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Design methodology for porous composites with tunable thermal expansion produced by multi-material topology optimization and additive manufacturing

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A B S T R A C T

To realize negative thermal expansion (NTE), porous composites made of two materials with different coefficients of thermal expansion are being actively researched. NTE can be realized by taking advantage of the thermal deformation mechanisms of a composite material's internal geometry. However, in addition to negative thermal expansion, materials with anisotropic and large positive thermal expansion are also desirable for various applications. Also, additive manufacturing provides new ways to fabricate composites by layering multiple materials at arbitrary points in three-dimensional space. In this study, we developed a design methodology for porous composites, which showed defined thermal expansion characteristics, including negative and positive thermal expansion as well as isotropic and anisotropic thermal expansion. Our approach was tested based on the fabrication of a multi-material photopolymer by additive manufacturing. The internal geometries required to produce such characteristics were designed by topology optimization, which is the most effective structural optimization method for realizing macroscopic inward deformation and for maintaining stiffness. The designed structures were converted to three-dimensional models and fabricated by multi-material photopolymer additive manufacturing. Using laser scanning dilatometry, we measured the thermal expansion of these specimens, revealing well-ordered thermal expansion, from anisotropic positive thermal expansion to anisotropic negative thermal expansion, over a wide range of about -3×10^{-4} K^{-1} to 1×10^{-3} K^{-1}.

1. Introduction

Thermal expansion is an important phenomenon in many applications. A large positive thermal expansion (PTE) is useful in thermal actuators and medical vessel dilators that operate based on human body temperature. A negative thermal expansion (NTE) is useful for canceling the thermal expansion of ordinary materials in high-temperature or high-precision devices. Because naturally occurring NTE is rare, materials that exhibit NTE have drawn considerable attention (e.g. Refs. [1–3]). However, NTE is limited to specific perovskite ceramics and tuning of NTE performance remains challenging.

Another way to realize NTE is by constructing a porous composite of two materials with different coefficients of thermal expansion (CTE). This approach can realize an effective (macroscopic average) NTE because of the internal geometry of the composite. For example, as the temperature rises, the system may exhibit inward deformation toward voids in the internal geometry, induced by bending of layers of materials that show different thermal expansion such as bimetals. Both theoretical and experimental studies of materials with negative thermal expansion and their internal structures, have been performed [4–13].

The design of the internal structure of porous composites, which allow for inward deformation, must consider the thermal deformation of the composite materials, which is related to their stiffness and CTE. Numerical structural optimization could be a powerful way to design complicated structures, because it allows for automatic structural optimization through numerical structural analysis and optimization techniques. In particular, topology optimization can be used to fundamentally optimize the target

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structure, including the number of void spaces [14]. This approach could be used in the design of composite materials and structures [4,11,12,15]. Some studies have used topology optimization to tune the negative thermal expansion of materials based on their internal geometry [4,11,12]. Although these approaches can generate structures that match arbitrary performance targets, the study of CTE topology optimization has been limited to isotropic NTE behavior. However, devices that require only axial NTE or an extra-large PTE might also have valuable applications.

On the experimental side, additive manufacturing and rapid prototyping have been used [16] to produce detailed 3D structures. Recent developments in technology have improved the manufacturing accuracy and the level of detail possible in 3D composites and porous materials to a scale of about 10 μm. Such small-scale fabrication can be used to develop novel composite materials [15,17–21]. Additive manufacturing could be another approach that can easily produce multi-material composites by controlling the location of the supplied material. This is a simpler process for the fabrication of NTE porous composites, which usually requires involved techniques such as micro-fabrication by co-extrusion and reduction sintering [6] or microelectromechanical fabrication [10]. Thus, additive manufacturing could be an effective way to simply fabricate porous composites that show NTE behavior [12,13].

In the present study, we developed a design methodology for porous composites with arbitrary thermal-expansion characteristics derived from their internal geometry. For the first time we also examined NTE together with isotropic and anisotropic, extra-large effective PTE behaviors in these structures. We used a numerical topology optimization based on the finite element method (FEM), to design the internal geometry and maximize the macroscopic inward or outward deformation while maintaining a certain stiffness. Test pieces with the designed internal structure were fabricated from a photopolymer by additive manufacturing. The internal thermal expansion of the test pieces was verified by measuring their thermal deformation with a laser scanning dilatometer.

2. Theoretical background of design methodology

2.1. Mechanics of porous composites

Here, we investigate the thermal expansion of a porous composite having an internal structure with a periodic layout in a plane using FEM. We assume that the thermal expansion of the material's internal structure follows linear elastic theory:

$$\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \Delta T \alpha_{kl}) = C_{ijkl}\beta_{kl}, \tag{1}$$

where $\boldsymbol{\sigma}$, C, ε, $\boldsymbol{\alpha}$, and $\boldsymbol{\beta}$ are the stress tensor, elastic tensor, strain tensor, CTE tensor, and thermal stress tensor, and ΔT is the temperature change from a reference temperature. The displacement $\mathbf{u}$ is related to the strain by $\varepsilon = \frac{1}{2}\{\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\}$. By solving this equation though FEM, after setting appropriate boundary conditions, one can determine the displacement distribution of the internal geometry of the porous composite caused by thermal expansion.

The effective physical properties of a porous material with a repeating unit cell can be calculated by numerical homogenization [22–24]. The effective elastic tensor C^H, CTE tensor α^H, and thermal stress tensor β^H of the periodic structure composed of a unit cell Y are calculated as:

$$C^H_{ijkl} = \frac{1}{|Y|}\int_Y \left(C_{ijkl} - C_{ijpq}\frac{\partial \chi_p^{kl}}{\partial y_q} \right) \mathrm{d}Y, \tag{2}$$

$$\alpha^H_{ij} = \left[C^H_{ijpq}\right]^{-1}\beta^H_{pq} = \left[C^H_{ijpq}\right]^{-1}\frac{1}{|Y|}\int_Y \left(\beta_{pq} - C_{pqkl}\frac{\partial \psi_k}{\partial y_l} \right) \mathrm{d}Y, \tag{3}$$

where $\boldsymbol{\chi}$ and $\boldsymbol{\psi}$ are the values of displacement obtained by solving the problem of Y-periodic cells expressed as:

$$\int_Y C_{ijpq}\left(\delta_{pk}\delta_{ql} - \frac{\partial \chi_p^{kl}}{\partial y_q} \right)\frac{\partial v_i}{\partial y_j}\mathrm{d}Y = 0, \tag{4}$$

$$\int_Y \left(\beta_{ij} - C_{ijkl}\frac{\partial \psi_k}{\partial y_l} \right)\frac{\partial v_i}{\partial y_j}\mathrm{d}Y = 0, \tag{5}$$

where $\mathbf{v}$ is an arbitrary test function. As for Eq. (1), these equations are solved by FEM.

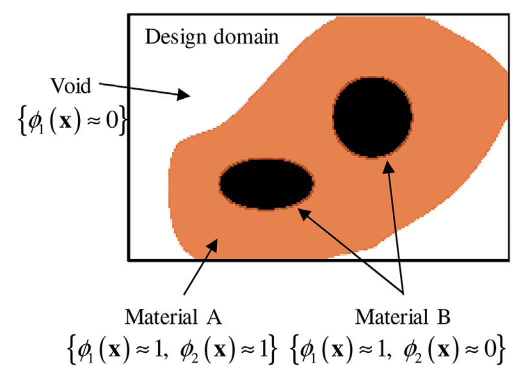

Fig. 1. Outline of the domain representation by multi-material topology optimization.

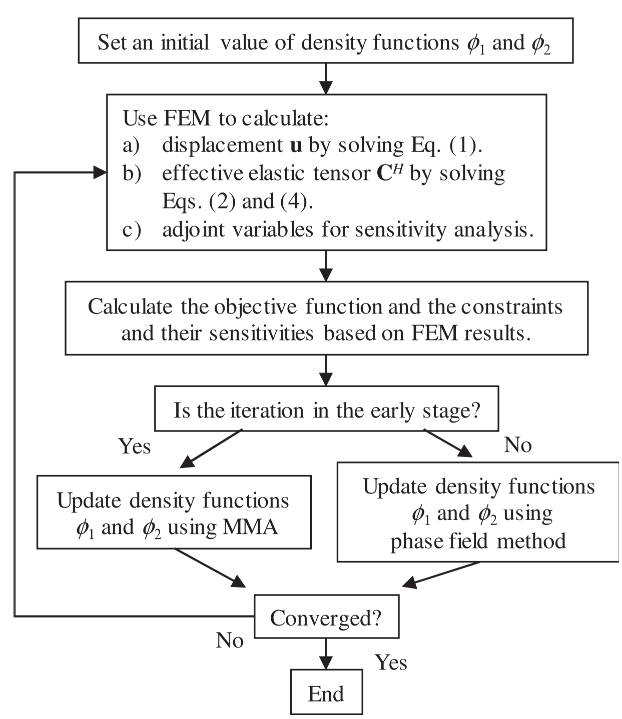

Fig. 2. Flowchart of the topology optimization procedure.