Analysis and optimization of thermoelastic structures with tension–compression asymmetry

Zongliang Du a,b, Yibo Jia a, Hayoung Chung c,x, Yupeng Zhang d, Yuan Li c,f, Hao Zhou g, Xu Guo a,b,*

a State Key Laboratory of Structural Analysis for Industrial Equipment, Department of Engineering Mechanics, Dalian University of Technology, Dalian, 116023, PR China
b Ningbo Institute of Dalian University of Technology, Ningbo, 315016, PR China
c Institute for Research and Development, Dalian Institute of Technology, Dalian, 116023, PR China
d Department of Mechanical Engineering, Ulsan National Institute of Science and Technology, Ulsan, 44919, Republic of Korea
e Innovation & Research Institute of Hiwing Technology Academy, Beijing, 100074, PR China
f Xi'an Jiaotong University, Xi'an, 710049, PR China
g Dongfang Electric Wind Power Co. LTD, Deyang, 618000, PR China
h Beijing Institute of Spacecraft System Engineering, China Academy of Space Technology, Beijing, 100094, PR China

ARTICLE INFO

Keywords:
Tension–compression asymmetry
Thermo-mechanical coupling
Variational principle
Numerical analysis
Topology optimization

ABSTRACT

Many engineering and biological materials have been found to have tension–compression asymmetry properties. An extension of the linear thermoelastic behavior called a bi-modulus constitutive model is proposed to study the impact of thermo-mechanical coupling in such materials and structures. The well-posedness of the corresponding bi-modulus thermoelasticity problems is confirmed via a variational approach. An efficient numerical analysis method is developed for such nontrivial material behavior and is further employed for structural topology optimization. The importance of the proposed analysis and design framework is demonstrated by the significant impact of the tension–compression asymmetry and thermal effect on structural responses and optimum structural configurations.

1. Introduction

Tension–compression asymmetric mechanical response has been reported in numerous materials and structures. In addition to many engineering materials such as concrete, fiber-reinforced composites (Ambartsumyan, 1986), shape memory alloys (Liu et al., 1998), numerous biological materials, such as skin (Romero et al., 2017) and brain tissues (Budday et al., 2017), show significant tension–compression asymmetry (TCA). TCA is often caused by microscale behavior such as microbuckling (Notbohm et al., 2015), unilateral contact (Bertoldi et al., 2008), and propagation or close of microcracks (Mattos et al., 1992). Recently, there has been growing research interest in TCA because of its effect on mechanically nontrivial behaviors.

By introducing different material parameters under tension and compression, the behavior of materials with TCA can be effectively described. In particular, Ambartsumyan’s monograph introduced the so-called bi-modulus elasticity theory with related experiments and analytical solutions, which assumes different Young’s modulus and Poisson’s ratio depending on the material’s tension and compression condition (Ambartsumyan, 1986). It has been shown that this bi-modulus constitutive model is useful not only for classical engineering materials (Ambartsumyan, 1986) but also very effective in accounting for the TCA effect in many soft matters (Sun et al., 2011; Notbohm et al., 2015; Du et al., 2020). Recently, variational principles (Du and Guo, 2014), advanced analytical solutions (Sun et al., 2010; Rosakis et al., 2015; Huang et al., 2016; Du et al., 2020), and efficient numerical analysis algorithms have all been developed based on the bi-modulus elasticity theory (Zhang et al., 2011, 2012; Du et al., 2016; Pan et al., 2020b; Kanno, 2022), and design optimization framework (Cai et al., 2016; Du et al., 2019). Additionally, the idea of asymmetric material constants for tension and compression is successfully extended to hyperelastic model (Du et al., 2020; Latorre and Montáns, 2020), fracture analysis (Zhang et al., 2019; Pan et al., 2020a), creep and damage mechanics (Guo et al., 2021).

It should be noted that the Ambartsumyan’s bi-modulus model is limited to three moduli and infinitesimal small deformation cases, and more generally applied hyperelastic constitutive models have been proposed recently to take the tension–compression asymmetry effect into account (Du et al., 2020; Latorre and Montáns, 2020). To the authors’ knowledge, however, most existing studies about the material...
with TCA focus on the structural responses under pure mechanical loads. There has not been much research done on how structures with TCA respond to the thermo-mechanical environment, or bi-modulus thermoelasticity, which is crucial for engineering applications. The motivation of the present work is to generalize the variational principles, efficient numerical algorithm, and topology optimization of bi-modulus elastic system to include the thermoelastic effect.

The constitutive model for bi-modulus thermoelasticity, which is developed in the principal stress/strain space, is initially proposed in Section 2. In Section 3, using the proposed variational principles, we studied the well-posedness of the bi-modulus thermoelasticity problem based on the unified energy densities expressed as semi-definite programming. In Section 4, an efficient numerical analysis method is developed and validated by comparing it with the analytical solutions for thermoelastic structures with TCA. In Section 5, the material model is further employed in the design optimization framework using the Moving Morphable Components method. Finally, concluding remarks are summarized in Section 6.

2. Constitutive model for thermo-mechanical behavior with TCA

It is well known that temperature variation causes a volumetric change for an unrestrained elastic solid. Thus, mechanical and thermal effects are coupled to produce the structural response. Under the isotropic thermal expansion and infinitesimal strain assumptions, the total strain can be decomposed into the mechanical and thermal parts (Sadd, 2009), i.e.,

\[ \varepsilon = \varepsilon + \theta = \varepsilon + a\Delta T \delta \]

where \( \varepsilon \) and \( \theta \) are the mechanical strain and thermal strain, respectively. \( a\Delta T \delta \) is the isotropic coefficient of thermal expansion tensor with \( \delta \) denoting the Kronecker delta, and \( \Delta T \) is a prescribed temperature change.

To analyze and design the structures with TCA behaviors undergoing temperature change, one needs a thermoelastic constitutive model containing the TCA.

2.1. A bi-modulus thermo-mechanical constitutive relation

As proposed by Ambartsumyan (1986), the TCA of mechanical behavior is described by the dissimilar material parameters under tension and compression, i.e., tensile Young’s modulus \( E^+ \) and Poisson’s ratio \( v^+ \) and their compressive counterparts \( E^−, v^− \). This is based on the assumptions of elasticity and isotropy of the material, infinitesimal deformation, and continuity of displacement. This concept successfully represents the pure mechanical TCA behavior of engineering and laboratory materials, as well as biological tissues (Ambartsumyan, 1986; Du and Guo, 2014; Du et al., 2020), especially when TCA behavior is significant. It is natural to generalize this bi-modulus model to account for thermoelastic behavior.

In the principal stress space, the corresponding constitutive relation is specifically defined in terms of:

\[ \begin{cases} \epsilon_i - \theta_i = \frac{\sigma_i}{E^+} - C_0 (\epsilon_j + \alpha_j) & \text{if } \sigma_i > 0 \\ \epsilon_i - \theta_i = \frac{\sigma_i}{E^-} - C_0 (\epsilon_j + \alpha_j) & \text{if } \sigma_i \leq 0 \end{cases} \]

(2)

where \( \epsilon_i \) and \( \theta_i \) are the \( i \)th principal stress and principal total strain, respectively. Here, the ratios between Young’s modulus and Poisson’s ratio are assumed to be the same, i.e., \( C_0 = v^+ / E^+ = v^- / E^- \), to satisfy the symmetry of stiffness matrix and the conservation of the system.

According to Eq. (2), the principal stress/strain space is divided into four thermally-determined subregions in a 2D case (eight for the 3D case). In each region, the elastic properties are kept constant. A schematic illustration is presented in Fig. 1.

2.2. Unified constitutive relation and strain energy density functional

As shown in Fig. 1, an exact estimation of each material point’s stress state is required to correctly identify the elastic constants present. However, this is challenging for engineering structures with complex geometry and loading conditions. In this regard, the strain energy model incorporating the unified constitutive model of the TCA behavior needs to be devised. Furthermore, the existence and uniqueness of the corresponding partial differential system need to be investigated to construct efficient numerical analysis algorithms.

The bi-modulus model incorporates inherent non-smoothness, in contrast to the linear thermoelastic theory, and its region-wise constitutive relations cannot be directly summarized as a unified law. The optimality condition of the complementary strain energy density functional, or strain energy density functional, is the constitutive law of a smooth elastic system, i.e.,

\[ \sigma = \frac{\partial u}{\partial \varepsilon} \quad \text{and} \quad \varepsilon = \frac{\partial u^\circ}{\partial \sigma} + \eta \]

where \( u \) and \( u^\circ \) are the strain energy density and complementary strain energy density functionals. This inspires us to construct a unified strain energy density functional inducing the nonsmooth bi-modulus thermoelastic constitutive relations.

Similar as the non-smooth constitutive relations, e.g., elasto-plastic, and no-tension/no-compression materials (Simó and Hughes, 2006; Kanno, 2011), internal variables are introduced within the proposed constitutive model. In the case of \( E^- \geq E^+ \), we propose a positive semi-definite internal variable \( z \in S^3 \) with \( S^3 \) denoting the set of real symmetric \( 3 \times 3 \) matrices \( z \geq 0 \), i.e., \( z \) is a positive semi-definite tensor. By setting \( \beta = (E^+ \cdot E^-)/((E^-)^3) \), Eq. (2) is expressed as the optimality condition of the following semi-definite programming,

\[ \phi \geq 0 : \min_{z \in S^3} u(z; \varepsilon, \theta) = \frac{1}{2} (\varepsilon - \theta - z) : C^- : (\varepsilon - \theta - z) + \frac{1}{2\beta} z : z \]

(4)

where \( C^- = \frac{E^-}{1 + v^-} (1 + \frac{v^-}{1 - 2v^-}) \delta \otimes \delta \) is the stiffness tensor of the linear elastic material with elastic constants \( E^-, v^- \), and \( \delta \) denotes as the fourth order unit tensor.

**Theorem 1.** For any prescribed \( \varepsilon \) and \( \theta \), the optimal objective function value of the semi-definite programming \( \phi \geq 0 \) is the strain energy density of the proposed bi-modulus thermoelastic material and the optimality requirement of problem (4) actually yields the nonsmooth bi-modulus thermoelastic constitutive relation as Eq. (5):

\[ \begin{cases} \sigma = C^- : (\varepsilon - \theta - z) \\ \varepsilon = D^- : \sigma + \theta + z \end{cases} \]

(5)

where \( D^- \equiv (1/E^- + C_0)1 - C_0 \delta \otimes \delta \) is the compliance tensor of the linear elastic material with elastic constants \( E^-, v^- \).

**Remark.** For the case \( E^- < E^+ \), we have \( \beta = (E^+ - E^-)/((E^-)^3) \) and the internal variable would be negative semi-definite, i.e., \( S^3 \ni z \leq 0 \). Eq. (2) can be formulated as the optimality condition of the following semi-definite programming:

\[ \phi \geq 1 : \min_{z \in S^3} u(z; \varepsilon, \theta) = \frac{1}{2} (\varepsilon - \theta - z) : C^+ : (\varepsilon - \theta - z) + \frac{1}{2\beta} z : z \]

(6)

where \( C^+ = \frac{E^+}{1 + v^+} (1 + \frac{v^+}{1 - 2v^+}) \delta \otimes \delta \) is the stiffness tensor of the linear elastic material with elastic constants \( E^+, v^+ \).

As shown in Appendix A, once the unified strain energy density is proposed, one can develop the variational principle naturally to further examine the fundamental properties of the corresponding partial differential equation system.
3. Variational principles and the existence and uniqueness of solutions

For an elastic solid composed of the proposed bi-modulus thermoelastic material, as shown in Fig. 2, the total potential energy is:

$$\Pi(u; \theta) = \int_\Omega \min \left\{ \epsilon(z) \phi, \theta \right\} \, d\Omega - \int_\Omega f \cdot u \, d\Omega - \int_{S_1} p \cdot u \, dS$$

(7)

where $\Omega$ is the elastic solid, $f$ is the body force density and $p$ is the surface traction density on the force boundary $S_1$, respectively. The principle of minimum potential energy requires minimization of the total potential Eq. (7), i.e., $\min_{u, \theta} \Pi(u, \theta)$, which leads to a complex bi-level programming. Alternatively, we propose the principle of minimum potential energy for bi-modulus thermoelastic system:

**Theorem 2.** For bi-modulus material with $E^+ \geq E^*$, among all the kinematically admissible displacement fields $u(x)$ and semi-definite positive internal fields $\Sigma \ni \epsilon(x) \geq 0$, the true solution fields make the following potential energy minimum:

$$\Pi(u, z; \theta) = \int_\Omega \left\{ \frac{1}{2} \epsilon(u) \phi - z + \frac{1}{2z} z : z \right\} \, d\Omega$$

$$- \int_\Omega f \cdot u \, d\Omega - \int_{S_1} p \cdot u \, dS$$

(8)

The Lagrangian functional of potential energy (Eq. (8)) reads as:

$$\mathcal{L}(u, \lambda, \theta) = \int_\Omega \frac{1}{2} \epsilon(u) \phi - z + \frac{1}{2z} z : z + \lambda \, d\Omega$$

$$- \int_\Omega f \cdot u \, d\Omega - \int_{S_1} p \cdot u \, dS$$

(9)

Due to convexity of the potential energy functional (8), its Karush–Kuhn–Tucker conditions, i.e., the necessary and sufficient condition of minimizer, can be grouped into two sets:

$$\begin{align*}
\nabla \Pi \phi &= f = 0 \quad \text{in } \Omega \\
\nabla \Pi \theta &= n = p \quad \text{on } S_1
\end{align*}$$

(10)

and

$$\begin{align*}
\kappa - z - z^* + z^* / \beta + \lambda^* &= 0 \quad \text{in } \Omega \\
z^* - z^* &= 0 \quad \text{in } \Omega
\end{align*}$$

(11)

According to Appendix A and Theorem 1, Eq. (11) ensures that the exact constitutive relation of Eq. (2) is adopted for each material point. Therefore, Eq. (10) yields the equilibrium equation and traction boundary conditions of the analyzed bi-modulus thermoelastic system.

In addition, the corresponding principle of minimum complementary energy is presented in Appendix B. As the potential energy functional in Eq. (9) is both convex about $u$ and $z$, and the complementary energy in Eq. (35) is both convex about $\sigma$ and $q$, the exact solution fields always exist and are uniquely determined via the proposed energy principles. This actually presents an extension of the existence and uniqueness of solutions, i.e., the well-posedness, in the linear thermoelastic system to the bi-modulus case.

4. Computational framework for analysis of bi-modulus thermoelastic structures

The variational principles in Section 3 uniquely determine the structural response. However, the corresponding computational cost is expensive, applying the finite element method, an individual semi-definite tensor (internal variable) needs to be introduced for each Gauss point. Both the internal variable tensors and the nodal displacement vector are determined by solving a semi-definite programming (Eq. (8)). Therefore, developing an efficient numerical method for analyzing the bi-modulus thermoelastic structures is imperative. For the ease of implementation, the forthcoming formulations and illustrative examples are restricted to the two-dimensional case, although generalizing them to the three dimensional case is straightforward (Du et al., 2016).

4.1. Iterative solution algorithm based on complemented constitutive relation

It should be noted that the proposed thermoelastic constitutive relation Eq. (2) is developed in the principal stress/strain space, whereas numerical analysis often requires the constitutive relation in the global coordinate system. When the constitutive matrix in the global coordinate system is obtained directly from the original bi-modulus constitutive relation defined in the principal coordinate system, it becomes
rank-deficient. This is because the constitutive matrix in the global coordinate system is expanded in dimension and singular (Ran and Yang, 2021).

To address this issue, consistent shear modulus is derived and added to the constitutive relation in principal coordinate system (Du et al., 2016). Similarly, for bi-modulus thermoelasticity in two-dimensional case, four complemented constitutive matrices are expressed as:

\[
\mathbf{C}_0^p = \begin{bmatrix}
\frac{E}{1-\nu^2} & \frac{E\nu}{1-\nu^2} & 0 \\
\frac{E\nu}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\
0 & 0 & G_1 \\
\end{bmatrix}
\]

for \((e_1, e_2) \in D_1, \; \mathrm{i.e.,}\)
\[
\nu^e e_1 + e_2 \geq 0 \\
e_1 + \nu^e e_2 \geq 0
\]

(12)

\[
\mathbf{C}_0^p = \begin{bmatrix}
\frac{E^-}{1-\nu^-} & \frac{E^-\nu^-}{1-\nu^-^2} & 0 \\
\frac{E^-\nu^-}{1-\nu^-^2} & \frac{E^-}{1-\nu^-^2} & 0 \\
0 & 0 & G_2 \\
\end{bmatrix}
\]

for \((e_1, e_2) \in D_2, \; \mathrm{i.e.,}\)
\[
\nu^- e_1 + e_2 < 0 \\
e_1 + \nu^- e_2 < 0
\]

(13)

\[
\mathbf{C}_0^p = \begin{bmatrix}
\frac{E^+}{1-\nu^+} & \frac{E^+\nu^+}{1-\nu^+^2} & 0 \\
\frac{E^+\nu^+}{1-\nu^+^2} & \frac{E^+}{1-\nu^+^2} & 0 \\
0 & 0 & G_3 \\
\end{bmatrix}
\]

for \((e_1, e_2) \in D_3, \; \mathrm{i.e.,}\)
\[
\nu^+ e_1 + e_2 \geq 0 \\
e_1 + \nu^+ e_2 < 0
\]

(14)

\[
\mathbf{C}_0^p = \begin{bmatrix}
\frac{E^-}{1-\nu^-} & \frac{E^-\nu^-}{1-\nu^-^2} & 0 \\
\frac{E^-\nu^-}{1-\nu^-^2} & \frac{E^-}{1-\nu^-^2} & 0 \\
0 & 0 & G_4 \\
\end{bmatrix}
\]

for \((e_1, e_2) \in D_4, \; \mathrm{i.e.,}\)
\[
\nu^- e_1 + e_2 < 0 \\
e_1 + \nu^- e_2 \geq 0
\]

(15)

Following a similar derivation in Du et al. (2016), the complemented shear moduli are

\[
G_1 = \frac{E^+}{2(1-\nu^+)}, \quad G_2 = \frac{E^-}{2(1-\nu^-)}, \quad G_3 = \frac{E^-}{2(1-\nu^+)}, \quad G_4 = \frac{E^-}{2(1-\nu^-)}
\]

(16)

with \(e_i = \theta_i \in [1,2].\) Obviously, the complemented constitutive matrices for pure tension and pure compression are identical to the linear elastic constitutive matrices with material constants \(E^+, \nu^+\) and \(E^-, \nu^-\). For the complex stress states, however, the shear moduli are highly dependent on the exact elastic deformation and this clearly shows the nonsmoothness and nonlinearity of the considered elastic system.

Due to the fact that the elastic strain and stress tensors of an arbitrary material point are always co-axial, they can be expressed as:

\[
\begin{cases}
\sigma = e_1 n_1 \otimes n_1 + e_2 n_2 \otimes n_2 \\
\sigma = \theta_1 n_1 \otimes n_1 + \theta_2 n_2 \otimes n_2
\end{cases}
\]  

(17)

with \(n_i = (l_i, m_i)\)

\[
\begin{bmatrix} l_1 \\ m_1 \\ l_2 \\ m_2 \\ l_1 m_1 + l_2 m_2 \end{bmatrix}
\]  

for \((e_1, e_2) \in D_i, \; i = 1, 2, 3, 4 \)

(18)

In light of the aforementioned results, the global stiffness matrix \(K\) and the effective thermal load \(F^0\) of the considered bi-modulus thermoelastic structures are calculated as:

\[
K = \sum_{c=1}^{N_c} \sum_{g=1}^{N_g} G_{c,g}^T \mathbf{B}_{c,g}^T \mathbf{D}_{c,g} \mathbf{B}_{c,g} |J| c,g \quad \text{for} \; (e_1, e_2) \in D_c
\]

(19)

\[
F^0 = \sum_{c=1}^{N_c} \sum_{g=1}^{N_g} G_{c,g}^T \mathbf{B}_{c,g}^T \theta u_{c,g} |J| c,g \quad \text{for} \; (e_1, e_2) \in D_c
\]

(20)

where \(c, g\) count the number of elements and number of Gauss points (GPs), \(G, B\) are the assembly matrix and the linear strain–displacement matrix, respectively. The symbols \(\mathbf{D}_{c,g}, u_{c,g}\) and \(|J| c,g\) denote the complemented constitutive matrix, the weight and the determinant of Jacobian of the \(g\)th GP in the \(e\)th element. \(\theta = a \Delta T(1, 1, 0)^T\) in the present work.

The iterative analysis process for bi-modulus thermoelastic structures is summarized in the following Table 1. The proposed algorithm is simple to parallelize, and the appropriate UMAT code is also developed in ABAQUS.

### 4.2. Numerical examples of analyzing bi-modulus thermoelastic structures

In this subsection, two benchmark examples are investigated to demonstrate the efficacy of the proposed analysis algorithm from the following aspects: (1) consistency with the analytical results; (2) computational efficiency and robustness.

#### 4.2.1. Tensile bar with thermal expansion

As shown in Fig. 3(a), a uniform column with a length of \(l\) and cross-sectional area of \(A\) is under a tensile load \(F\) and temperature variation of \(\Delta T\). Suppose this bar is made of bi-modulus material with a density \(\rho\), the thermal expansion coefficient of \(a\) and tensile and compressive moduli \(E^+, E^-\), respectively.

The location of its neutral cross section, i.e., \(\sigma = 0\), can be determined as \(x(c) = l - F/(\rho g A)\). Then according to the stress states on the two sides of \(x = c\) and the continuity of displacement field, the analytical solution is:

\[
u(x) = \begin{cases}
\frac{\rho g l^2}{F} x^2 + \frac{F}{E} a \Delta T - \frac{\rho g l^2}{F} c^2 & 0 \leq x < c \\
\frac{\rho g l^2}{F} (x - c)^2 + a \Delta T x - \frac{\rho g l^2}{F} c^2 & c \leq x \leq l
\end{cases}
\]

(21)

For the case \(\Delta T = 0\), the above solution degenerates to the displacement field obtained in Ambartsyun (1986).

To show the effect of TCA and thermal expansion, without loss of generality, we set \(l = 10\; \text{m}, A = 1\; \text{m}^2, \rho g = 1.5\; \text{N/m}^2, a = 1.2 \times 10^{-4}\; \text{K}^{-1}, E^- = 500\; \text{Pa}, F = 6.0\; \text{N.}\) The analytical displacement
field is shown in Fig. 3(b). It is discovered that, for this statically determinate problem, the regions of bar under tension and compression (i.e., compression in 0 ≤ x < 6 m and tension in 6 m < x ≤ 10 m) are kept constant while ΔT and E′/E″ vary. This is consistent with the fact that, when the compressive modulus and ΔT are fixed, the u(x) remains constant for 0 ≤ x < 6 m for different E′/E″ as shown in Fig. 3(b). The displacement field across the entire bar is examined, and it is discovered that both the temperature variation and TCA play a significant role. This exhibits the accuracy of the proposed bi-modulus thermoelastic model.

By discretizing the bar into 4 × 4 quadrilateral plane stress elements with v′ = v″ = 0 and a convergence criterion of ∥u(k) − u(k−1)∥/∥u(k)∥ ≤ 10−4, the benchmark example is also solved using the proposed numerical algorithm. The nodal values of displacement at y = 0 are identical to the corresponding analytical solutions, as shown in Table 2. This again validates the effectiveness of the proposed numerical algorithm.

4.2.2. A cantilever beam example

As illustrated in Fig. 4(a), we study a cantilever beam composed of the proposed bi-modulus thermoelastic material experiencing a traction force and uniform thermal expansion. Without loss of generality, it is set as l = 2 m, h = 1 m, F = 1 kN, α = 2 × 10−5 K−1 and the thickness is 0.01 m.

To illustrate the significance of the proposed iterative algorithm with the shear-modulus complemented constitutive matrix obtained by Eq. (18), this problem is first analyzed using a classical iterative algorithm without shear modulus (Du et al., 2016). The domain is discretized by 4 × 2 quadrilateral plane stress elements. We examine two cases with different temperature conditions and degrees of TCA: (1) ΔT = −20 K, E′ = 1 GPa, v′ = 0.3, E″/E′ = v″/v′ = 0.5 and (2) ΔT = 50 K, E′ = 1 GPa, v′ = 0.06, E″/E′ = v″/v′ = 5. The vertical displacement x = l, y = 0 and norm difference between the nodal displacement vectors of two successive iterations are shown in Fig. 4(b). It clearly shows that the classical algorithm does not always converge. On the other hand, when the proposed iterative approach with the shear-modulus complemented constitutive matrix is utilized, such divergence is not seen from the identical initial guess. The solutions rapidly converge within five iterations for the convergence criteria of ∥u(k) − u(k−1)∥ < 10−6 for both of those cases, as shown in Table 3.

Table 1

<table>
<thead>
<tr>
<th>Initialization: Implement linear thermoelastic analysis with material constants E′, v′ or E″, v″ to obtain u(l); While: ε = 0.001; ε can be defined as ∥u(l) − u(l−1)∥/∥u(l)∥ or ∥(K′′−1 u(l) − F − F0)/(F + F0)∥; 1. For each GP, determine the stress state based on its elastic strain in principal coordinate system and calculate the corresponding complemented constitutive matrix according to Eqs. (12)–(16); ii. Assemble the global stiffness matrix K′′ and thermal load F0 according to Eqs. (19) and (20); III. Update the displacement vector u(l+1) according to K′′u(l+1) = F + F0; IV. k = k + 1.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Table 2</strong> Comparison of the analytical displacement field (u*) with numerical solutions (u).</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>x = 1 m</th>
<th>x = 3 m</th>
<th>x = 7 m</th>
<th>x = 10 m</th>
</tr>
</thead>
<tbody>
<tr>
<td>u* (m)</td>
<td>u (m)</td>
<td>u* (m)</td>
<td>u (m)</td>
<td>u* (m)</td>
</tr>
<tr>
<td>ΔT = −20 K</td>
<td>E′/E″ = 0.1</td>
<td>−0.0189</td>
<td>−0.0189</td>
<td>−0.0477</td>
</tr>
<tr>
<td>E′/E″ = 1</td>
<td>−0.0189</td>
<td>−0.0189</td>
<td>−0.0477</td>
<td>−0.0477</td>
</tr>
<tr>
<td>E′/E″ = 20</td>
<td>−0.0189</td>
<td>−0.0189</td>
<td>−0.0477</td>
<td>−0.0477</td>
</tr>
<tr>
<td>ΔT = 50 K</td>
<td>E′/E″ = 0.1</td>
<td>−0.0105</td>
<td>−0.0105</td>
<td>−0.0225</td>
</tr>
<tr>
<td>E′/E″ = 1</td>
<td>−0.0105</td>
<td>−0.0105</td>
<td>−0.0225</td>
<td>−0.0225</td>
</tr>
<tr>
<td>E′/E″ = 20</td>
<td>−0.0105</td>
<td>−0.0105</td>
<td>−0.0225</td>
<td>−0.0225</td>
</tr>
</tbody>
</table>

Fig. 4. (a) A bi-modulus cantilever beam subject to a traction and thermal expansion; (b) values of u(x, 0) and ∥u(l) − u(l−1)∥ during loops of the iterative algorithm without shear modulus (u(l) obtained by linear thermoelastic analysis with E = E′, v = v″).
In particular, for the $\phi_i$ during the optimization process (Guo et al., 2014; Zhang et al., 2016).

## 5.1. MMC-based topology optimization framework

Under the Eulerian mesh, the topological description function (TDF) of the MMC can be formulated as:

$$
\phi(x,y) = 1 - \left( \left( \frac{x}{l_i} \right)^{6} + \left( \frac{y}{l_i} \right)^{6} \right)^{1/6}
$$

(22)

Table 3

<table>
<thead>
<tr>
<th>Loop</th>
<th>Case (1)</th>
<th>Case (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_i(l,0)$ (m)</td>
<td>$</td>
<td>u_i^{(0)} - u_i^{(0-1)}</td>
</tr>
<tr>
<td>1</td>
<td>$-4.888 \times 10^{-3}$</td>
<td>$2.857 \times 10^{-2}$</td>
</tr>
<tr>
<td>2</td>
<td>$-3.132 \times 10^{-3}$</td>
<td>$4.002 \times 10^{-3}$</td>
</tr>
<tr>
<td>3</td>
<td>$-3.149 \times 10^{-3}$</td>
<td>$6.626 \times 10^{-3}$</td>
</tr>
<tr>
<td>4</td>
<td>$-3.149 \times 10^{-3}$</td>
<td>$2.957 \times 10^{-3}$</td>
</tr>
<tr>
<td>5</td>
<td>$-3.149 \times 10^{-3}$</td>
<td>$8.932 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

10 iterations even for large TCA case and indifference against different initial guesses.

## 5. Structural topology optimization of bi-modulus thermoelastic structures

Topology optimization of the bi-modulus thermoelastic structure, which is thought to be able to conceive a novel structure without predefined structural geometry, is shown in this part to show the applicability of the suggested method to structural design. Herein, we adopt the Moving Morphable Component (MMC) method to describe the structures and update the geometry accordingly.

### 5.1. MMC-based topology optimization framework

In the MMC method, as shown in Fig. 6, optimized structures are explicitly described by the geometric parameters of a set of components, which can move, deform, disappear and overlap with each other during the optimization process (Guo et al., 2014; Zhang et al., 2016). In particular, for the $i$th MMC with quadratically varying thickness shown in Fig. 6(a), its design variable is $d_i = (x_0, y_0, L_i, y_i, r_i, \theta_i)^T$. Under the Eulerian mesh, the topological description function (TDF) of the $i$th MMC can be formulated as:

$$
\phi_i(x,y) = 1 - \left( \left( \frac{x-x_0}{L_i} \right)^{6} + \left( \frac{y-y_0}{L_i} \right)^{6} \right)^{1/6}
$$

(23)

with

$$
\begin{align*}
\frac{x'}{y'} &= (x-x_0) \cos \theta_i + (y-y_0) \sin \theta_i \\
\frac{y'}{y'} &= -(x-x_0) \sin \theta_i + (y-y_0) \cos \theta_i \\
L_i &= \frac{t_i^1 + t_i^2 - 2t_3^3}{2L_i^2} (x')^2 + \frac{t_i^2 - t_i^1}{2L_i} + t_i^3
\end{align*}
$$

(24)

Denoting the design domain as $D$, the solid region $\Omega'$ occupied by this component is determined as

$$
\begin{align*}
\phi'^{(i),y}(x,y) &= 0, \quad \text{if } (x,y) \in \Omega' \cap D \\
\phi'^{(i),y}(x,y) &= 0, \quad \text{if } (x,y) \in \partial \Omega' \cap D \\
\phi'^{(i),y}(x,y) &< 0, \quad \text{if } (x,y) \in D \setminus (\Omega' \cup \partial \Omega')
\end{align*}
$$

Similarly, the optimized structure is identified by the global TDF (Du et al., 2022), i.e., $\Omega = \{(x,y)|(x,y) \in D, \phi'^{(i),y}(x,y) > 0\}$ with

$$
\phi = \max(\phi'^{(1),y}, \ldots, \phi'^{(n),y}) \approx \left( \sum_{i=1}^{n} \exp(d_i) \right) / \lambda
$$

(25)

where $n$ denotes the total number of MMCs and $\lambda = 100$ in this work. In this manner, the optimized structure is described explicitly by the design variable vector $d = (d^1, d^2, \ldots, d^n)^T$.

Furthermore, for the finite element analysis with fixed mesh, elemental densities are introduced and the ersatz material model (Zhang et al., 2016) is adopted for the tensile and compressive Young’s moduli $E^\varepsilon$ and $E^\varepsilon = \rho E^\varepsilon$

$$
\rho_i(d) = \frac{1}{4} \sum_{i=1}^{4} H_i^\varepsilon(\phi_i^e) \quad \text{and} \quad E_i^\varepsilon = \rho_i E^\varepsilon
$$

(26)

where $\phi_i^e$ is the $i$th nodal value of the global TDF of $e$th element and the smoothed Heaviside function $H_i^\varepsilon$ is defined as

$$
H_i^\varepsilon(x) = \begin{cases} 1, & \text{if } x > \varepsilon \\
\frac{1}{4} \left( 1 - \frac{4}{\varepsilon} \left( \frac{x}{\varepsilon} - \frac{1}{2} \right) + \frac{1}{4} \frac{1}{\varepsilon^2} \right), & \text{if } |x| \leq \varepsilon \\
0, & \text{otherwise}
\end{cases}
$$

(27)

with $\varepsilon = 0.15$ and $\xi = 10^{-3}$ unless otherwise stated.
Fig. 8(b). The corresponding optimized design and the iteration history difference with the perturbation constant \( \Delta d \) design variables) as shown in Fig. 8 (a). The analytical sensitivity is \( E \) and it is to obtain the optimal designs corresponding to \( E \) design domain. Fixing \( F \) structural layout.

5.3. Illustrative examples

Numerous formulations for thermoelastic topology optimization have been proposed in the literature (Xia and Wang, 2008; Zhang et al., 2014; Takallozadeh and Yoon, 2017; Chung et al., 2020). Here, the mean compliance minimization with a volume constraint is formulated as:

\[
\begin{align*}
\text{min } & f = (F + F^0(u, d))^T u(d) \\
\text{subject to } & K(u, d)u(d) = F + F^0(u, d) \\
& g = V(d)/D - v \leq 0
\end{align*}
\]

where \( F^o \) is the admissible set of design variable vector; \( V, D, v \) are the volume of the optimized structure, volume of the design domain, upper bound of allowable volume fraction, respectively.

Notably, in contrast to the linear elastic counterparts, the global stiffness matrix and thermal load depend on the stress states determined by the displacement field through the iterative process following Table 1. As demonstrated in Appendix C, the design sensitivity of the bi-modulus thermoelastic structures has a similar form of the sensitivity of linear thermoelastic structures (Xia and Wang, 2008), i.e.,

\[
\frac{df}{dd_j} = -\sum_{i=1}^{n} \left( -u_i^T k_{ij} u_i + 2u_i^T f_i^{th} \frac{\partial v_i}{\partial d_j} \right) \quad \text{and} \quad \frac{dg}{dd_j} = \sum_{i=1}^{n} V_i \frac{\partial V_i}{\partial d_j} \quad (28)
\]

where \( d_j \) is the \( j \)th variable of the \( i \)th component, \( u_i, V_i \) are the elemental displacement vector and volume of each element. The symbols \( k_{ij} \) and \( f_i^{th} \) are the elemental stiffness matrix and elemental thermal load vector of each element with \( \rho_1 = 1 \), respectively. For conciseness of the main text, the expressions of \( \partial f/\partial d_j \) are presented in Appendix D.

5.3.1. Two-bar structure example

As shown in Fig. 7(a), a 1 m × 4 m design domain with a uniform thickness of \( \delta = 0.01 \) m is fixed on the left side. A concentrated load of \( F = -10^8 \) Pa is applied on the middle point of the right edge of the design domain. Fixing \( E^+ = 2 \) GPa, \( v^+ = v^- = 0, \alpha = 1.54 \times 10^{-6} \) K \(^{-1} \), it is to obtain the optimal designs corresponding to \( E^+/E^- = 0.125, 1, 1.3, \) and \( \Delta T = -20 \) K, 0 K, 100 K with a maximum volume fraction of 10%.

The design domain is discretized by \( 40 \times 160 \) uniform bilinear quadrilateral plane stress elements. The optimization problem is solved using MMCs with a uniform thickness (i.e., \( t^i = t^o = t^f \)). The number of maximum iterations is set to 100, while the converged result is obtained far earlier. Without loss of generality, we assume \( E^+/E^- = 3 \) and \( \Delta T = -20 \) K, and the initial distributions of 8 MMCs (i.e., 40 design variables) as shown in Fig. 8(a). The analytical sensitivity is consistent with the finite difference result (obtained by the central difference with the perturbation constant \( \Delta d_i = 10^{-6} \)) as shown in Fig. 8(b). The corresponding optimized design and the iteration history

<table>
<thead>
<tr>
<th>Case (3)</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
<th>Case (4)</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
</tr>
</thead>
<tbody>
<tr>
<td>-9.793 × 10^{-2}</td>
<td>8</td>
<td>-9.792 × 10^{-2}</td>
<td>8</td>
<td>-5.981 × 10^{-5}</td>
<td>9</td>
<td>-5.981 × 10^{-5}</td>
<td>9</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fig. 7. (a) Illustration of the tensile bar under thermal expansion; (b) the displacement field with respect to different temperature variations and tension to compression asymmetries.

Table 4

| Converged values of \( u_i(0) \) and loop numbers of the iterative algorithm with the shear-modulus complemented constitutive matrix from different initial guesses ((\( |u_i^{(1)} - u_i^{(0)}|/|u_i^{(0)}| \leq 10^{-4} \), subscripts and – imply \( u_i^{(1)} \) obtained by linear thermoelastic analysis with \( E = E^+, \) = \( v^+ \) and \( E = E^-, \) = \( v^- \), respectively). |

<table>
<thead>
<tr>
<th>Case (3)</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
<th>Case (4)</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
<th>( u_i^{(1)} / 0 ) (m)</th>
<th>Loop</th>
</tr>
</thead>
<tbody>
<tr>
<td>-9.793 × 10^{-2}</td>
<td>8</td>
<td>-9.792 × 10^{-2}</td>
<td>8</td>
<td>-5.981 × 10^{-5}</td>
<td>9</td>
<td>-5.981 × 10^{-5}</td>
<td>9</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Since the optimal design of this example is a two-bar structure shown in Fig. 7(b), we can determine the corresponding optimal configurations by the following parametric programming (which also accounts the effect of thermal expansion perpendicular to the axial direction of the two bars):

\[
\begin{align*}
\text{find} & \quad a_1, a_2, \theta_1, \theta_2 \\
\text{min} & \quad \frac{1}{E_1} + F a_1 \sin \theta_1 \cos \theta_2 + \sin \theta_1 \cos \theta_1 \theta_1 \right)^2 \\
+ & \quad \left[ -F \sin \theta_1 + E_1 a_1 \sin \theta_1 \cos \theta_2 + \sin \theta_1 \cos \theta_1 \right)^2 \\
+ & \quad \frac{E_1 a_1 \sin \theta_1 \cos \theta_1}{\sin \theta_1} \\
+ & \quad \frac{E_1 a_1 \sin \theta_1 \cos \theta_1}{\sin \theta_1} \\
\text{s.t.} & \quad a_1, a_2 \leq 0.4 \\
& \quad 0 \leq 1/\tan \theta_i \leq 2, \quad i = 1, 2
\end{align*}
\]

The optimal parameters of the two-bar trusses about different degrees of TCA and temperature changes are shown in Table 5. The volume fractions and objective function values are obtained by analyzing the truss structures using the same setting of finite element analysis. The proposed method’s analytic results and optimized structures are consistent. Some minor mismatch is possibly due to the influence of the cut elements near the structural boundary and the concentrated loading.

5.3.2. A bi-clamped beam

As shown in Fig. 10(a), a 2 m x 1 m design domain with a uniform thickness of \( \delta = 0.01 \text{ m} \) is fixed on the two sides. A concentrated load of \( F = -5 \times 10^4 \text{ Pa} \) is applied at the bottom center of the design domain. By fixing \( E^* = 199.5 \text{ GPA} \), \( \max (\nu^*, \nu^*) = 0.3, a = 1.54 \times 10^{-5} \text{ K}^{-1} \) and \( \nu = 20\% \), it is to determine the optimized designs for \( E^*/E^* = 0.1, 1.1, 5 \) and \( \Delta T = -5 \text{ K}, 0 \text{ K}, 5 \text{ K}, 10 \text{ K} \), respectively.

With the initial design shown in Fig. 10(b), the design domain is discretized into \( 160 \times 80 \) uniform bilinear quadrilateral plane stress elements, and the optimization problem is solved using the proposed MMC-based method. There are 20 MMCs and 140 design variables. Note that the number of active design variables may decrease throughout the iteration, since some of the components are eliminated during the design process (Du et al., 2022). As shown in Fig. 11(a), which corresponds to the case of \( E^* = 39.9 \text{ GPA}, \nu^* = 0.06 \) and \( \Delta T = 10 \text{ K} \),

### Table 5

<table>
<thead>
<tr>
<th>Case</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
<th>( \theta_1 )</th>
<th>( \theta_2 )</th>
<th>( V/\text{f} )</th>
<th>( f(\times 10) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/8</td>
<td>0.2259</td>
<td>0.0513</td>
<td>0.7552</td>
<td>0.8156</td>
<td>0.1000</td>
<td>2.637</td>
</tr>
<tr>
<td>F. E.</td>
<td>( \Delta T = -20 )</td>
<td>0.2043</td>
<td>0.0557</td>
<td>0.6891</td>
<td>0.7844</td>
<td>1.000</td>
</tr>
<tr>
<td>Ana.</td>
<td>( \Delta T = 0 )</td>
<td>0.1756</td>
<td>0.0176</td>
<td>0.1036</td>
<td>0.5439</td>
<td>0.1000</td>
</tr>
<tr>
<td>F. E.</td>
<td>( \Delta T = 50 )</td>
<td>0.1921</td>
<td>0.0354</td>
<td>1.1729</td>
<td>0.4636</td>
<td>0.0582</td>
</tr>
<tr>
<td>Ana.</td>
<td>( \Delta T = 50 )</td>
<td>0.1332</td>
<td>0.0994</td>
<td>1.1478</td>
<td>0.4636</td>
<td>0.0577</td>
</tr>
<tr>
<td>1/8</td>
<td>0.1512</td>
<td>0.1258</td>
<td>0.6940</td>
<td>0.8767</td>
<td>0.0985</td>
<td>3.866</td>
</tr>
<tr>
<td>F. E.</td>
<td>( \Delta T = -20 )</td>
<td>0.1543</td>
<td>0.1294</td>
<td>0.6968</td>
<td>0.8818</td>
<td>0.1000</td>
</tr>
<tr>
<td>Ana.</td>
<td>( \Delta T = 0 )</td>
<td>0.1414</td>
<td>0.1414</td>
<td>0.7854</td>
<td>0.7854</td>
<td>0.0983</td>
</tr>
<tr>
<td>F. E.</td>
<td>( \Delta T = 0 )</td>
<td>0.1442</td>
<td>0.1442</td>
<td>0.7854</td>
<td>0.7854</td>
<td>0.1000</td>
</tr>
<tr>
<td>Ana.</td>
<td>( \Delta T = 50 )</td>
<td>0.0978</td>
<td>0.1530</td>
<td>1.0018</td>
<td>0.5690</td>
<td>0.0989</td>
</tr>
<tr>
<td>F. E.</td>
<td>( \Delta T = 50 )</td>
<td>0.1009</td>
<td>0.1565</td>
<td>1.0084</td>
<td>0.5728</td>
<td>0.1000</td>
</tr>
</tbody>
</table>

\( \nu^* = 20\% \), it is to determine the optimized designs for \( E^*/E^* = 0.1, 1.1, 5 \) and \( \Delta T = -5 \text{ K}, 0 \text{ K}, 5 \text{ K}, 10 \text{ K} \), respectively.
Z. Du et al.

Fig. 10. (a) Design domain of the bi-clamped beam example; (b) the initial design.

Fig. 11. For the case $E^*/E^- = 5.0$ and $\Delta T = 10$ K (a) iteration history of objective function and constraint values; (b) some intermediate designs.

Table 6
Optimized designs with different temperature changes and degrees of TCA.

| $\Delta T$ | $E^*/E^-$ | $V/|D|$ | $f$ |
|----------|----------|--------|-----|
| $-5K$    | 0.1      | 12.9%  | 21.76 |
| $0K$     | 1.0      | 18.7%  | 12.66 |
| $5K$     | 5.0      | 20.0%  | 7.86  |
| $10K$    | 0.1      | 20.0%  | 14.85 |
|          | 1.0      | 20.0%  | 37.57 |
|          | 5.0      | 20.0%  | 70.47 |

Iteration histories of objective and constraint values are found to be stable. Some representative configurations of optimized structures are also shown in Fig. 11(b). The first 25 iterations reveal that there is still no solid material at the loading point, and the structure gradually changes to more effectively withstand the mechanical load, resulting in a connected load path. After that, the objective function value decreases drastically and components not contributing to the load path disappear. An optimized design with an objective function value of 70.47 and a volume fraction of $V/|D| = 16\%$ is obtained in the iteration 100.

Table 6 collects the corresponding optimized designs of different $a\Delta T$ and degrees of TCA. The optimized designs of $E^+ = E^-$ is consistent with the linear thermoelastic designs found in literature (Xia and Wang, 2008). It should be noted that, the interplay between temperature variation and the TCA plays a significant role on the optimized layout, even leading to the design with inactive volume constraint.

High-fidelity numerical analysis is used to investigate the structural responses of these optimized designs to further demonstrate the rationality of the optimized designs. Four representative layouts in Table 7 are straightforwardly imported to ABAQUS and analyzed using conformal mesh with our in-house UMAT by taking the advantages of explicit description of the MMC method. In each column, contours of displacement amplitude of the optimized design for different degrees of TCA and temperature variations are presented. The diagonal one boxed by red lines are the optimized design among the ones in the same row, verifying the optimality of the optimized solution. In particular, among
the designs in the first row, the thermal expansion further increases the deformation of the second and the fourth designs. The volume fraction of the third one is much smaller and the mechanical deformation would be larger compared to the first design. For the designs in the fourth row, the compressive modulus is ten times of the tensile modulus and thermal shrink exists. The structural components in tension of the first and third designs are thinner and the corresponding mechanical deformation would be excessive, while the two thin components fixed of the second design would pull the structure downside to increase the mechanical deformation. Therefore, it can be concluded that the fourth design fully takes the advantage of coupling between the mechanical and thermal effect.

6. Concluding remarks

The following main achievements are obtained in this work, to systematically study the thermoelastic behavior of materials and structures with TCA: (1) a constitutive model based on bi-modulus elasticity is proposed to describe the corresponding thermo-mechanical behavior; (2) variational principles, as well as the well-posedness of the related boundary value problems, are developed; (3) with analytical solutions, an effective numerical framework is constructed to analyze structures made of such materials; and (4) with the analytical sensitivities derived, optimal design of thermoelastic structures with TCA is studied. It has been shown that both the TCA and thermal expansion play a key role in the structural responses and optimized layout. Extending the proposed work to three-dimension and the multi-material cases is in progress. It would also be interesting to further focus on the novel applications of the bi-modulus thermoelasticity, e.g., prediction of wrinkling regions in the membrane under mechanical and thermal loading (Blandino et al., 2002), and strut-and-tie model design considering thermal effects (Du et al., 2019).

CRediT authorship contribution statement


Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

This work is supported by the National Natural Science Foundation of China (No. 11821202, 11732004, 12002073), China National Key Research and Development Plan Project (2020YFB1709401), and the Fundamental Research Funds for the Central Universities, China (No. DUT20RC(3)020). The financial support from the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIT) (No. NRF-2020R1C1C1005741) and the AI Incubation Research Fund of Ulsan National Institute of Science and Technology (UNIST)(1.210090.01) are also gratefully acknowledged.

Appendix A. Semi-definite programming for the bi-modulus thermoelastic material

First a preliminary lemma from the convex analysis of positive semi-definite matrices is introduced as follows (Alizadeh et al., 1997):

Lemma 1. Denoting $S^+$ as the set of all $n \times n$ real symmetric matrices, for $S^+ \ni A \geq 0$ and $S^+ \ni B \leq 0$, $A : B = 0$ if and only if there exists $Q \in R^{n \times n}$ with $Q^TQ = I$, such that $A = Q^T\text{Diag}(A_1, A_2, \ldots, A_n)Q$, $B = Q^T\text{Diag}(B_1, B_2, \ldots, B_n)Q$, $A_1 \geq 0$, $B_i \leq 0$ and $A_i B_i = 0$, $i = 1, \ldots, n$. 
With a Lagrangian multiplier $S^3 \ni \lambda \leq 0$, the optimality conditions of $\phi \theta$ in Eq. (4) read as
\begin{align}
-C^* : \varepsilon + z^* + \beta \lambda^* = 0 \\
z^* - \lambda^* = 0 \\
z^* \geq 0, \quad \lambda^* \leq 0
\end{align} (31)

According to Lemma 1, $z^*$ and $\lambda^*$ are co-axial, and $\lambda^* z^* = 0, i = 1, 2, 3$. Then from the first equation of Eq. (31), it is obvious that $z^*$ is also co-axial with $\lambda^*$ and $z^*$.

For the case $\lambda^* < 0$, the complementary condition implies $z^* = 0$. The $i$th component of Eq. (5) can be simplified as $\sigma_i = (C^* : \varepsilon - \theta) = \lambda^*_i - \varepsilon_i - \theta_i = (\varepsilon_i - \theta_i)$. On the other hand, for the case $\lambda^*_i > 0, z^*_i = 0, i = 1, 2, 3$, then $\lambda^*_i - \varepsilon_i - \theta_i = (\varepsilon_i + \theta_i)$. Those cases are consistent with the proposed bi-modulus thermoelastic constitutive relation exactly.

Furthermore, denote the $i$th component of the optimal objective function value as
\begin{align}
w^i = 1/2(\varepsilon - \theta - z^*), \quad (C^* : (\varepsilon - \theta - z^*))^{1/2} = \frac{1}{2\beta}(z^*)^2
\end{align} (32)

According to the above discussions, Eq. (32) can be classified into the following cases:
\begin{align}
w^i = (\varepsilon_i - \theta_i) \sigma_i = \frac{1}{2}(\varepsilon_i - \theta_i) \sigma_i/2 \quad \text{if } \sigma_i \leq 0 \\
w^i = (\varepsilon_i - \theta_i - \beta \sigma_i) \sigma_i/2 + (\beta \sigma_i)^2/2(\beta) \sigma_i \sigma_i/2 \quad \text{if } \sigma_i > 0
\end{align} (33)

Therefore, the proposed bi-modulus constitutive relations can be unified by Eq. (5) with internal variable determined by the optimality condition of the semi-definite programming $\phi \theta$, and the corresponding optimal objective function value is the strain energy density.

Appendix B. The principle of minimum complementary energy of the bi-modulus thermoelastic system

**Theorem 3.** For bi-modulus material with $E^* \geq E^*$, the thermoelastic constitutive relation (2) can be unified as $\varepsilon - \theta = D^* : \sigma - \beta q$. Among all the statically admissible stress fields $\sigma(x)$ and negative semi-definite internal fields $S^3 \ni q(x) \leq 0$, the true solution fields make the following complementary energy minimum:
\begin{align}
\Pi^*(\sigma; q; \theta) = \int \left( \frac{1}{2} \sigma : D^* : \sigma + \frac{\beta}{2} (\sigma - q) : (\sigma - q) + \sigma : \theta \right) d\Omega \\
- \int_{S_S} (\sigma \cdot n) \cdot u dS
\end{align} (34)

By introducing a complementary field $S^3 \ni \lambda(x) \geq 0$, the true solutions, i.e., $\sigma^*, \varepsilon, q^*, \lambda^*$, are uniquely determined by the following equation systems:
\begin{align}
\left\{ \begin{array}{l}
D^* : \sigma^* - \beta q^* = (\nabla u + \nabla v)/2 - \theta \\
u = \bar{u} \quad \text{on } S_S
\end{array} \right.
\end{align} (35)

and
\begin{align}
\beta (\sigma^* - \beta q^*) + \lambda^* = 0 \quad \text{in } \Omega \\
q^* : \lambda^* = 0 \quad \text{in } \Omega \\
q^* \leq 0, \quad \lambda^* \geq 0 \quad \text{in } \Omega
\end{align} (36)

According to Lemma 1, Eq. (36) and the unified constitutive relation $\varepsilon - \theta = D^* : \sigma - \beta q$ imply $\sigma^*, \varepsilon, q^*$ and $\lambda^*$ are co-axial. Then it is obvious that Eq. (36) is equivalent to the thermoelastic constitutive relation (2). Furthermore, Eq. (35) leads to the strain–displacement relation at infinitesimal deformation case and displacement boundary condition.

Appendix C. Derivation of the sensitivity

The potential energy functional of the bi-modulus thermoelastic system can be formulated as
\begin{align}
P(u; \rho; \theta) = \frac{1}{2} \int_\Omega (\varepsilon(u) - \theta) : C(u; \rho) : (\varepsilon(u) - \theta) d\Omega \\
- \int_\Omega f \cdot v d\Omega - \int_{S_S} p \cdot v dS
\end{align}

\begin{align}
= \frac{1}{2} \int_{\Omega} \varepsilon(u) : C(u; \rho) : (\varepsilon(u) + \frac{1}{2} \theta d\Omega \\
- \int_{\Omega} \varepsilon(u) : C : \theta d\Omega - \int_{\Omega} v \cdot \nabla \theta - \int_{S_S} p \cdot v dS
\end{align} (37)

The actual potential energy reads as
\begin{align}
P^*(u(\rho; \rho; \theta) = \frac{1}{2} \int_\Omega u^T (p) K(u(\rho); p) u(\rho) + \Delta(u(\rho); \rho)
\end{align}

\begin{align}
- u^T (p) F^{th}(u(\rho); p) - u^T (p) F
\end{align}

\begin{align}
= -\frac{1}{2} u^T (F + F^{th}) + \Delta
\end{align} (38)

with $\Delta(u(\rho); \rho) = \frac{1}{2} \int_\Omega \varepsilon(u(\rho); \rho) : \theta d\Omega$. Therefore, the following relation holds
\begin{align}
\frac{\partial \Pi}{\partial \rho_c} = \frac{\partial}{\partial u} \left( -2 \left( \Pi^* - \Delta \right) \right) \frac{\partial \Pi}{\partial \rho_c} - \frac{\partial}{\partial \rho_c} \left( -2 \left( \Pi^* - \Delta \right) \right)
\end{align}

\begin{align}
\approx -u^T \frac{\partial^2}{\partial \rho_c} F + 2u^T \frac{\partial^2}{\partial \rho_c} F^{th} = -u^T k^{th} K + 2u^T f^{th}
\end{align} (39)

where the facts $\delta_{i} \Pi^* = 0$ and $\frac{\partial^2}{\partial \rho_c} = 0$ are used.

Appendix D. Exact expressions of $\frac{\partial \rho_c}{\partial f_c}$

Since $\psi$ is only dependent on the design variable of the $i$th component, $\frac{\partial \rho_c}{\partial f_c}$ can be calculated following the chain rule as
\begin{align}
\frac{\partial \rho_c}{\partial f_c} = \frac{\partial \rho_c}{\partial \psi ^{i}} \frac{\partial \psi ^{i}}{\partial f_c}
\end{align} (40)

For the MMC with quadratically varying thickness illustrated in Fig. 6(a), we have the following facts
\begin{align}
\frac{\partial \psi ^{i}}{\partial x} &= -\cos \theta_i \\
\frac{\partial \psi ^{i}}{\partial y} &= \sin \theta_i \\
\frac{\partial \psi ^{i}}{\partial z} &= -\cos \theta_i \\
\frac{\partial \psi ^{i}}{\partial y} &= y' \\
\frac{\partial \psi ^{i}}{\partial x} &= x'
\end{align} (41)

$\eta$ is the thickness of the beam, $f_i$ is the thickness of the cross section $i$, $l_i$ is the corresponding length of the cross section $i$, and $L$ is the total length of the beam.

Note that $C$ keeps constant for $u$ except for the boundary (with a Lebesgue measure of 0 on $\mathbb{R}^2$) of four different stress states in the principal strain space.
And the exact expressions of $\frac{\partial f}{\partial n}$ are

\[
\frac{\partial f}{\partial n} = \left[ \left( \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \right) \frac{\partial \phi}{\partial n} \right]^6 \left[ \left( \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \right)^2 - \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} - \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right] \times \cos \theta - \frac{1}{2} \sin \theta \left( \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right)
\]

\[
\frac{\partial f}{\partial n} = \left[ \left( \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \right) \frac{\partial \phi}{\partial n} \right]^6 \left[ \left( \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \right)^2 - \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} - \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right] \times \sin \theta + \frac{1}{2} \cos \theta \left( \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right)
\]

\[
\frac{\partial f}{\partial n} = \left[ \left( \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \right) \frac{\partial \phi}{\partial n} \right]^6 \left[ \left( \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \right)^2 - \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} - \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right] \times \cos \theta - \frac{1}{2} \sin \theta \left( \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial y} \right)
\]

The references are:


