldsymbol{\eta}$ is defined as

$$\eta_{ijk} = \varepsilon_{ij,k} = \frac{1}{2}\left(u_{i,jk} + u_{j,ik}\right). \tag{7}$$

Then, the elastic strain gradients are defined as

$$\eta^e_{ijk} = \varepsilon^e_{ij,k} = \left(\varepsilon_{ij} - \beta_{ij}\theta\right)_{,k} \tag{8}$$

2.2. Governing equations

The governing equations derived earlier for the elastic and electrical fields are then formally unchanged

$$\sigma_{ij,j}(\mathbf{x},\tau) - \tau_{ijk,jk}(\mathbf{x},\tau) = 0 \tag{9}$$

$$D_{k,k}(\mathbf{x},\tau) = 0 \tag{10}$$

The governing equations (9)-(10) have to be supplemented by the generalized heat conduction equation (1).

3. Numerical implementation

The weak-form of a boundary value problem in gradient thermo-piezoelectricity can be derived from the principle of virtual work. The weak form and boundary conditions have been implemented into the commercial software Comsol. The C^1 continuity shape functions of the Argyris type have been utilized [12].

$$\int_V \left(\lambda_i \delta\theta_{,i} - \tau_0 \dot{\lambda}_i \delta\theta_{,i} - \rho c \dot{\theta} \delta\theta\right) dV = \int_{\Gamma_\lambda} \left(\bar{\Lambda} - \tau_0 \dot{\bar{\Lambda}}\right) \delta\theta d\Gamma \tag{11}$$

$$\int_V \left(\sigma_{ij}\delta u_{i,j} + \tau_{ijk}\delta u_{i,jk} + D_k\delta\phi_{,k}\right)dV = \int_{\Gamma_t} \overline{t}_i\delta u_i\,d\Gamma + \int_{\Gamma_R} \overline{R}_i\delta s_i\,d\Gamma + \int_{\Gamma_Q} \overline{Q}\delta\phi\,d\Gamma \quad (12)$$

where the heat flux vector is denoted as $\lambda_i = -k_{ij}\theta_{,j}$.

The corresponding FE-mesh has about 4027 of Argyris type elements with a local refinement near the crack tip (Fig. 1).

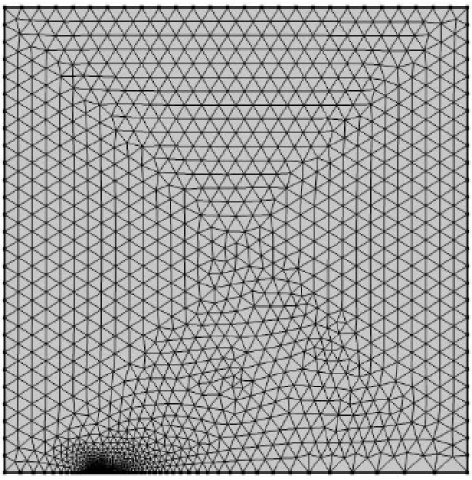

Fig. 1. A square plate with an edge crack: Finite element mesh

4. Numerical experiments

To analyze the problem via numerical simulation, a square plate with an edge crack has been considered. The plate possesses a side length of $w = 5\times10^{-7}\,\mathrm{m}$ and a crack length $a = 1\times10^{-7}\,\mathrm{m}$ (Fig. 2). For the non-stationary analysis, the plate was subjected to a thermal shock $\theta(\tau) = \theta_0 H(\tau)$ where $H(\tau)$ is Heaviside step function, and temperature $\theta_0 = -1K$ is applied on the top. The heat flux on the left and right lateral sides of the plate is zero. Furthermore, the external boundaries and the crack surfaces are free of tractions and electrical displacements. In this example, the crack faces are assumed to be electrically impermeable. The material constants of piezoelectric material are the following: The ceramic PZT-5H is considered [13]:

$c_{11} = 12.6\times10^{10}\,\mathrm{Pa}$, $c_{13} = 5.3\times10^{10}\,\mathrm{Pa}$, $c_{33} = 11.7\times10^{10}\,\mathrm{Pa}$, $c_{44} = 3.53\times10^{10}\,\mathrm{Pa}$

$e_{31} = -6.5\,\mathrm{C\,m^{-2}}$, $e_{33} = 23.3\,\mathrm{C\,m^{-2}}$, $e_{15} = 17.0\,\mathrm{C\,m^{-2}}$,

$a_{11} = 15.1\times10^{-9}\,\mathrm{C^2/N/m^2}$, $a_{33} = 13.0\times10^{-9}\,\mathrm{C^2/N/m^2}$

$k_{11} = 50\,\mathrm{W/K\,m}$, $k_{33} = 75\,\mathrm{W/K\,m}$,

$\beta_{11} = 0.88\times10^{-5}\,\mathrm{1/K}$, $\beta_{33} = 0.5\times10^{-5}\,\mathrm{1/K}$

$c = 420\,\mathrm{Ws/kg/K}$, $\rho = 7500\,\mathrm{kg/m^3}$

In order to assess the effects of the strain-gradients, the size-factor q is introduced, with $l^2 = q \cdot l_0^2$, $m^2 = q_m \cdot m_0^2$.

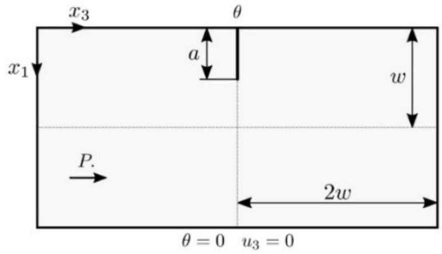

Fig. 2. A square plate with an edge crack: Geometry and boundary conditions

Figure 3 illustrates the crack opening displacements for classical piezolectricity $q = 0$ with varying characteristic time τ_0. It is worth mentioning that in classical piezoelectricity, the crack tip displacements exhibit square root behaviour near the crack tip. In Figure 4, the strain gradient elasticity $q = 4$ eliminates the singularity of Cauchy stresses, the shape of the curve is different, and the crack opening displacement exhibits asymptotic beahvior. The influence of the characteristic time τ_0 is more pronounced for short time instances. However, in both cases, if the characteristic time increases, the crack opening displacements are reduced. The influence of another effect, socalled flexoelectric effect, on the crack opening displacements can be seen in Figure 5a. With increaseing flexoelectric coefficient more mechanical energy is converted into the electric energy, and the crack opening displacements are decreasing. In Figure 5b, the pyroelectric effect causes a reduction in the crack opening displacements. If the pyroelectric coefficient is increasing, the more thermal energy is converted into electrical energy.

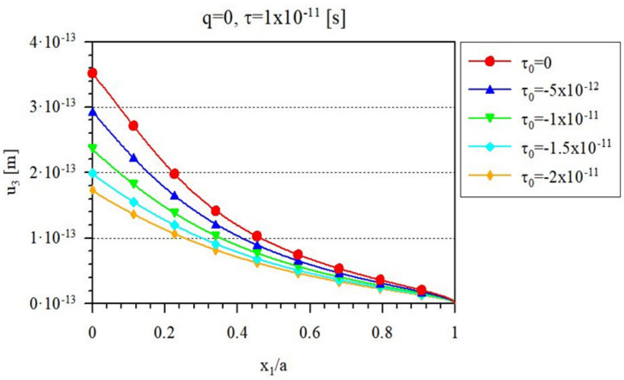

Fig. 3. Crack opening displacements for various characteristic time parameters within classical piezoelectricity $q = 0$

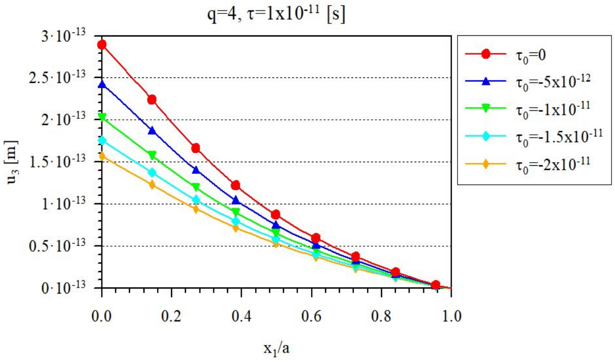

Fig. 4. Crack opening displacements for various characteristic time parameters within strain gradient elasticity $q = 4$

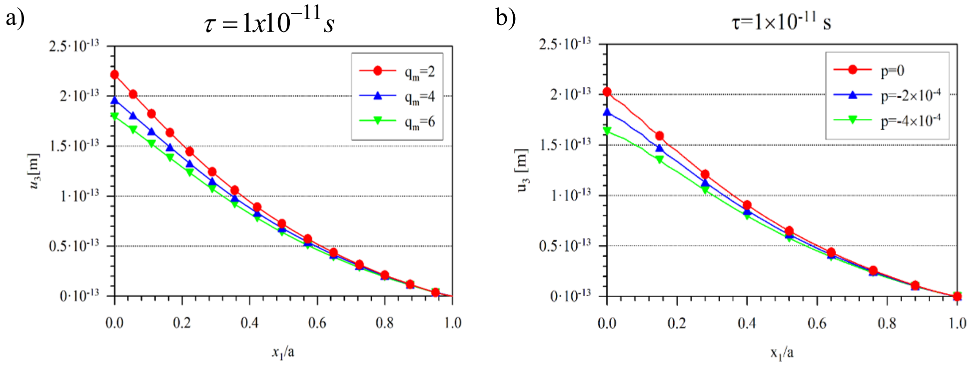

Fig. 5. Crack opening displacements for various flexoelectric coefficients q_m (a) influence of the pyroelectric coefficient p on crack opening displacement (b)

5. Conclusions

The influence of thermal load on the piezoelectric solid at micro/nano scale is investigated in this paper. The influence of the characteristic time parameter that is present in generalized heat conduction, as well as of the strain-gradient size-factor is studied in this paper. The present theory can be applied to general 2D boundary value problems of piezoelectric nano-sized structures with cracks under a transient thermal load. The variational principle is applied to derive the governing equations, including the corresponding boundary conditions in the framework of uncoupled thermoelasticity. The characteristic time in the generalized heat conduction equation is also shown to have an influence on crack opening displacements in this study, albeit for a short instant after the application of a thermal shock. The flexoelectric effect, which is present at micro/nano scales, has been studied as well as influence of the pyroelectric effect on crack opening displacements. The further research will focus on developing of 3D numerical model using and advanced computational method, known as the mixed finite element method.

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