

Thermo-electro-mechanical behaviour of Nano-sized structures

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Abstract. Thermo-electro-mechanical behaviour of the nano-sized structures is analysed by the finite element method (FEM). The mechanical response of the nano-sized structures cannot be modelled with classical continuum theories due to the size effect phenomenon. The strain gradient theory with one length scale parameter has been applied to study size effect phenomenon. The coupled theory of thermo-electricity has been used together with strain gradient theory of elasticity. The governing equations have been derived and incorporated into the commercial software Comsol via weak form module. The influence of the length scale parameter on mechanical response of the structures is investigated by some numerical examples.

1 Introduction

In the small scale energy harvesting devices the thermo-electric materials are conveniently utilized to convert thermal energy into the electrical through so called Seebeck effect. The maximum efficiency of thermo-electric material is function of its thermo-electric material properties. The higher electric conductivity and lower thermal conductivity lead to the better efficiency [1]. One of the potential techniques how to improve efficiency is to use nano-structured materials [2]. However, the application of advanced materials in nano-sized thermo-electric devices requires sophisticated design process to assess the structural integrity of these small scale devices. The large temperature gradients which can be easily generated in nano-sized structures can have significant influence on mechanical behaviour of these structures. Therefore, it is important to study heat conduction and thermal stresses induced by an electric current [3]. However, applications of classical continuum mechanics theories is insufficient to describe size effect phenomenon which has been experimentally observed in nano-sized structures [4-6]. Due to the lack of length scale information in classical continuum theories, the results are size independent. To this end strain gradient elasticity theory can be applied in order to model size effect phenomenon in thermo-electro-mechanical nano-sized structures. It is the aim of this paper to study thermo-electro-mechanical behaviour of the nano-sized structures. For this purpose the finite element method [7] has been utilized to solve related boundary value problem and investigate influence of the size effect parameter on mechanical response of the structure. We present comparison of results from different commercial codes.

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2 Equations and mathematics

In order to describe mechanical behaviour of nano-sized thermo-electric material the constitutive equations for Cauchy stress tensor and higher order stress tensor within strain gradient elasticity are given as: [8-9].

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} - \gamma_{ij}\theta \quad (1)$$

$$\tau_{jkl} = g_{jklmni}\eta_{nmi}^e \quad (2)$$

where the temperature difference is $\theta = T - T_0$ with the reference temperature denoted as T_0 . The stress-temperature modulus γ_{ij} is calculated through stiffness coefficients c_{ijkl} and the coefficients of linear thermal expansion β_{kl}

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

The coefficient \mathbf{g} denotes the nonlocal elastic effects, i.e., the strain-gradient elasticity and higher order stress tensor is denoted as τ_{ijk} . The total strain tensor ε_{ij} is related to the displacements u_i by

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

The elastic strain-gradient tensor is defined as

$$\eta_{ijk}^e = \varepsilon_{ij,k}^e = (\varepsilon_{ij} - \beta_{ij}\theta)_{,k} \quad (5)$$

The mechanical constitutive equations (1) and (2) should be supplied in a thermoelectric materials by constitutive equations for electric current density J_i and the heat flux vector h_i .

$$J_i = s_{ij}(E_j - \Sigma_{jk}\theta_{,k}) \quad (6)$$

$$h_i = \bar{\Sigma}_{ij}E_j - \kappa_{ij}\theta_{,j} \quad (7)$$

Where s_{ij} is the electrical conductivity at a uniform temperature, Σ_{ij} and $\bar{\Sigma}_{ij}$ are Seebeck and Peltier coefficients which are calculated via Seebecks coefficients and absolute temperature $\bar{\Sigma}_{ij} = \Sigma_{ij}T$ and κ_{ij} is the thermal conductivity. The electric field vector E_j is related to the electric potential ϕ by

$$E_j = -\phi_{,j} \quad (8)$$

The governing equations for thermo-electro-mechanics are following:

$$\sigma_{ij,j} - \tau_{ijk,jk} = 0 \quad (9)$$

$$J_{i,i} = 0 \quad (10)$$

$$h_{i,i} = E_i J_i \quad (11)$$

where the source term in last equation is the joule heating. Substituting the constitutive equations into the governing equations gives fully coupled set of equations which means that the energy is transformed in both ways, from thermal to electrical and vice versa while transformation of energy from mechanical to thermal is neglected.

3 Numerical results

The governing equations (9-11) has been implemented and solved via the FEM software Comsol. The finite element model consists of 5000 Argyris elements which possess C^1 continuity of shape functions. The thermoelectric material, titanium alloy Ti-6Al-4V is considered in this study. It has the following material constants [10]:

$$c_{11} = 12.8 \times 10^{10} \text{ [Pa]}, \quad c_{12} = 4.22 \times 10^{10} \text{ [Pa]},$$

$$c_{22} = 12.8 \times 10^{10} \text{ [Pa]}, \quad c_{44} = 4.28 \times 10^{10} \text{ [Pa]},$$

$$s_{11} = 5.83 \times 10^5 \text{ [Am/V]}, \quad s_{22} = 5.7 \times 10^5 \text{ [Am/V]},$$

$$\Sigma_{11} = -2.947 \text{ [A/mK]}, \quad \Sigma_{22} = -2.793 \text{ [A/mK]},$$

$$\kappa_{11} = 7.373 \text{ [W/Km]}, \quad \kappa_{22} = 7.3 \text{ [W/Km]},$$

$$\beta_{11} = 8.7 \times 10^{-6} \text{ [1/K]}, \quad \beta_{22} = 8.7 \times 10^{-6} \text{ [1/K]}.$$

In order to evaluate the influence of the size effect, the size-factor q is introduced, with

$$l^2 = q \cdot l_0^2,$$

where $l_0 = 5 \times 10^{-9} \text{ [m]}$.

In this study a square plate with central crack is analyzed, with dimensions $w = 5a$, $a = 1.0 \times 10^{-7} \text{ [m]}$ (see Fig. 1). The boundary conditions have been imposed according to the Fig.1. The cracked plate is symmetric with respect to the horizontal and vertical mid-planes. On the top and right side of the quarter plate it is prescribed temperature $\theta = 283 \text{ [K]}$. The zero temperature is considered on the crack face. The electric potential is vanishing ahead the crack tip in the plane $x_2 = 0$.

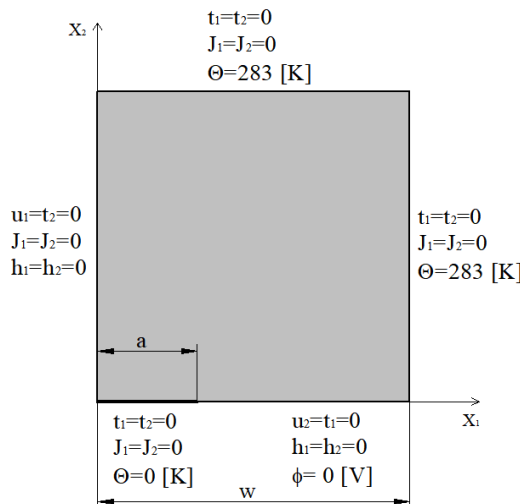


Fig. 1. Geometry and boundary conditions of the plate with a central crack.

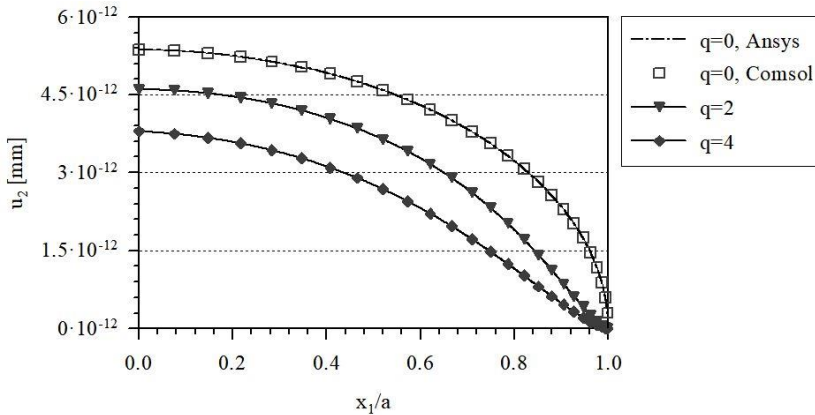


Fig. 2. Crack opening displacement u_2 [mm] for different size factors q .

The influence of the size effect on the crack opening displacement is depicted in Fig. 2. If the size effect parameter increases crack opening displacements decrease. The structure appears to behave as stiffer. It is evidently seen that presence of strain-gradients has a significant influence on the crack opening displacements u_2 . For the classical thermo-electro-mechanical model with size factor $q=0$, the crack opening displacements exhibit the well-known square-root behavior near the crack-tip and the stresses possess the square-root singularity. It can be seen in Fig. 2 that the presence of the strain-gradients with $q>0$ changes the asymptotic crack-tip behavior of the crack-opening-displacements. The numerical results obtained for $q=0$ agree very well indeed with the reference results from Ansys.

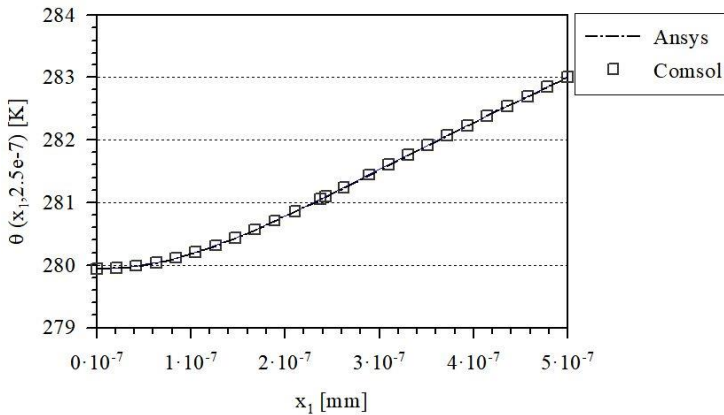


Fig. 3. Variation of the temperature along x_1 - coordinate.

Since the transformation of energy is in both ways in coupled thermo-electricity from thermal to electrical energy and vice versa the heat source is generated due to the joule heating. In nano-sized structures where large gradients can occur the joule heating can be more pronounced. The heat source caused by the joule heating influences the distribution of the temperature. The comparison of the temperature profiles is shown in Fig.3. The results obtained by Comsol are in good agreement with those obtained by the Ansys where

coupled thermo-electricity is implemented. Due to independence of temperature on mechanical fields the temperature distribution in the domain is only affected by heat sources due to the Joules heating. Then, the gradient theory has no influence on the temperature distribution, and it can be analyzed by the classical theory. The temperature variation along x_1 coordinate is shown in Fig.3. One can observe a very good agreement of with results obtained from Ansys.

4 Conclusion

The thermo-electro-mechanical nano-sized plate with central cracks under a thermal load has been analysed. The strain gradient elasticity theory has been applied in order to describe size effect phenomenon. Strain-gradients are considered in the constitutive equations for the higher order stress tensor. Since uncoupled thermo-elasticity is considered, the heat conduction problem is computed independently of the mechanical fields in the first step. The finite element method has been utilized for the solution of related boundary value problems. The numerical example is presented and discussed. The results are verified with Ansys software for classical theory ($q=0$). The influence of the size effect on the crack-opening-displacements is investigated. The crack opening displacements decrease as the size factor increases and exhibit lower values than in classical theory ($q=0$).

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