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Research Paper

A finite element computational scheme for transient and nonlinear coupling thermoelectric fields and the associated thermal stresses in thermoelectric materials

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HIGHLIGHTS

- A transient finite element computational model for thermoelectric materials is developed.
- The model can consider temperature dependence of material properties with strong nonlinear thermoelectric coupling.
- A computation code is developed in commercial programming software Matlab.
- Thermal stress analysis can be carried out with the finite element solution of temperature field.

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ABSTRACT

This paper proposes a finite element model for the determination of time dependent thermoelectric coupling fields. The model takes into account all thermoelectric effects, including Joule heating, Thomson effect, Peltier effect and Fourier's heat conduction. Temperature-dependent material properties are also taken into account. The method uses the finite element space discretization to obtain a first-order system of differential equations. The system is solved by employing finite difference scheme to resolve the time dependent response. A computation code is developed in commercial programming software Matlab. Once the temperature field is obtained, the thermal stress analysis can be conducted through standard thermoelasticity or finite element analysis. An equation to evaluate the stress level in the thermoelectric materials is identified. This is the first finite element scheme to deal with transient and nonlinear thermoelectric coupling fields in thermoelectric materials.

1. Introduction

Because of their capability in converting waste heat directly into electricity, thermoelectric materials have attracted significant interests recently [1]. They are often used for power generation and refrigeration. Thermoelectric material devices have many significant advantages. For example, they do not have any moving parts, are portability, do not produce any noise, show good durability and high reliability. Under operation conditions, thermoelectric materials are subjected to thermal gradients, which are produced by both the temperature difference applied at the hot and cold ends of the thermoelectric element and the Joule heating due to the thermoelectric effects.

Recent renaissance of research in thermoelectrics has been focusing on determining the effective properties of layered thermoelectric materials [2–5]. Analysis of such type of materials is considerably more difficult since the thermoelectric properties of thermoelectric materials are coupling and non-homogeneous. Although the thermoelectric coupling has been formulated analytically in the classic books of physics, numerical techniques able to solve problems with complicated geometries, material behavior and working conditions are rare. In Ref. [6], a finite element model has been formulated for the analysis of sensors based on semiconductors. The method considers the potential and fluxes of the thermal field and also of the electron and hole distributions using thermodynamics of irreversible processes and statistics. Other examples include that of [7] that analyses the functioning of aluminum production using electrolytic cells. The excellent work of [8] conducts a finite element analysis of nonlinear fully coupled thermoelectrics.

On the other hand, many engineering materials may operate in transient heating environments [9–11]. Dynamic characteristics are extremely important for design and operation of thermoelectric

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coolers (TECs) [12]. The difficulty in continuum analysis of thermoelectric is due to the nonlinear nature and coupling of electric conduction and heat transfer. In addition, for most of semiconductor materials, Seebeck coefficient, electric conductivity and thermal conductivity are strongly temperature-dependent. Time dependence of thermoelectric coupling also greatly increases the difficulty of the analysis. All of these challenging issues have not been sufficiently elucidated in the literature and motivate me to establish a comprehensive transient finite element method based on continuum mechanics concept.

The present transient finite element model is used to capture the dynamic temperature variations in thermoelectric materials with constant and variable material properties. The paper is organized as follows. In Section 2, the governing equations of thermoelectric coupling are given. This is the root of the finite element formulation. Different forms of the governing equations, which may satisfy different analysis requirements, will also be given. In Section 3 the implementation of finite element scheme together with the solution strategy by using the finite difference in time domain are outlined. In Section 4, iterative solution procedure for the steady finite element equation system is presented. Section 5 discusses some simple test cases to show the feasibility of the approach. These include numerical results for the transient and steady-state temperature for a thermoelectric element, with and without considerations of temperature-dependence of the material properties. Section 6 presents the thermal stress associated with the temperature change in a typical thermoelectric element. Conclusions are drawn in Section 7.

2. Governing equations of thermoelectric coupling

2.1. Thermoelectric coupling equations

Suppose in a coordinate system $\boldsymbol{x}$ (whose components are x_i, where $i = 1, 2, 3$) there is a thermoelectric body occupying a space Ω, which is surrounded by a surface S. The electric and temperature fields inside the body may vary from point to point, and with time. Assume the electric potential $V(\boldsymbol{x}, t)$ and the temperature $T(\boldsymbol{x}, t)$ are continuous functions of the coordinates x_i and time t. The basic law of electric and heat conductions for isotropic thermoelectric materials may be stated as [8,13,14]

$$j_i = -\sigma\frac{\partial V}{\partial x_i} - \sigma s\frac{\partial T}{\partial x_i}, \tag{1a}$$

$$q_i = -\sigma sT\frac{\partial V}{\partial x_i} - (k + \sigma s^2 T)\frac{\partial T}{\partial x_i}. \tag{1b}$$

These are also known as the constitutive equations, in which, σ is the electric conductivity, k is the heat conductivity, s is the so-called Seebeck coefficient, j_i are the components of the electric current vector $\boldsymbol{j}$, $\partial V/\partial x_j$ are the electric field gradients, q_i are the components of the heat flow vector $\boldsymbol{q}$ and $\partial T/\partial x_j$ are the temperature gradients. Hereafter, the summations over the indices i and j will be assumed when appearing twice in an equation. Because the body is isotropic, electricity and heat flow in the direction of the electric potential and temperature gradients.

From the energy balance of the body, the electric and thermal fluxes are controlled by the following equilibrium equations

$$-j_{i,i} = 0 \tag{2a}$$

$$-q_{i,i} - j_i\frac{\partial V}{\partial x_i} = \rho c\frac{\partial T}{\partial t} \tag{2b}$$

where $\rho(\boldsymbol{x})$ is the mass density, $c(\boldsymbol{x})$ the specific heat. The constitutive equations can also be written in terms of the electric current vector. For example, substitution of Eq. (1a) into Eq. (1b) gives:

$$q_i = -k\frac{\partial T}{\partial x_i} + sTj_i. \tag{3}$$

The equilibrium Eqs. (2a) and (2b) can also be converted to

$$V_{,ii} + sT_{,ii} = 0, \quad kT_{,ii} + \frac{1}{\sigma}j_i j_i = \rho c\frac{\partial T}{\partial t}. \tag{4}$$

Eqs. (3) and (4) are useful when the electric flux vector is known. For example, in one-dimensional problem, from (2a) it can be seen that j should be a constant. In this situation, the solution of Eq. (4) will be quite straightforward.

2.2. Alternative form of the governing equations

For a more systemic analysis, a generalized electric current vector $\boldsymbol{J} = \boldsymbol{j}T$ and the symbols $D_{11} = \sigma T$, $D_{12} = sD_{11}$, $D_{21} = D_{12}$ and $D_{22} = k + s^2 D_{11}$ will be introduced. By such definitions, the constitutive Eqs. (1a) and (1b) become

$$J_i = -D_{11}\frac{\partial V}{\partial x_i} - D_{12}\frac{\partial T}{\partial x_i}, \tag{5a}$$

$$q_i = -D_{21}\frac{\partial V}{\partial x_i} - D_{22}\frac{\partial T}{\partial x_i}. \tag{5b}$$

where J_i are the components of the vector $\boldsymbol{J}$. By such operation, the global matrices of the finite element formulation will be symmetric, enabling us to use standard numerical method to solve the system of the finite element equations. With the substitution of Eqs. (5a) and (5b), the equilibrium Eqs. (2a) and (2b) can be written in terms of electric potential and temperature:

$$D_{11}\nabla^2 V + D_{12}\nabla^2 T + J_E = 0, \tag{6a}$$

$$D_{21}\nabla^2 V + D_{22}\nabla^2 T + Q_q = \rho c\frac{\partial T}{\partial t}, \tag{6b}$$

where

$$J_E = j_i\frac{\partial T}{\partial x_i}, \quad Q_q = -j_i\frac{\partial V}{\partial x_i}. \tag{7}$$

It can be seen that the coefficients D_{11}, D_{12} and D_{22} are temperature-dependent. Since thermoelectric materials may work in relatively large temperature range and temperature gradient, the materials properties σ, k and s may also be temperature-dependent. As a result, Eqs. (6a) and (6b) are transient, highly non-linear and fully coupled.

The conduction Eqs. (6a) and (6b) must be solved for prescribed boundary and initial conditions. The initial condition specifies the electric potential and temperature distributions at time zero. These are, $V(x_j, 0) = \overline{V}_0(x_j, 0)$ and $T(x_j, 0) = \overline{T}_0(x_j, 0)$. Conduction boundary conditions take several forms. The frequently encountered conditions are specified surface electric potential and temperature and specified surface electric and heat fluxes. Therefore, the boundary conditions are summarized as:

$$J_i n_i = \bar{J}, \quad \text{on boundary } S_j \tag{8a}$$

$$q_i n_i = \bar{q}, \quad \text{on boundary } S_q \tag{8b}$$

and

$$V = \overline{V}, \quad \text{on boundary } S_V \tag{9a}$$

$$T = \overline{T}, \quad \text{on boundary } S_T \tag{9b}$$

where $S_j + S_V = S_q + S_T = S$, S the surface surrounding the thermoelectric body, the over bar represents the known value, n_i are components of the unit vector $\boldsymbol{n}$ normal to the exterior of S. Eqs. (8) indicate that on the boundaries S_j and S_q the electric and thermal fluxes are prescribed, which are positive if they are directed towards the exterior of the body.