

## THE TOPOLOGICAL DESIGN OF MATERIALS WITH SPECIFIED THERMAL EXPANSION USING A LEVEL SET-BASED PARAMETERIZATION METHOD

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In this paper, a level set-based parameterization method is proposed to design the three-phase composite material with specified thermal expansion coefficient. The composites are comprised by periodic base cells, and made of a three-phase material (two different material phases and a void phase). The numerical homogenization method is applied to compute effective elastic and thermal expansion properties of the composite based on a finite-element discretization of the base cell. The optimal distribution of material phases within the periodical unit cell is found using level set-based parameterization method under certain constraints, such as elastic symmetry, volume fractions of the constituent phases, and lower limit of bulk modulus. A MATLAB program is developed to conduct the composite material design and the results demonstrate that materials with zero and negative effective thermal expansion coefficients can be achieved by three-phase materials.

## Introduction

Topology optimization has been identified as one of the most promising structural optimization disciplines due to its establishing an overall framework of the conceptual design without prior knowledge of an optimal shape and size design. The discipline has experienced considerable progress during the past decades, and is being extended to a wide variety of engineering areas, especially since the prominent research work of Bendsøe and Kikuchi [1] and the recently published works of Wang et al. [2] and Allaire et al. [3]. Topology optimization actually consists of determining the best arrangements of a prescribed sum of material to iteratively eliminate and redistribute them throughout the design space to get the best structural performance. Topology optimization has been identified as one of the most promising structural optimization disciplines due to its establishing an overall framework of the conceptual design without prior knowledge of an optimal shape and size design.

The level set methods were originally developed for tracking, modelling, and simulating the evolution of moving boundaries with topology changes of merging and breaking naturally. They have found a wide range of successful applications, such as in fluid mechanics, solids modeling, computer animation, material science, crack propagation, and image processing. Sethian and Wiegmann [4] are among the first researchers to initially introduce the level set methods into structural optimization areas with an Eulerian representation, in which the shape and topology changes of the design boundary are achieved in accordance with the equivalent stresses on the boundaries. A family of level set structural optimization works has been reported using an implicit boundary representation. The highlight of these works is to bridge the classical shape derivative with the powerful level set method. Wang and Wang [5] introduced globally supported radial basis functions (RBFs) into conventional level set methods to interpolate the level set function, and the original partial differential equation (PDE) is transformed into a set of mathematically more convenient ordinary differential equations (ODEs). Their work has explored the promising characteristics of RBF-based level set structural optimization approaches, but further investigation is needed to study numerical considerations such as convergence, sparseness, stability, and errors accumulation.

Here, an efficient parameterization method [6] is developed as an alternative to perform structural shape and topology optimization. The compactly supported radial basis function (CS-RBF) is employed to interpolate the level set function with a desirable smoothness and accuracy. Then, the temporal and spatial initial value problem, defined as the Hamilton–Jacobi PDE, is converted to a parametric problem. The shape functions are spatial only while the expansion coefficients, being posed as design variables, are temporal. An efficient convex programming is applied to solve the parametric optimization, leading to higher computational efficiency.

Materials with specific or unusual thermal expansion behaviour are of interest from both a technological and fundamental standpoint. Examples include materials with zero thermal expansion or negative thermal expansion.

Zero thermal expansion materials are needed in structures subject to temperature changes such as space structures, bridges, and piping systems. A fastener made of a negative thermal expansion material, upon heating, can be inserted easily into a hole. Upon cooling it will expand, fitting tightly into the hole. Three phases are used as opposed to two phases, since one can achieve composite properties beyond those of the individual components [7]. In this

paper we use a level set-based parameterization method to determine the distribution of two different bulk material phases and a void phase to design 2D composites with specific thermal expansion behaviour.

### Parameterization of level set-based model

In this level set method, the interface is embedded into a higher-dimensional level set surface as a set of constant level-sets (e.g. 2D boundary to 3D surface), compared to the zero level set in the standard level set method [8] [9]. A level set function  $\Phi(\mathbf{x}, t)$  with Lipschitz continuous is defined over a reference domain  $D \subset R^d$  ( $d = 2$  or  $3$ ). The three-dimensional structure is embedded as follows:

$$\begin{cases} \Phi(\mathbf{x}, t) > 0 & \forall \mathbf{x} \in \Omega \setminus \partial\Omega \text{ (inside)} \\ \Phi(\mathbf{x}, t) = 0 & \forall \mathbf{x} \in \partial\Omega \cap D \text{ (boundary)} \\ \Phi(\mathbf{x}, t) < 0 & \forall \mathbf{x} \in D \setminus \Omega \text{ (outside)} \end{cases} \quad (1)$$

To enable the dynamic motion, introducing the pseudo-time  $t$  into the level set function leads to the following first-order ‘Hamilton-Jacobi type’ PDE by differentiating it on both sides with respect to pseudo-time  $t$ :

$$\frac{\partial\Phi(\mathbf{x}, t)}{\partial t} + \mathbf{v}_n |\nabla\Phi| = 0, \quad \Phi(\mathbf{x}, 0) = \Phi_0(\mathbf{x}) \quad (2)$$

The normal velocity is expressed as follows:

$$\mathbf{v}_n = \mathbf{v} \cdot \mathbf{n} = \mathbf{v} \cdot \frac{\nabla\Phi}{|\nabla\Phi|} = \frac{d\mathbf{x}}{dt} \cdot \frac{\nabla\Phi}{\sqrt{\nabla\Phi \cdot \nabla\Phi}} \quad (3)$$

Hence, moving boundary  $\Gamma = \{\mathbf{x} | \Phi(\mathbf{x}) = C\}$  along normal direction  $\mathbf{n} = \nabla\Phi/|\nabla\Phi|$  is equivalent to transporting  $\Phi$  by solving the Hamilton-Jacobi PDE with explicit time-marching schemes [2] [3] on a fixed Eulerian rectilinear grids. The velocity field is generally determined using the shape derivative analysis. As aforementioned, numerical difficulties in solving the complicated Hamilton-Jacobi PDEs limit the further application of the level set method to topology optimization [6].

In the present work, the CS-RBF designed by Wendland [10] with desired smoothness is introduced to interpolate the higher-dimensional level set function. We adopt the following popular CS-RBF with C2 smoothness,

$$\phi(r) = \max\{0, (1-r)^4\} (4r+1) \text{ (Wendland - C2)} \quad (4)$$

Using the CS-RBF, the level set function can be described by centrally positioning the CS-RBFs at their pre-specified knots over the whole design domain, as

$$\Phi(\mathbf{x}) = \boldsymbol{\varphi}(\mathbf{x})^T \boldsymbol{\alpha} = \sum_{i=1}^N \phi_i(\mathbf{x}) \alpha_i \quad (5)$$

with a vector of the shape functions

$$\boldsymbol{\varphi}(\mathbf{x}) = [\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \dots, \phi_N(\mathbf{x})]^T \in \mathbb{R}^N \quad (6)$$

and the expansion coefficient vector

$$\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \dots, \alpha_N]^T \in \mathbb{R}^N \quad (7)$$

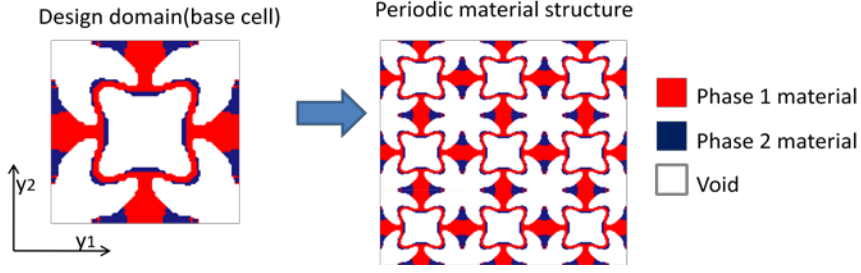
The interpolant of the level set function is uniquely determined in terms of the given interpolating data of the level set function located at the knots, owing to the property of strict positive definiteness of the CS-RBFs.

### Topology optimization for three-phase composite

The aim of this work is to optimize microstructural topologies of the composite under given effective thermal tensors  $\alpha_{ij}^H$  and amounts of two material phases and void (three-phase in total) within the design domain. It should also be possible to specify elastic symmetries such as orthotropy, square symmetry or isotropy of the resulting materials. An optimization problem including these features can be written as:

$$\left\{ \begin{array}{l} \text{Minimize : Some function of the effective thermal coefficient } \alpha_{ij}^H, \\ \text{Variables : Distribution of Two material phases and void in the base cell,} \\ \text{Subject to : Constrains on volume fractions,} \\ \quad \text{Orthotropy, square symmetry or isotropy constrains,} \\ \quad \text{Lower bound constraints on stiffness,} \\ \quad \text{Bounds on design variables.} \end{array} \right. \quad (8)$$

The material type, that is, material phase 1, phase 2 or void, can vary from finite element to finite element as seen in Fig. 1. With a fine finite-element discretization, this allows us to define complicated bimaterial topologies within the design domain. Having discretized the design domain (the periodic base cell) with finite elements, the design problem consists in assigning either phase 1, 2 or void to each element such that the objective function is minimized. Since the base cell has been assumed small enough and be periodically repeated in the material, the macro property of the periodic material is computed using homogenization method [11].



**Figure 1: Design domain for the three-phase topology optimization problem.**

Using a simple artificial mixture assumption, the local stiffness and thermal strain coefficient tensor,  $C_{ijkl}^e$  and  $\alpha_{ij}^e$ , in element  $e$  can be written as a function of the two design variables  $\varphi_1^e$  and  $\varphi_2^e$ .

$$C_{ijkl}^e(\varphi_1^e, \varphi_2^e) = H(\varphi_1^e)((1 - H(\varphi_2^e))C_{ijkl}^1 + H(\varphi_2^e)C_{ijkl}^2) \quad (9)$$

$$\alpha_{ij}^e(\varphi_1^e, \varphi_2^e) = (1 - H(\varphi_2^e))\alpha_{ij}^1 + H(\varphi_2^e)\alpha_{ij}^2 \quad (10)$$

Where  $H(\varphi)$  is the Heaviside function.

For a base cell  $Y$  which is discretized by finite elements, the homogenized stiffness tensor and thermal stress tensor can be computed by

$$C_{ijkl}^H = \frac{1}{|Y|} \int_Y (\varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^{*(ij)}) C_{pqrs}^e (\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^{*(kl)}) dy \quad (11)$$

$$\beta_{kl}^H = \frac{1}{|Y|} \int_Y (\alpha_{pq}^e - \varepsilon_{pq}^{C*}) C_{pqkl}^e (\varepsilon_{kl}^{0(ij)} - \varepsilon_{kl}^{*(ij)}) dy \quad (12)$$

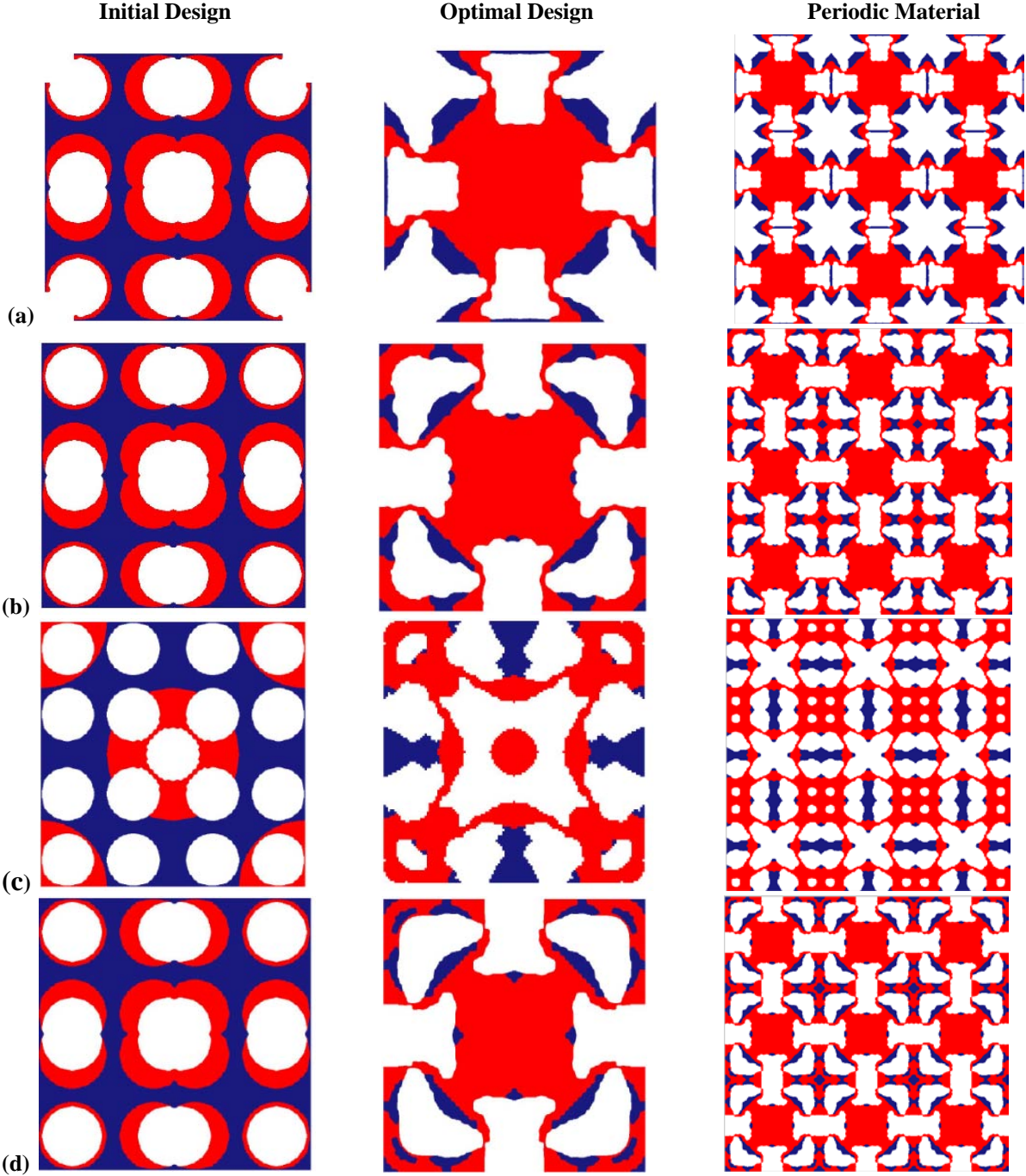
$$\alpha_{ij}^H = (C_{ijkl}^H)^{-1} \beta_{kl}^H \quad (13)$$

where  $C_{ijkl}^H$  is the effective stiffness tensor,  $\beta_{kl}^H$  is the effective thermal stress tensor,  $\alpha_{ij}^H$  is the effective thermal strain tensor,  $\varepsilon^0$  and  $\varepsilon^*$  are the unit test strain fields and the strains tensor with the displacement field,  $|Y|$  is the volume of the cell.

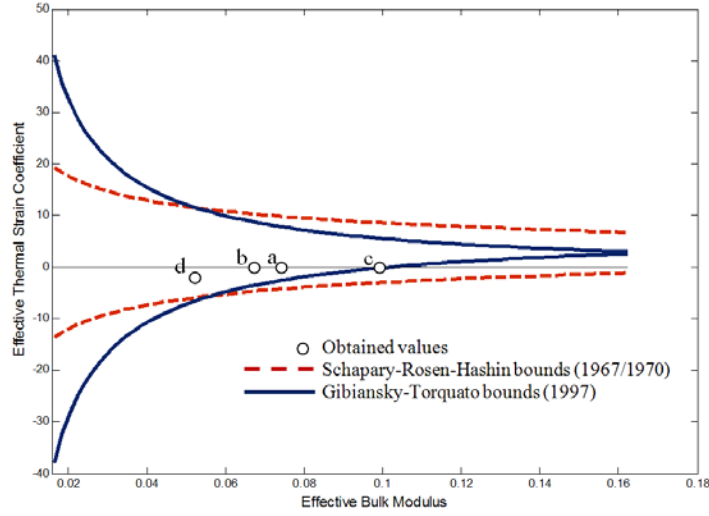
## Design Examples

In this section, we investigated by unusual examples for three-phase composites to illustrate the effectiveness of the proposed scheme. The phase data are taken as  $E_1 = E_2 = 1$ ,  $\nu_1 = \nu_2 = 0.3$ ,  $\alpha_1 = 1$ ,  $\alpha_2 = 10$ . We consider the design material to achieve zero and negative effective thermal expansion with horizontal, vertical and diagonal geometric symmetry is

specified. The volume fractions are prescribed to be  $c_1 = 40\%$ ,  $c_2 = 10\%$  and the volume of void is  $c_0 = 50\%$  and there is a lower bound of effective bulk modulus is constraint  $k^H \geq 0.05$ .



**Figure 2: Cases (a) (b) (c): optimal microstructures for zero effective thermal strain coefficient with different initial design; Cases (d): optimal microstructures for negative effective thermal strain coefficient**



**Figure 3: Bounds for three-phase design example. The circles with letters a-d denote the obtained values for the microstructures shown in Figure 2.**

TABLE I. Thermoelastic parameters for optimal microstructures

Case	Objective	$\alpha^H$	$k^H$
(a)	$\alpha^H = 0$	0.0005000	0.067
(b)	$\alpha^H = 0$	0.0002996	0.0622
(c)	$\alpha^H = 0$	0.0005088	0.0992
(d)	$\alpha^H = -0.5$	-0.5000000	0.0525

The resulting topologies are shown in Figure 2 and their effective properties are shown in Table 1 and plotted as small circles in Fig. 3. There is a good agreement between the effective properties is observed and two property bounds, the old and new theoretical bounds are given by [12] and [13], respectively. Design cases (a) and (c) in Figure 2 demonstrate how, topologically, very different microstructures can have (almost) the same value of the objective function. The only difference among the three cases is the initial design. It is due to that the topology optimization problem is very prone to converge to local minima.

The actual mechanisms behind the extreme thermal expansion coefficients of the material structures can be difficult to understand. From the optimal microstructure topologies, we can estimate that the displacements, due to an increase in temperature of the microstructure appear to be contact between parts of the microstructure. When allowing low bulk modulus, the main mechanics behind the negative thermal expansion is the re-entrant cell structure having multi-material components which bend and cause large deformation when heated. The multi-material interfaces of design examples bend and make the cell contract, similar to the behaviour of negative Poisson's ratio materials [14].

## Conclusions

We have applied a level-set based parameterization method to design material microstructures with specified thermoelastic properties. For the topology optimization method in general, the

results in this paper show, that the method produces designs which are optimal indeed. We note that the method is applicable to design of smart materials. In a future paper, the procedure described here will be used to find the structures that optimize the bio-material. The method can also be modified to handle three-dimensional microstructures. The extension to three dimensions is straightforward, but computer time will increase dramatically.

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