



# Crack analysis of size-dependent piezoelectric solids under a thermal load



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## ABSTRACT

General 2D boundary value problems of piezoelectric nano-sized structures with cracks under a thermal load are analyzed by the finite element method (FEM). The size-effect phenomenon observed in nano-sized structures is described by the strain-gradient effect. The strain gradients are considered in the constitutive equations for electric displacement and the high-order stress tensor. For this model, the governing equations and the corresponding boundary conditions are derived using the variational principle. Uncoupled thermoelasticity is considered; thus, the heat conduction problem is analyzed independently of the mechanical fields in the first step. The veracity of the derived formulations and their implementation into the finite element scheme is demonstrated by some numerical examples.

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## 1. Introduction

The advent of nanotechnology has resulted in the development and production of small microelectronic components and devices for various engineering applications. The classical electromechanical coupling theory of piezoelectricity fails to describe the size-dependent phenomenon observed experimentally (e.g., [43,4–7,17,30,51]), when the dimensions of the structure are of the same order of magnitude as the material length scale. Classical continuum mechanics neglects the interaction of material microstructure and the results from it are size-independent. Experimental techniques as well as discrete atomistic methods such as molecular dynamics (MD) simulations can be utilized for the analysis of nano-sized structures. However, the cost of using these methods can be quite prohibitive. An appropriate but less expensive approach can be employed provided it is sufficiently reliable. In this regard, a promising strategy is to adopt an advanced continuum mechanics model which can account for the size effect phenomenon, where the strain gradients are included in the constitutive equations. If the dielectric polarization is dependent on the strain gradient or curvature strain, it is referred in the literature as the flexoelectric effect [23,32,40]. In the theory of elastic dielectric with electric quadrupoles, the electric field gradients are considered in the constitutive equations [8,21,31]. Later, Hu and Shen [18] applied a variational principle to derive the governing equations in a theory for nano-sized elastic dielectrics with the electric field-gradient and strain gradients. The surface effect for nano-sized dielectrics is also considered in their formulation [41]. The constitutive equations as given by Hu and Shen [18] for a pure electro-mechanical case are modified in the present work for thermo-piezoelectricity. This involves providing the thermal term from the Duhamel-Neuman constitutive equation for the stresses.

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Gradient elasticity theory appears to be also suited for modeling macro-sized structures if the strain gradients are relatively large. For crack problems, it has also been noted that there is a substantial increase of the stress singularity at the crack-tip when the couple-stresses are considered [29,38]. Numerous studies have been reported in the literature to determine the stress and strain fields near the crack-tip under modes I, II and III load conditions in plane strain or anti-plane deformation in the framework of the gradient theory of elasticity (see, e.g., [2,9–11,13,20,25,42,47]). Huang et al. [19] have also derived the expressions for the near-tip fields for a crack in elastic or elastic-plastic materials with strain-gradient effects under mixed mode loadings. A problem which involves the strain gradients is, in general, relatively complex and a reliable computational tool is required to obtain accurate solutions. To this end, Karlis et al. [22] has developed a boundary element method for the 2D fracture mechanics analysis of gradient elastic solids under static loading.

The theory of thermo-piezoelectricity in macro-sized structures was first proposed by Mindlin [33,34]. The physical laws for thermo-piezoelectric materials were also explored by Nowacki [35]. Piezoelectric materials are brittle; therefore, it is important to understand the fracture and damage behaviors of a cracked piezoelectric solid under coupled thermal, mechanical and electrical loads [49,50]. A book on fracture of thermo-piezoelectric materials has also been written by Qin [37]. Boundary value problems for coupled fields are very complex indeed, and analytical solutions are available only for simple geometries and boundary conditions [39]. For solving a general boundary value problem of a piezoelectric medium, the finite element method (FEM) has been shown to be an effective technique [15,24] to employ. The meshless Petrov-Galerkin method has also been developed for treating cracks in piezoelectric solids under a thermal load by Sladek et al. [44]. There is, however, paucity of reported works on problems of thermo-piezoelectricity of nano-sized structures in the literature. This is due to the computational difficulties involved. To the best of the authors' knowledge, there are only papers in which non-local thermo-piezoelectricity is applied to beams or plates [1,3,28].

In this study, the gradient theory for thermo-piezoelectricity is developed which can account for the size-dependent behavior of in-plane cracks in nano-sized piezoelectric structures under a thermal load. A physically similar, but simpler, problem has been analyzed very recently by the authors for nano-sized cracks in piezoelectric solid [46]. Only coupling of mechanical and electrical fields was considered in that work. In the present study, a thermal field is added to the load conditions. A successful attempt to this end has not been reported previously, as far as the authors are aware. Uncoupled thermoelasticity is considered in which the heat conduction problem is analyzed independently of the mechanical fields in the first step. The size-effect phenomenon in nano-sized structures is described by the strain-gradients in the constitutive equations of a piezoelectric material. The governing equations with the corresponding boundary conditions are derived from the variational principle. With these equations, the FEM formulation is then developed. Some numerical examples are presented and discussed to demonstrate the veracity of the computational scheme developed.

## 2. Basic equations for electric-strain gradient theory in thermoelasticity

Consider the electric field-strain gradient coupling and pure nonlocal elastic effect under a thermal load of a nano-dielectric material. The constitutive equations given by Hu and Shen [18] for a pure electro-mechanical case have to be augmented by the thermal term from the Duhamel-Neuman constitutive equation for stresses

$$\begin{aligned}\sigma_{ij} &= c_{ijkl}\varepsilon_{kl} - e_{kij}E_k - \gamma_{ij}\theta, \\ \tau_{jkl} &= -f_{ijkl}E_i + g_{jklmni}n_{nmi}^e, \\ D_k &= a_{kl}E_l + e_{kij}\varepsilon_{ij} + f_{klmn}n_{lmn},\end{aligned}\quad (1)$$

and the Fourier law for the heat flux vector

$$\lambda_i = -k_{ij}\theta_{,j}, \quad (2)$$

where the temperature differences are denoted by  $\theta = T - T_0$  with the reference temperature  $T_0$  at which the thermal strains are zero, i.e.  $\varepsilon_{ij}^T = 0$ . Also, the stress-temperature modulus can be expressed through the stiffness coefficients and the coefficients of linear thermal expansion  $\beta_{kl}$

$$\gamma_{ij} = c_{ijkl}\beta_{kl}. \quad (3)$$

The other coefficients in (1), namely,  $\mathbf{a}$ ,  $\mathbf{c}$ ,  $\mathbf{e}$ ,  $\mathbf{f}$  and  $\mathbf{g}$  are the material property tensors. Symbols  $\mathbf{a}$  and  $\mathbf{c}$  are used for the second-order permittivity and the fourth-order elastic constant tensors, respectively. The symbol  $\mathbf{e}$  denotes the piezoelectric coefficient and  $\mathbf{f}$  is the electric field-strain gradient coupling coefficient tensors representing the higher-order electromechanical coupling induced by the strain gradient. The tensor  $\mathbf{g}$  denotes the purely nonlocal elastic effects, i.e., the strain-gradient elasticity. The symbols  $\tau_{ijk}$  and  $D_i$  represent the higher-order stress and electric displacement components, respectively.

The strain tensor  $\varepsilon_{ij}$  and the electric field vector  $E_j$  are related to the displacements  $u_i$  and the electric potential  $\phi$  by

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad E_j = -\phi_{,j}, \quad (4)$$

where the latter assumption is justified when the quasi-static approximation for electromagnetic fields is applicable.

When the macroscopic strain coincides with the micro-deformation [10], the strain-gradient tensor  $\boldsymbol{\eta}$  is defined as

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