Designing composite microstructures with targeted properties

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We present a numerical method to find specific composite microstructures with targeted effective properties. The effective properties that may be prescribed are quite diverse and include transport, mechanical, and electromagnetic properties, as well as properties associated with coupled phenomena, such as piezoelectric and thermoelectric coefficients. We formulated the target problem as an optimization problem. To illustrate our general target optimization technique, we have successfully found two-phase composite microstructures having specified effective electrical or thermal conductivities at fixed volume fractions. The method can also be used to design microstructures with multifunctional characteristics.

I. INTRODUCTION

An important goal of materials science is to have exquisite knowledge of structure/property relations in order to design material microstructures with desired properties and performance characteristics. Although this objective has been achieved in certain cases through trial and error, a systematic means of doing so is currently lacking. For certain physical phenomena at specific length scales, the governing equations are known and the only barrier to achieving the aforementioned goal is the development of an appropriate method to attack the problem.

The purpose of this article is to introduce a methodology to design at will composite microstructures with targeted effective properties under required constraints. In general terms, this is accomplished by formulating the task as an optimization problem that we call target optimization. Target optimization is an adaptation of traditional structural optimization techniques.[1,2] Specifically, an initial microstructure is allowed to evolve to the targeted state by extremizing an appropriately defined objective function. The types of effective properties that we can address are quite general and include transport, mechanical, and electromagnetic properties, as well as properties associated with coupled phenomena, such as piezoelectric and thermoelectric coefficients.

To illustrate our general target optimization technique, we find two-phase composite microstructures in two dimensions having specified effective electrical or thermal conductivities at fixed volume fractions. In the first example, we use the geometric-mean formula for the targeted effective conductivity. In the second example, we use the target optimization technique to find the structures that lie between the optimal Hashin–Shtrikman (HS) bounds for the effective conductivity.

In Sec. II, we summarize the basic local and homogenized equations. Section III introduces the target optimization method to identify microstructures with prescribed effective properties. The formulations for the objective function and constraints are provided. Section IV reviews pertinent theoretical results for the effective conductivity. In Sec. V, we apply the technique to find microstructures having specified effective conductivities. We make concluding remarks in Sec. VI.

II. LOCAL AND HOMOGENIZED EQUATIONS

Consider a two-phase composite material consisting of a phase with a property K_1 and volume fraction ϕ_1 and another phase with a property K_2 and volume fraction ϕ_2 $(= 1 - \phi_1)$. The property K_i is perfectly general: It may represent a transport, mechanical, or electromagnetic property, or properties associated with coupled phenomena, such as piezoelectricity or thermoelectricity. For steady-state situations, the generalized flux $\mathbf{F}(\mathbf{r})$ at some local position $\mathbf{r}$ in the composite obeys the following conservation law in the phases:

$$\nabla \cdot \mathbf{F}(\mathbf{r}) = 0 \quad . \tag{1}$$

In the case of electrical conduction and elasticity, $\mathbf{F}$ represents the current density and stress tensor, respectively.

The local constitutive law relates $\mathbf{F}$ to a generalized gradient $\mathbf{G}$, which in the special case of a linear relationship is given by

$$\mathbf{F}(\mathbf{r}) = K(\mathbf{r})\mathbf{G}(\mathbf{r}) \quad , \tag{2}$$

where $K(\mathbf{r})$ is the local property. In the case of electrical conduction, Eq. (2) is just Ohm's law, and K and $\mathbf{G}$ are

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the conductivity and electric field, respectively. For elastic solids, Eq. (2) is Hooke's law, and K and $\mathbf{G}$ are the stiffness tensor and strain field, respectively. For piezoelectricity, $\mathbf{F}$ is the stress tensor, K embodies the compliance and piezoelectric coefficients, and $\mathbf{G}$ embodies both the electric field and strain tensor. The generalized gradient $\mathbf{G}$ must also satisfy a governing differential equation. For example, in the case of electrical conduction, $\mathbf{G}$ must be curl free.

One must also specify the appropriate boundary conditions at the two-phase interface. For nonideal interfaces, interfacial properties are associated with the interface. In the case of ideal interfaces, certain components of the local fields are continuous across the interface. For example, for pure conduction across an ideal interface, the tangential component of the electric field and normal component of the current vector remain continuous.

One can show that the effective properties are found by homogenizing (averaging) the aforementioned local fields. In the case of linear material, we have that the effective property K_e is given by

$$\langle \mathbf{F}(\mathbf{r}) \rangle = K_e \langle \mathbf{G}(\mathbf{r}) \rangle \quad , \tag{3}$$

where angular brackets denote a volume average. Our interest is in determining composite microstructures that have specified effective properties.

III. TARGET OPTIMIZATION

To find composite microstructures that have targeted properties, we introduce the target optimization technique. This numerical technique is adapted from the conventional structural optimization methods.[1,2] However, the target optimization technique is different from the latter in an important way. While the conventional optimization methods determine microstructures possessing optimal properties, the target optimization technique determines microstructures for targeted properties that may or may not be optimal. Thus, the objective functions are different. Target optimization uses a modified objective function that consists of the effective properties of the composite as well as the targeted properties. The optimization portion of the algorithms can be performed in a variety of ways. For example, one can use the topology optimization method[1,2] when the topology is not specified or the shape optimization method[1] when the topology is fixed. In this article, we will adapt the topology optimization technique to perform the target optimization. Moreover, an additional penalty function in the objective function is needed to achieve the final two-phase microstructures. Finally, as opposed to previous work, we introduce the interior-point method to carry out the linear programming, as described below.

The design domain (cubic unit cell) is discretized into a number of finite elements and periodic boundary conditions are employed (see Fig. 1). One could begin by making an initial guess for the distribution of the two phases among the elements, solve for the local fields using finite elements, and then evolve the microstructure to the targeted properties. However, even for a small number of elements, this integer-type optimization problem becomes a huge and intractable combinatorial problem. Following the idea of standard topology optimization procedures, the problem is therefore relaxed by allowing the material at a given point to be a gray-scale mixture of the two phases. This makes it possible to find sensitivities with respect to design changes, which in turn allows us to use mathematical programming methods to solve the optimization problem. At the end of the optimization procedure, however, we desire to have a design where each element is either phase-1 or phase-2 material.

Therefore, let $x_i \in [0, 1]$ be the local density of the ith element, so that when $x_i = 0$, the element corresponds to phase 1 and when $x_i = 1$, the element corresponds to phase 2. Let $\mathbf{x}$ (x_i, $i = 1, \ldots, n$) be the vector of design variables. For any $\mathbf{x}$, the local fields are computed using finite elements and the effective property $K_e(K_1, K_2; \mathbf{x})$, which is a function of K_1, K_2, and $\mathbf{x}$, is computed from Eq. (3).

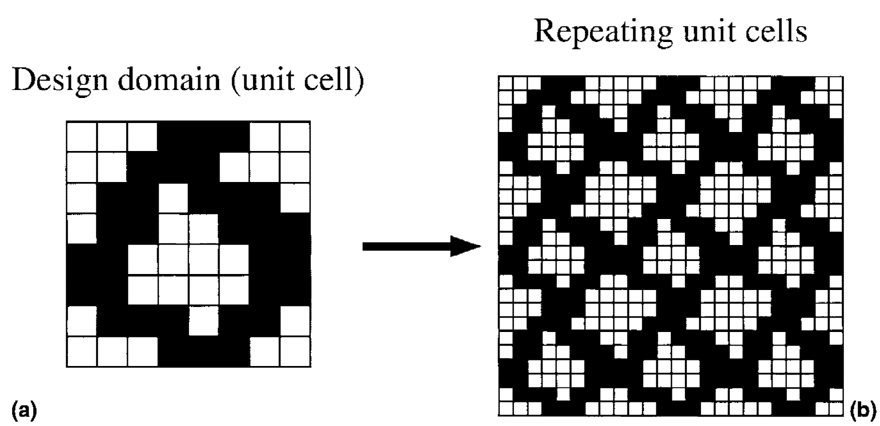


FIG. 1. (a) The design domain is the unit cell of a periodic material which is discretized into finite elements, white representing phase 1 and black representing phase 2. (b) 3 × 3 repeating unit cells.

We take the objective function Φ for the target optimization problem to be given by a least-square form involving the effective property $K_e(\mathbf{x})$ and a target property K_0. The target optimization problem for the target property $K_e(K_1, K_2; \mathbf{x})$ is defined by

$$\text{Minimize: } \Phi = [K_e(\mathbf{x}) - K_0]^2 \quad , \tag{4}$$

$$\text{subject to: } \frac{1}{n}\sum_{i=1}^{n} x_i = \phi_1 \quad ,$$

$0 \leqslant$ xi $\leqslant 1$, i = 1, . . . , n
and prescribed symmetries.

Typically, the volume fraction ϕ_1 is fixed in the simulation. We also impose geometrical constraints (e.g., reflection symmetry) to obtain simple microstructures that achieve the targeted properties.

The objective function Φ is nonlinear but we linearize it to take advantage of sequential linear programming, a well-established optimization technique. The effective property $K_e(\mathbf{x})$ in the objective function Φ is expanded in Taylor series for a given microstructure $\mathbf{x}_0$:

$$\Phi \simeq [K_e(\mathbf{x}_0) + \nabla K_e \cdot \Delta\mathbf{x} - K_0]^2 \quad , \tag{5}$$

$$\simeq [K_e(\mathbf{x}_0) - K_0]^2 + 2[K_e(\mathbf{x}_0) - K_0]\nabla K_e \cdot \Delta\mathbf{x} \quad , \tag{6}$$

where $\Delta\mathbf{x} = \mathbf{x} - \mathbf{x}_0$. An initial microstructure is determined by randomly assigning the design variables x_i to take values between 0 and 1. In each iteration, the microstructure evolves to the targeted state by determining the design variables x_i. Linear programming finds the optimum solution of the design variables $\mathbf{x}$ for the given linearized objective function Eq. (6). Following usual sensitivity analysis,[2] the required derivatives ∇K_e of the objective function with respect to the design variables are determined by the local fields of each element obtained by one finite element calculation.

To carry out the linear programming of the target optimization problem, we introduce the interior-point method,[3] which becomes especially efficient as the number of design variables becomes large. The reason for this is that it is not necessary to define the move limits of all the design variables. Previous topology optimization techniques have used the simplex methods for the linear programming.

The penalization factor scheme[1] is used for the artificial material phase in the relaxation process, which is required to resolve the ill-posedness of the general "0–1" optimization problem. In a design problem for the conductance, the penalization factor p is defined by

$$K(x_i) = K_1 x_i^p + K_2(1 - x_i)^p \quad , \tag{7}$$

where $K(x_i)$ is the conductivity of *i*th element. Note that $K(x_i) = K_1$ when $x_i = 1$ and $K(x_i) = K_2$ when $x_i = 0$. During the optimization procedure, each element is generally in a "composite" state because the relaxed density x_i lies between 0 and 1. By using a high value for the penalization factor p, the density x_i tends to move toward 0 or 1 because it is more economical in the optimization.

In the conventional topology optimization, assigning the penalization factor (p >3) normally works to achieve the final two-phase composite. However, this alone does not work well for target optimization because gray (intermediate) phases tend to remain after many iterations. The reason for this is that target optimization is not a true optimization problem in the sense that it does not necessarily maximize or minimize the properties. Instead, the target optimization method determines a microstructure that achieves targeted properties that generally lie between the optimal properties. Therefore, in addition to Eq. (7), it is necessary to use another constraint to achieve the final two-phase composite. Specifically, in the final stage of the optimization procedure, we add a simple penalty function

$$\Phi_p = -w_p \sum_{i=1}^{n} x_i(x_i - 1) \quad . \tag{8}$$

to the original objective function Eq. (6), where w_p is a weighting factor.

Finally, a conventional filtering scheme[2] is adapted to avoid microscale structures. Normally, the filtering range is initially set up to be similar to the size of the unit cell to achieve a single-scale structure in the design domain. The filtering range is gradually decreased during the course of the simulation.

IV. BACKGROUND ON CONDUCTIVITY PROBLEM

To illustrate the target optimization technique, we will carry out specific calculations for the effective conductivity problem. However, before presenting our calculations, it is necessary to review some important basic work in the theory of composites that is particularly pertinent to the optimization problem at hand.

Consider isotropic two-phase composites with phase conductivities $K_1 \equiv \sigma_1$ and $K_2 \equiv \sigma_2$ and phase volume fractions ϕ_1 and ϕ_2. For simplicity, we assume ideal interfaces. A very fundamental question in the theory of composites is the following: What are the microstructures that either maximize or minimize the effective conductivity σ_e for a prescribed volume fraction? This question was answered in three dimensions by Hashin and Shtrikman[4] who found the best possible bounds on σ_e (given volume fraction information) and microstructures that realize them. Analogous two-dimensional bounds were found by Hashin.[5] In any dimension, we refer to these as the Hashin–Shtrikman (HS) bounds. In two dimensions and for $\sigma_2 \geqslant \sigma_1$, they are given by

$$\sigma_L \leqslant \sigma_e \leqslant \sigma_U \quad , \tag{9}$$

where

$$\sigma_L = \langle\sigma\rangle - \frac{\phi_1\phi_2(\sigma_1 - \sigma_2)^2}{\langle\tilde{\sigma}\rangle + \sigma_1} \quad , \tag{10}$$

$$\sigma_U = \langle\sigma\rangle - \frac{\phi_1\phi_2(\sigma_1 - \sigma_2)^2}{\langle\tilde{\sigma}\rangle + \sigma_2} \quad . \tag{11}$$

Here

$$\langle\sigma\rangle = \sigma_1\phi_1 + \sigma_2\phi_2 \quad , \tag{12}$$

$$\langle\tilde{\sigma}\rangle = \sigma_1\phi_2 + \sigma_2\phi_1 \quad . \tag{13}$$

The reason why the HS bounds Eq. (9) are the best possible (optimal) bounds given volume fraction information is that they are realizable by a special dispersion of circular inclusions.[5] Specifically, the lower bound is realized by a dispersion consisting of composite circular inclusions that are composed of a circular core, of conductivity σ_2 and radius a, which is surrounded by a concentric shell of conductivity σ_1 with an outer radius b. The ratio $(a/b)^2$ is fixed and equal to the inclusion volume fraction ϕ_2. The composite inclusions fill all space, implying that there is a distribution in their sizes ranging to the infinitesimally small. Thus, the more conducting phase always disconnected (except at the trivial point $\phi_2 = 1$). Indeed, as far as the effective conductivity σ_e is concerned, the HS lower bound construction may be regarded as the most "disconnected" arrangement of the conducting material since phase-2 elements are well separated from each other. The upper bound is realized by the same microstructure but with the phases interchanged. Here the conducting phase is always a connected phase (except at the trivial point $\phi_2 = 0$) and hence may be regarded as the most "connected" arrangement of the conducting material.

However, these multisized coated inclusions are not the only structures that realize the bounds Eq. (9). For example, the single-scale Vigdergauz[7,8] constructions that realize the HS bounds on the effective planar bulk modulus also realizes the bounds Eq. (9). In so far as the effective conductivity is concerned, the connectivities of the Vigdergauz constructions are identical to those of the HS constructions.

Importantly, since the HS bounds are optimal, all isotropic composites must have effective conductivities that lie between them. Although certain classes of optimal structures are known (as discussed above), the structures that lie between the extreme values of the effective conductivity are not known. As one application of the target optimization technique, we will find the intermediate structures.

V. ILLUSTRATIVE EXAMPLES

A. Geometric-mean effective conductivity

To begin, we choose the target effective conductivity σ_e at the volume fraction $\phi_1 = \phi_2 = ½$ to be the geometric average of the phase conductivities, i.e.,

$$\sigma_e = \sqrt{\sigma_1\sigma_2} \quad . \tag{14}$$

We make this choice because it is one of the rare instances in the theory of composites in which we have exact results. Specifically, Eq. (14) is exact for any two-phase, two-dimensional composite whose phase topologies are statistically equivalent to one another.[6] This class encompasses a variety of different composites, including the regular checkerboard as well as the random checkerboard. Therefore, it will be of interest to see what microstructure our target optimization algorithm yields when Eq. (14) is employed.

Starting from a random initial guess, we have carried out the simulation for a target effective conductivity σ_0 given by Eq. (14) in which $\sigma_1 = 1$ and $\sigma_2 = 10$; i.e., $\sigma_0 = \sqrt{10} \approx 3.1623$. We imposed reflection symmetry about the horizontal and vertical axes. Figure 2 shows the resulting microstructure for 2 × 2 repeated unit cells. Interestingly, we see that our algorithm finds the regular checkerboard. This particular geometry is found because of the symmetries that we impose and the size of the "filter" that we use to avoid local minima.[2] Note that conduction is dominated by transport through the "necks" (corner points) connecting the conducting phase, especially for high phase contrast ratio. The effective conductivity of the composite structure shown in Fig. 2 is

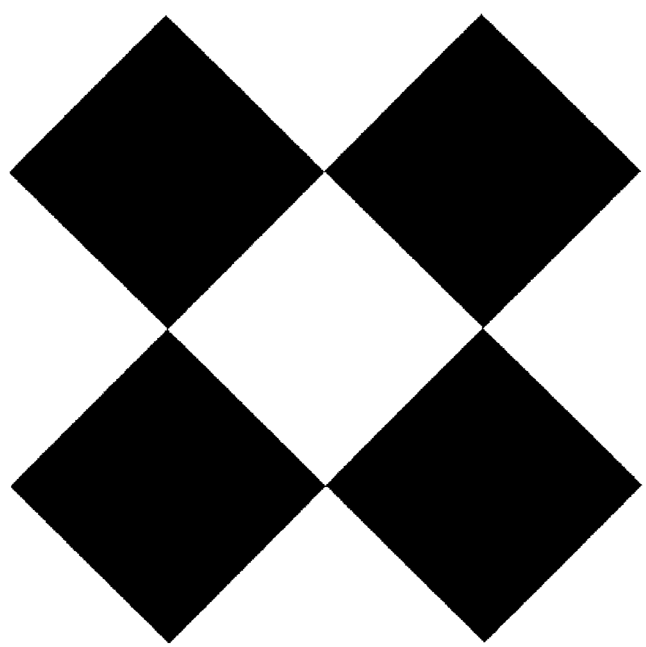
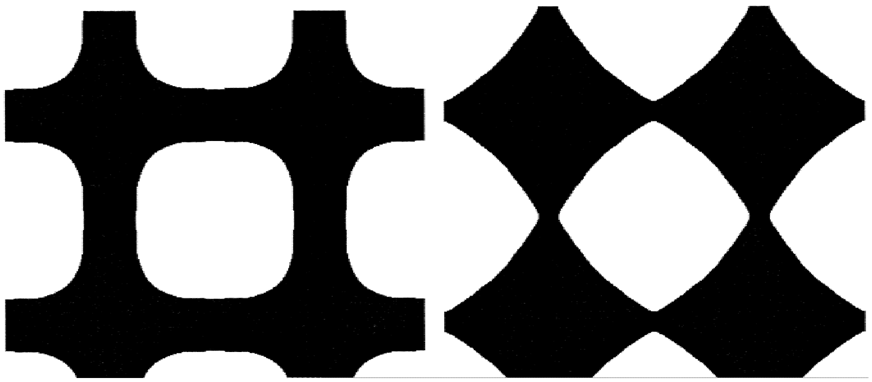


FIG. 2. Regular checkerboard (2 × 2 unit cells) found by target optimization for $\phi_2 = ½$, $\sigma_1 = 1$, and $\sigma_2 = 10$.

given by $\sigma_e = 3.12$. Most of the error of about 1% from the targeted value is due to discretization error in resolving the corner connections in the checkerboard, not the optimization part of the routine.

This example clearly shows that our target optimization procedure can yield microstructures with targeted properties with minimal error. Therefore, it is an important benchmark.



B. Structures lying between HS bounds

Here our aim is to generate the possible structures that lie between the HS bounds (9) at a fixed volume fraction, including the known optimal Vigdergauz structures[7,8] that lie at the extremes. Obtaining the extremal structures will be another test of the target optimization method since it must also be able to yield these optimal structures when the target is specified as such.

Finding the structures that lie between them will enable us to study how the degree of connectivity of the conducting phase changes from the extreme values. Recall that the structures corresponding to the HS lower and upper bounds may be regarded to be the most disconnected and connected arrangements of the conducting phase, respectively.

Accordingly, let the target effective conductivity be given by

$$\sigma_0 = \sigma_L + \alpha(\sigma_U - \sigma_L) \quad , \tag{15}$$

where σ_L and σ_U are the lower and upper bounds given by Eqs. (10) and (11) and $\sigma_U - \sigma_L$ is the bound width. Thus, by varying the parameter α between 0 and 1, one can continuously span between the lower bound value and the upper bound value, respectively.

As in the previous example, we have carried out simulations for $\phi_2 = ½$ with $\sigma_1 = 1$ and $\sigma_2 = 10$ and have imposed reflection symmetry about the horizontal and vertical axes. Here we use the target conductivity Eq. (15) and consider the cases $\alpha = 0$, 0.2, 0.4, 0.6, 0.8 and 1. Figure 3 depicts the resulting microstructures for 2 × 2 repeated unit cells. Table I shows that associated effective conductivities are in very good agreement with the targeted effective conductivities.

First, we observe that our program correctly finds the optimal Vigdergauz constructions at the extremes; i.e., $\alpha = 0$ and $\alpha = 1$. This provides further evidence that our optimization algorithm accurately yields targeted microstructures. We see that as α increases from 0 to 0.4, the conducting phase remains disconnected but changes to squarelike inclusions. At $\alpha = 0.4$, the structure is very close to the regular checkerboard but the corners of adjacent squarelike conducting inclusions do not touch; i.e., the system does not percolate. At $\alpha = 0.43$ (not shown in Fig. 3), we know from our previous calculation that the structure is indeed the regular checkerboard, which percolates due to touching conducting corners. At $\alpha = 0.6$, the conducting phase consists of squarelike inclusions on a checkerboard but with small "bridges" between the corners. At $\alpha = 0.8$, the bridges are more pronounced.

TABLE I. Comparison of the effective conductivities σ_e to be targeted conductivities σ_o for points between the HS bounds for $\phi_2 = 0.5$, $\sigma_1 = 1$, and $\sigma_2 = 10$.

$\alpha \times 100\%$	σ_0	σ_e
100%	4.194	4.188
80%	3.832	3.852
60%	3.470	3.487
40%	3.109	3.042
20%	2.747	2.760
0%	2.385	2.393

VI. CONCLUDING REMARKS

In this article, we have introduced a numerical method to identify specific microstructures of composite materials that have targeted properties that we call target optimization. The conventional topology optimization is adapted to perform this target optimization with a revised objective function. Moreover, unlike previous work, we use the interior-point method to perform the linear programming. The method is quite general and can treat transport, mechanical, and electromagnetic properties, as well as properties associated with coupled phenomena, such as piezoelectric and thermoelectric coefficients. To illustrate the technique, we have successfully found two-phase composite microstructures in two dimensions having specified effective electrical or thermal conductivities at fixed volume fractions. Although we have focused on a single targeted property, the method can also treat several properties by simply adding quadratic terms to the objective function as follows:

$$\Phi = \kappa_1[K_e^{(1)} - K_0^{(1)}]^2 + \kappa_2[K_e^{(2)} - K_0^{(2)}]^2 + \kappa_3[K_e^{(3)} - K_0^{(3)}]^2 + \cdots \quad , \tag{16}$$

where $K_e^{(1)}, K_e^{(2)}, K_e^{(3)}, \cdots$ are the effective properties of interest, $K_0^{(1)}, K_0^{(2)}, K_0^{(3)}, \cdots$ are the associated target properties and $\kappa_1, \kappa_2, \kappa_3, \cdots$ are scalar weights. Therefore, the method can also be used to design microstructures with multifunctional characteristics.

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