29th International Conference
ENGINEERING MECHANICS 2023
Milovy, Czech Republic, May 9 – 11, 2023

ADVANCED CONTINUUM MODEL FOR THERMOELECTRIC ANALYSES

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Abstract: *The Seebeck effect is utilized in the thermoelectric materials to convert the waste heat directly to electricity. A high electrical conductivity, low thermal conductivity and high Seebeck coefficient are desirable for high thermoelectric conversion efficiency. For generation of a large voltage it is needed to keep sustained large temperature gradients. Therefore, some research efforts are devoted to develop thermoelectric composites with low thermal and high electric conductivities. Earlier research on macro-sized structures has not been successful. Nanotechnology open a door to reduce thermal conductivity without affecting the electrical conductivity. The heat transfer is realized by "larger" phonons than electrons responsible for the electric conduction. The scattering of phonons is increased in nano-sized structures and the thermal conductivity is reduced owing to the mean-free path of phonons becoming comparable with the size of sample. Then, the classical Fourier heat conduction model appears to be insufficient because of ignoring size effects. To consider the size effect an advanced continuum model for heat transfer is developed here with including second order temperature gradients in constitutive law. The governing equations involve higher-order derivatives of field variables. Therefore, it is necessary to develop also a powerful computational tool to solve general boundary-value problems. The mixed finite element method (FEM) is developed in this paper.*

Keywords: ***Gradient theory for thermal conduction, Coupled problem, Seebeck effect, Size effect, Mixed finite element method.***

1. Introduction

Thermoelectric materials have a potential to convert waste heat directly into electricity (Minnich et al., 2009; Bies et al., 2002). However, this thermoelectric material property has not been utilized up to date in engineering applications because of low thermoelectric conversion efficiency. A high electrical conductivity, low thermal conductivity and high Seebeck coefficient are required for high thermoelectric conversion efficiency. It is not easy to satisfy these requirements simultaneously even in composite materials (Cao et al., 2008) in macro-sized structures. The classical continuum model is applicable to simulations in such structures. However, in nano-sized samples it is possible to reduce thermal conductivity without a reduction of the electrical conductivity (Boukai et al., 2008). The heat transport in nano-sized structures is decreased because of increasing scattering of phonons when the mean-free path of phonons is comparable with the size of samples . Thus, the size effect is observed in nano-sized structural elements. Obviously, the classical Fourier heat conduction model becomes inapplicable because of absence of sample size dependence in classical models.

Allen (2014) has introduced a generalized continuum model based on the nonlocal expression of the heat flux with temperature gradients. Introducing a spatial size effect into the governing equations for heat transfer it is possible to explain the incorrect results obtained by classical thermal wave models (Yu et al. 2016). A similar nonlocal model was also applied to nonlocal thermoelasticity using

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ISSN: 1805-8256, doi: 10.21495/em2023-227

Eringen's nonlocal theory (Yu et al., 2015; Sarkar, 2020). Numerical results showed that thermal nonlocal parameters may become a new indicator required for a real modelling of the heat transport in nano-sized structures.

In the present paper, an advanced continuum model for heat transfer is applied to the coupled thermoelectric problem in nano-sized structures. Higher-order derivatives of temperature and higher-grade heat flux are occurring in this model. Boundary-value problems for coupled fields with higher-order derivatives in governing equations are very complex, and a powerful computational tool to solve them is required. The finite element method (FEM) is often convenient to solve similar problems. However, the standard C^0-continuous elements cannot be applied here due to the higher-order derivatives involved in this new gradient theory. A mixed FEM formulation is developed here with C^0 continuous interpolation independently applied to the temperature and its gradients. For the electric field, there is no need to employ gradient theory and the standard C^0 elements are used. The computational method is verified on simple examples where analytical solution is available.

2. The mixed FEM in gradient theory of thermoelectricity

The constitutive equations for the heat conduction vector λ_i and the electric current J_i in the classical theory of thermoelectricity are given as (Yang et al., 2013)

$$\lambda_i = -\kappa_{ij}\theta_{,j} + \bar{\zeta}_{ij}E_j$$

$$J_i = s_{ij}E_j - \zeta_{ij}\theta_{,j} \tag{1}$$

where κ_{ij} and s_{ij} are the heat and electrical conductivities, respectively. Symbols ζ_{ij} and $\bar{\zeta}_{ij}$ are used for the generalized Seebeck and Peltier coefficients, which are correlated via the absolute temperature T as $\bar{\zeta}_{ij} = \zeta_{ij}T_0$, with T_0 being the reference temperature and $\theta = T - T_0$.

The electric intensity vector E_j is related to the electric potential ϕ by

$$E_j = -\phi_{,j} \ . \tag{2}$$

Electric processes are much faster than thermal ones and a quasi-static approximation for the electric fields is assumed. Then, the stationary governing equation is valid

$$J_{i,i} = 0 \ . \tag{3}$$

The heat conduction equation in the gradient theory is given as (Sladek et al. 2020)

$$\lambda_{i,i}(\mathbf{x}) - m_{ik,ik}(\mathbf{x}) + \rho c\dot{\theta} = 0 \, , \tag{4}$$

where m_{ik} is the higher-grade flux considered as canonically conjugated field with $\theta_{,ik}$. In linear theory, $m_{ik} = \alpha_{ikjl}\theta_{,jl}$ and assuming the new material coefficients as $\alpha_{ikjl} = -l^2\delta_{lk}\kappa_{ij}$, we have the additional constitutive relationship

$$m_{ik} = -l^2\kappa_{ij}\theta_{,jk} \ . \tag{5}$$

Furthermore, ρ and c are the mass density and specific heat, respectively. Note that the number of additional material coefficients is reduced to only one internal material structure parameter l.

The amount of boundary conditions (b.c.) is increased and the definition of boundary densities are modified in higher-grade theory of heat conduction. Possible boundary conditions in considered thermo-electric problem are given as:

Essential b.c.:
$$\begin{aligned} &\theta(\mathbf{x}) = \bar{\theta}(\mathbf{x}) \ \text{on} \ \Gamma_\theta \, , \ \Gamma_\theta \subset \Gamma \\ &p(\mathbf{x}) = \bar{p}(\mathbf{x}) \ \text{on} \ \Gamma_p \, , \ \Gamma_p \subset \Gamma \\ &\phi(\mathbf{x}) = \bar{\phi}(\mathbf{x}) \ \text{on} \ \Gamma_\phi \, , \ \Gamma_\phi \subset \Gamma \end{aligned} \tag{6}$$

Natural b.c.:
$$\begin{aligned} &\Lambda(\mathbf{x}) = \bar{\Lambda}(\mathbf{x}) \ \text{on} \ \Gamma_t \, , \ \Gamma_\Lambda \cup \Gamma_\theta = \Gamma \, , \ \Gamma_\Lambda \cap \Gamma_\theta = \emptyset \\ &P(\mathbf{x}) = \bar{P}(\mathbf{x}) \ \text{on} \ \Gamma_R \, , \ \Gamma_P \cup \Gamma_p = \Gamma \, , \ \Gamma_P \cap \Gamma_p = \emptyset \\ &Q(\mathbf{x}) = \bar{Q}(\mathbf{x}) \ \text{on} \ \Gamma_Q \, , \ \Gamma_Q \cup \Gamma_\phi = \Gamma \, , \ \Gamma_Q \cap \Gamma_\phi = \emptyset \, . \end{aligned} \tag{7}$$

In above b.c. , $Q = n_k J_k$, is the flux of electric current and the generalized heat flux is defined as

$$\Lambda = n_i\left(\lambda_i - m_{ik,k}\right) - \frac{\partial \mu}{\partial \boldsymbol{\tau}} + \sum_c \left[\!\left[\mu(\mathbf{x}^c) \right]\!\right] \delta(\mathbf{x} - \mathbf{x}^c) , \tag{8}$$

$$\mu = n_k \tau_i m_{ik} \tag{9}$$

with n_i and τ_i the Cartesian components of the unit outward normal and tangent vector on ∂V, respectively, and the possible jump at a corner on the oriented boundary contour ∂V, defined as

$$\left[\!\left[\mu(\mathbf{x}^c) \right]\!\right] := \mu(\mathbf{x}^c - 0) - \mu(\mathbf{x}^c + 0) . \tag{10}$$

Additional boundary quantities occurring in the gradient theory of heat conduction are:

$p = \partial\theta / \partial\mathbf{n}$, $P = n_k n_i m_{ik}$.

For an isotropic material, the heat and electrical conductivities, and Seebeck coefficient are given as

$$s_{ij} = \sigma\delta_{ij} , \zeta_{ij} = \alpha\sigma\delta_{ij} , \ \kappa_{ij} = \bar{\kappa}\delta_{ij} = \left(\alpha^2\sigma T + \kappa\right)\delta_{ij} ,$$

and the thermoelectric conversion efficiency in the classical theory, $ZT = \alpha^2\sigma T / \kappa$, is replaced by

$$ZT = \frac{\alpha^2\sigma T}{\kappa - \kappa(l/L)^2} > \frac{\alpha^2\sigma T}{\kappa} ,$$

in higher-grade thermoelectricity (Sladek et al. 2020).

The FEM equations are derived from the weak-form of the governing equations (3) and (4)

$$\int_V \left(\lambda_i \delta\theta_{,i} + m_{ik}\delta\theta_{,ik} + J_i\delta\phi_{,i} - \rho c\dot{\theta}\delta\theta\right) dV = \int_{\Gamma_\Lambda} \bar{\Lambda}\delta\theta d\Gamma + \int_{\Gamma_P} \bar{P}\delta p d\Gamma + \int_{\Gamma_Q} \bar{Q}\delta\phi d\Gamma . \tag{11}$$

Standard 2D elements with C^0-continuous approximation are used for temperature and electric potential

$$\theta = \mathbf{N}_\theta\left(\xi_1, \xi_2\right)\mathbf{q}_\theta , \qquad \phi = \mathbf{N}_\phi\left(\xi_1, \xi_2\right)\mathbf{q}_\phi , \tag{12}$$

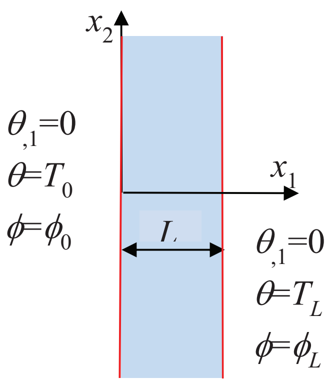
where $\mathbf{q}_\theta$ and $\mathbf{q}_\phi$ are the nodal temperature and electric potential, respectively.

The electric intensity vector, and temperature gradients are approximated according Eq. (12) as:

$$-\mathbf{E} = -\begin{bmatrix} E_1 \\ E_2 \end{bmatrix} = \begin{bmatrix} \partial_1 \\ \partial_2 \end{bmatrix} \phi = \mathbf{B}_\phi(\xi_1, \xi_2)\mathbf{q}_\phi , \qquad \boldsymbol{\varepsilon} = \begin{bmatrix} \theta_{,1} \\ \theta_{,2} \end{bmatrix} = \begin{bmatrix} \partial_1 \\ \partial_2 \end{bmatrix} \theta = \mathbf{B}_\theta(\xi_1, \xi_2)\mathbf{q}_\theta , \tag{13}$$

In the mixed FEM an independent approximation of temperature gradients, $\boldsymbol{\varepsilon}$, is required

$$\hat{\boldsymbol{\varepsilon}}^{In} = \mathbf{A}_\varepsilon\left(\xi_1, \xi_2\right)\boldsymbol{\alpha} , \tag{14}$$



where $\boldsymbol{\alpha}$ is a vector composed of undetermined coefficients and the polynomial function matrix for 4-node quadrilateral element can be selected as

$$\mathbf{A}_\varepsilon\left(\xi_1, \xi_2\right) = \left[1 \quad \xi_1 \quad \xi_2 \quad \xi_1\xi_2\right] .$$

The coincidence of the two independent approximations of the temperature gradients at Gauss quadrature points $\boldsymbol{\xi}^c = (\xi_1^c, \xi_2^c)$, gives unknown coefficients

$$\boldsymbol{\alpha} = \mathbf{A}_\varepsilon^{-1}(\boldsymbol{\xi}^c)\mathbf{B}_\theta(\boldsymbol{\xi}^c)\mathbf{q}_\theta$$

and the final expression for the independent approximation of $\boldsymbol{\varepsilon}$ is given as

$$\hat{\boldsymbol{\varepsilon}}^{In} = \mathbf{A}_\varepsilon(\xi_1, \xi_3)\mathbf{L}\mathbf{q}_\theta ,$$

where $\mathbf{L} = \mathbf{A}_\varepsilon^{-1}(\boldsymbol{\xi}^c)\mathbf{B}_\theta(\boldsymbol{\xi}^c)$.

To verify our FEM formulation and the corresponding computer code, an infinite strip – 1D problem is analyzed. An analytical solution is derived in work (Sladek et al. 2020)

$$\theta(0) = T_0 - T_0 = 0\,,\quad \theta(L) = T_L - T_0\,,\quad \theta'(0) = 0 = \theta'(L)\,,\quad \phi(0) = \phi_0\,,\quad \phi(L) = \phi_L\,.$$

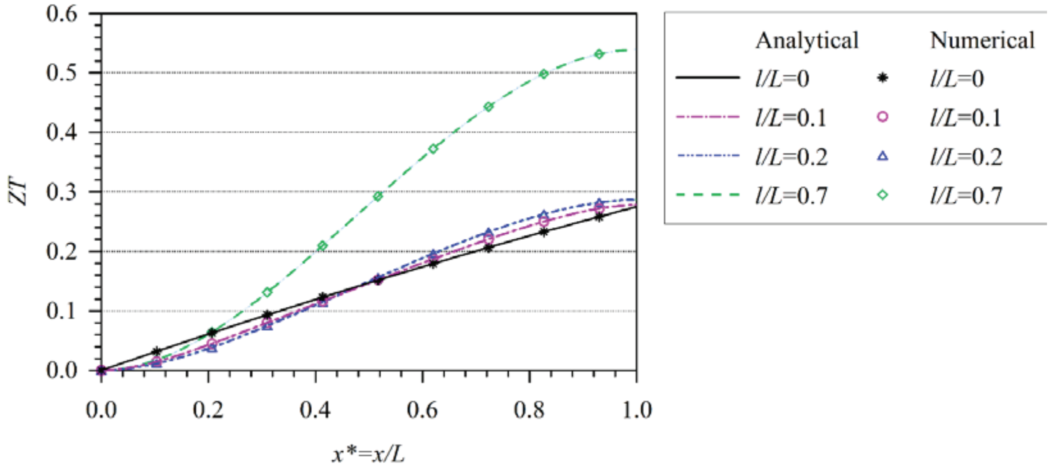


Fig 1: Variation of conversion efficiency *ZT* with different ratios *l*/*L*.

One can observe a significant enhancement on the *ZT* parameter when the internal size parameter *l* is increased.

Acknowledgement

The authors acknowledge the support by the Slovak Science and Technology Assistance Agency registered under number SK-UA-21-0010 and VEGA-2/0061/20.

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