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Asymptotic homogenization of three-dimensional thermoelectric composites

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A B S T R A C T

Thermoelectric composites are promising for high efficiency energy conversion between thermal flows and electric conduction, though their effective behaviors remain poorly understood due to nonlinear thermoelectric coupling. In this paper, we develop an asymptotic homogenization theory to analyze the effective behavior of three-dimensional (3D) thermoelectric composites, built on the observation that the equations governing microscopic field fluctuations in the composite are actually linear instead of nonlinear after separation of length scales. A set of solutions similar to Green's function method are used to construct the unit cell problem, and appropriate interfacial continuity conditions and boundary conditions are derived. The homogenized governing equations are then developed for thermoelectric composites, and they are further reduced for a special case wherein the heat flow and electric conduction in the composite remains one-dimensional (1D) at macroscopic scale, even though the composite itself is 3D in general. The general homogenization theory is implemented using finite element method, and a key constant in the constructed solutions is determined using the reformulated eigenvalue problem. The algorithm is validated, and is applied for a number of case studies for the effective behavior of thermoelectric composites.

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1. Introduction

Thermoelectric materials are capable of converting heat directly into electricity and vice versa based on the Seebeck effect and the Peltier effect (Callen, 1960; Harman and Honig, 1967), and thus they have been widely pursued for applications in waste heat recovery and solid state thermal management (Yang and Caillat, 2006; Narducci, 2011; Kraemer et al., 2011; Tritt and Subramanian, 2006). High efficiency thermoelectric conversion, however, requires simultaneously high electric conductivity and low thermal conductivity, which is rather difficult to achieve in a single-phase material (Nolas et al., 1999). In addition, high electric conductivity and the Seebeck coefficient also impose conflicting requirements on the desired concentration of charge carriers (Snyder and Toberer, 2008), making it even more challenging to improve thermoelectric conversion efficiency. As a result, substantial efforts have been devoted into developing high performance thermoelectric composites (Alboni et al., 2008; Cao et al., 2008; Gothard et al., 2008; Poudel et al., 2008).

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While significant advances have been accomplished in the last decade on experimental investigations of thermoelectric composites with enhanced properties (Arachchige et al., 2008; Heremans et al., 2002; Poudeu et al., 2010; Pei et al., 2011; Xie et al., 2010), theoretical understanding remains rather limited. The difficulty lies primarily in the nonlinear coupling between heat flow and electric conduction, and much confusion exists even in the correct form of governing equation (Milton, 2002; Yang et al., 2013b; Liu, 2012). Earlier analysis concluded that figure of merit of a thermoelectric composite is bounded by that of its constituent (Bergman and Levy, 1991; Bergman and Fel, 1999), though the conclusion was drawn based on linearized thermoelectric transport equations. It has been shown recently that under nonlinear coupling, thermoelectric conversion efficiency of a composite material can be higher than its constituents (Yang et al., 2013a, 2014). These studies suggest that better understanding on the effective behavior of thermoelectric composites is needed for their design, analysis, and optimization, which we seek to develop in this work.

In an earlier paper, we developed asymptotic homogenization theory for one-dimensional (1D) layered thermoelectric composites (Yang et al., 2013b), with which homogenized governing equations have been derived in terms of thermoelectric properties of constituent phases. A key observation there is that the electric current density remains uniform in the layered composites, regardless of the detailed microstructural features. While this attribute makes the analysis much simpler for 1D composites, it is no longer valid for two- (2D) and three-dimensional (3D) systems, and thus complicating the analysis substantially. On the other hand, constant current density in 1D composites imposes a rather strong constraint on the field distribution, making it much harder to optimize for enhanced thermoelectric properties (Yang et al., 2013b). Relaxing such constraint in 2D and 3D composites could offer additional opportunities to fine tune the field distributions and thus further improve thermoelectric performance, and in order to materialize such promises, the effective behavior of 2D and 3D thermoelectric composites has to be understood first.

In this paper, we develop asymptotic homogenization to analyze the effective behaviors of 3D thermoelectric composites. The preliminaries of thermoelectricity are presented in Section 2, where a concise notation is introduced for the convenience of later analysis. Asymptotic homogenization theory is then developed in Section 3, and a key observation is that for general 3D composites, the equations governing microscopic field fluctuations are actually linear instead of nonlinear after separation of length scales, and there exists a unique solution to this microscopic field fluctuation. This allows us to construct a set of solutions similar to Green's function method, with which the governing equations on the unit cell are formulated, and appropriate interfacial continuity conditions and boundary conditions are derived. The homogenized governing equations are then developed for thermoelectric composites. In Section 4, the general theory is reduced to a special case that is more relevant to engineering practices, wherein the heat flow and electric conduction in the composite remain to be 1D at macroscopic scale, even though the composite itself is 3D in general. This effectively decouples unit cells lateral to the macroscopic flows, enabling further simplifications in the analysis. We then implement the general homogenization theory into finite element simulation in Section 5, by decomposing the unit cell problem into two sub-problems. A key constant in the constructed solution is determined first using reformulated eigenvalue problem, from which the field distributions in the unit cell can be solved. Numerical results and discussions are presented in Section 6. The algorithm is validated first against known analytic results in 1D, followed by some case studies. We then conclude in Section 7 by summaries and outlook for future studies.

2. Thermoelectricity

We consider the coupled transports of heat and electricity in a thermoelectric material, with the respective transport equations given by (Callen, 1960; Harman and Honig, 1967; Yang et al., 2012)

$$-\mathbf{J} = \sigma\nabla\phi + \sigma\alpha\nabla T, \tag{1}$$

$$\mathbf{J}_Q = -T\alpha\sigma\nabla\phi - (T\alpha^2\sigma + \kappa)\nabla T = T\alpha\mathbf{J} - \kappa\nabla T, \tag{2}$$

where the thermoelectric flows are driven by both electric field $\nabla\phi$ and temperature gradient ∇T, and the resulting electric current density $\mathbf{J}$ and heat flux $\mathbf{J}_Q$ are coupled together through the Seebeck coefficient α, electric conductivity σ, and thermal conductivity κ. For simplicity all the thermoelectric properties are assumed to be isotropic, though this constraint can be relaxed. This set of thermoelectric transport equations can be derived from irreversible thermodynamics, as detailed in Callen (1960), Harman and Honig (1967), and Yang et al. (2013b). Note that both temperature gradient ∇T and temperature T enter the thermal transport equation (2), making the coupling nonlinear in general and thus much more difficult to solve than normal electric conduction or heat transfer problems in an uncoupled medium.

Since energy is transported by both electricity and heat, the energy flux $\mathbf{J}_U$ can be derived from the current density and heat flux as

$$\mathbf{J}_U = \mathbf{J}_Q + \phi\mathbf{J}. \tag{3}$$

We are interested in a system wherein both charges and energy are conserved, such that both current density and energy flux are divergence-free:

$$\nabla\cdot\mathbf{J} = 0, \tag{4}$$

$$\nabla\cdot\mathbf{J}_U = 0. \tag{5}$$

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