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Influence of BESO topology optimization parameters on the design of periodic cellular material with zero thermal expansion

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Topology optimization design of periodic cellular materials depends on the topology optimization method being used, as well as on their parameter setting, which in general are defined arbitrarily or based on the literature. In this work, the influence of the design parameters of the Bi-directional Evolutionary Structural Optimization method in the design of metamaterials with zero thermal expansion is investigated. The effects of the evolutionary ratio, addition ratio, filter radio, and volume percentages on the objective function are studied. The different sets of parameters show that the objective function is dependent on some BESO parameters while it is independent of others. It is also verified that for a final topology with 50% solid material, there is a better volume percentage ratio between materials with low and high thermal expansion coefficients.
Topology optimization, Thermal expansion coefficients, Homogenization method, BESO method

INTRODUCTION

Metamaterials are materials that present properties that are not found in nature. The inverse homogenization associated with a topology optimization method can be used to design metamaterials by looking for the best material distribution within a base cell that results in an aimed property (Babuska,1976).

The same effective material property can be obtained by different material distributions in the base cell. This material distribution is what we call the topology of the metamaterial. The final topology depends on the topology optimization method, used to solve the topology optimization problem, and on its setting parameters (Faure et al., 2017; Sigmund and Torquato, 1997; Takezawa et al., 2017; Takezawa et al., 2018; Wang et al, 2004; Wang et al., 2016).

The BESO method is easy to implement and allows to obtain topologies with well-defined boundaries between solid phases (Xie and Steven, 1993; Xie and Steven, 1997; Huang and Xie, 2010), however, the application of this method to the design of metamaterials using topology optimization is not common in literature, due to the discrete nature of the design variables(Anaya et al., 2018). This characteristic suggests the application of numerical strategies not covered in this work.

The specific objective of this study was to investigate the influence of the BESO parameters on the final value of the objective function considering the topology design of metamaterials with zero thermal expansion.

The BESO parameters studied in this work are the evolutionary ratio, the addition ratio, the filter radio, and the final volume fraction of each solid material phase (Huang and Xie, 2010b).

This study aims to contribute to the use of the BESO method in the design of metamaterials with extreme thermal properties by knowing the influence of the principal parameters of the methodology on the final value of the objective function.

This paper has been divided into three parts. The first part deals with the effective properties calculation using the homogenization method, the material interpolation scheme, the topology optimization problem, the sensitivity numbers calculation, and the Bi-directional evolutionary structural optimization methodology, the second part presents the findings of this research, obtained for the BESO parameter analysis, and finally, the third section presents the concluding remarks.

EFFECTIVE PROPERTIES

Considering a periodic base cell as the design domain, the effective thermal expansion coefficients are calculated using the asymptotic homogenization (Hassani and Hinton, 1998a;Hassani and Hinton, 1998b;Hassani and Hinton, 1998c;

Rodrigues and Fernandes,1995), as follows:

$$\boldsymbol{D}^H = \frac{1}{|Y|}\int_Y \boldsymbol{D}(\boldsymbol{I}-\boldsymbol{B}\boldsymbol{U})\,dy \tag{1}$$

$$\boldsymbol{\beta}^H = \frac{1}{|Y|}\int_Y \boldsymbol{D}(\boldsymbol{\alpha}-\boldsymbol{B}\boldsymbol{\phi})\,dy \tag{2}$$

$$\boldsymbol{\alpha}^H = \left(\boldsymbol{D}^H\right)^{-1}\boldsymbol{\beta}^H \tag{3}$$

where $\boldsymbol{D}^H$, $\boldsymbol{\beta}^H$ and $\boldsymbol{\alpha}^H$, are the homogenized elasticity matrix, the effective thermal stress vector and the effective vector of thermal expansion coefficients, respectively. $|Y|$, $\boldsymbol{I}$ and $\boldsymbol{B}$ are the base cell volume, the identity matrix and the strain/displacement matrix, respectively. The displacement fields $\boldsymbol{U}$ and $\boldsymbol{\phi}$ ate calculatedi by solving the followign equations:

$$\underbrace{\mathop{\mathrm{A}}_{e=1}^{Nel}\left(\int_{\Omega_e}\boldsymbol{B}_e^T\boldsymbol{D}_e\boldsymbol{B}_e d\Omega_e\right)}_{\boldsymbol{K}}\boldsymbol{U} = \underbrace{\mathop{\mathrm{A}}_{e=1}^{Nel}\left(\int_{\Omega_e}\boldsymbol{B}_e^T\boldsymbol{D}_e\boldsymbol{\varepsilon}d\Omega_e\right)}_{\boldsymbol{F}} \tag{4}$$

$$\underbrace{\mathop{\mathrm{A}}_{e=1}^{Nel}\left(\int_{\Omega_e}\boldsymbol{B}_e^T\boldsymbol{D}_e\boldsymbol{B}_e d\Omega_e\right)}_{\boldsymbol{K}}\boldsymbol{\phi} = \underbrace{\mathop{\mathrm{A}}_{e=1}^{Nel}\left(\int_{\Omega_e}\boldsymbol{B}_e^T\boldsymbol{\beta}_e\Delta_t d\Omega_e\right)}_{\boldsymbol{f}_t} \tag{5}$$

where, A is the finite element assembly operator, Nel is the total number of elements, Ω_e is the domain of the eth element,$\boldsymbol{D}$ and $\boldsymbol{\beta}$ are the isotropic elasticity matriz and the thermal stress vector of each element e, and $\boldsymbol{\varepsilon}$ is the matrix of the three unitary strains applied to the cell,

$$\boldsymbol{\varepsilon} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{6}$$

Material interpolation

To obtain a metamaterial with zero thermal expansion, it is necessary to allow two material phases and void in the design domain. The material interpolation used in this work takes into account the material change of the element e between neighboring materials (Huang and Xie, 2008), as follows:

$$\boldsymbol{D}_e^j = (X_{ej})^{p_j}\boldsymbol{D}_j + [1-(X_{ej})^{p_j}]\boldsymbol{D}_{j+1}, \tag{7}$$

$$\boldsymbol{\alpha}_e^j = (X_{ej})^{q_j}\boldsymbol{\alpha}_j + [1-(X_{ej})^{q_j}]\boldsymbol{\alpha}_{j+1} \tag{8}$$

for $j = 1,2$, where $j = 1$ when considering a change between material 1 and material 2 and $j = 2$ for a change between material 2 and void. The discrete design variables are grouped in the matrix $\boldsymbol{X}$,

$$\boldsymbol{X} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ X_{Nel1} & X_{Nel2} \end{bmatrix}, \tag{9}$$

and only take values of 1 and $x_{\min}$. To characterize that the element is filled with material 1, the first and the second design variable are equal to 1, for material 2, the first design variable ate $x_{\min}$ while the second one is 1. Finally, for the void elements both design variables are $x_{\min}$.

Topology Optimization problem

The specific objective of this study was to study the influence of the parameters of the bi-directional evolutionary structural optimization method on the final value of the thermal expansion coefficients. Data for this study were collected solving the following topology optimization problem:

$$
\begin{aligned}
find: \quad & \boldsymbol{X} \\
minimize: \quad & (\alpha_{11}^H)^2 + (\alpha_{22}^H)^2 \\
subject\ to: \quad & V_1^* - \sum_{e=1}^{Nel} V_e X_{e1} = 0 \\
& V_2^* - \sum_{e=1}^{Nel} V_e X_{e2} - V_1^* = 0 \\
& \boldsymbol{KU} = \boldsymbol{F} \\
& \boldsymbol{K}\boldsymbol{\phi} = \boldsymbol{f}_t \\
& X_{ej} = x_{\min} \quad or \quad 1, \quad for \quad e = 1,..,Nel \quad and \quad j = 1,2.
\end{aligned}
\tag{10}
$$

Sensitivity analysis

The BESO method modifies the topology of the design domain according to the relative ranking of the elemental sensitivities. The elemental sensitivities, sn_{ej}, of the objective function with respect to the design variable can be calculated as follows,

$$
sn_{ej} = 2\left(\alpha_{11}^H\right)\frac{\partial \alpha_{11}^H}{\partial X_{ej}} + 2\left(\alpha_{22}^H\right)\frac{\partial \alpha_{22}^H}{\partial X_{ej}}; \quad for \quad e = 1,...,Nel \quad and \quad j = 1,2. \tag{11}
$$

where $\frac{\partial \alpha_{11}^H}{\partial X_{ej}}$ and $\frac{\partial \alpha_{22}^H}{\partial X_{ej}}$ are the derivatives of the first and second component of the vector of the equivalent vector of the thermal expansion coefficients, $\boldsymbol{\alpha}^H$, with respect to the design variables, given by:

$$
\frac{\partial \boldsymbol{\alpha}^H}{\partial X_{ej}} = \left(\boldsymbol{D}^H\right)^{-1}\left(\frac{\partial \boldsymbol{\beta}^H}{\partial X_{ej}} - \frac{\partial \boldsymbol{D}^H}{\partial X_{ej}}\boldsymbol{\alpha}^H\right); \quad for \quad e = 1,...,Nel \quad and \quad j = 1,2. \tag{12}
$$

where the derivatives of the homogenized elasticity matrix and the effective thermal stress vector, with respect to the design variables, are calculated as follows:

$$
\frac{\partial \boldsymbol{D}^H}{\partial X_{ej}} = \frac{1}{|Y_e|}\int_{Y_e} (\boldsymbol{I}_e - \boldsymbol{B}_e\boldsymbol{U}_e)^T \frac{\partial \boldsymbol{D}_e}{\partial X_{ej}} (\boldsymbol{I}_e - \boldsymbol{B}_e\boldsymbol{U}_e)\, dy; \quad for \quad e = 1,...,Nel \quad and \quad j = 1,2. \tag{13}
$$

and

$$
\begin{aligned}
\frac{\partial \boldsymbol{\beta}^H}{\partial X_{ej}} = & \frac{1}{|Y_e|}\int_{Y_e} (\boldsymbol{I}_e - \boldsymbol{B}_e\boldsymbol{U}_e)^T \frac{\partial \boldsymbol{D}_e}{\partial X_{ej}} (\boldsymbol{\alpha}_e - \boldsymbol{B}_e\boldsymbol{\phi}_e)\, dy \\
& + \frac{1}{|Y_e|}\int_{Y_e} (\boldsymbol{I}_e - \boldsymbol{B}_e\boldsymbol{U}_e)^T \boldsymbol{D}_e \frac{\partial \boldsymbol{\alpha}_e}{\partial X_{ej}} dy; \quad for \quad e = 1,...,Nel \quad and \quad j = 1,2.
\end{aligned}
\tag{14}
$$

where, $\frac{\partial \boldsymbol{D}_e}{\partial X_{ej}}$ and $\frac{\partial \boldsymbol{\alpha}_e}{\partial X_{ej}}$ are the derivatives of the material interpolation equations with respect to each design variables, which are given by:

$$
\frac{\partial \boldsymbol{D}_e}{\partial X_{e1}} = p_1 X_{e1}^{p_1 - 1}\left(\boldsymbol{D}_1 - \boldsymbol{D}_2\right), \tag{15}
$$

$$
\frac{\partial \boldsymbol{\alpha}_e}{\partial X_{e1}} = q_1 X_{e1}^{q_1 - 1}\left(\boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2\right), \tag{16}
$$

$$
\frac{\partial \boldsymbol{D}_e}{\partial X_{e2}} = p_2 X_{e2}^{p_2 - 1}\left(\boldsymbol{D}_2\right) \quad \text{and,} \tag{17}
$$

$$
\frac{\partial \boldsymbol{\alpha}_e}{\partial X_{e2}} = q_2 X_{e2}^{q_2 - 1}\left(\boldsymbol{\alpha}_2\right). \tag{18}
$$

(19)

Bi-directional evolutionary structural optimization method

The study was conducted using the results obtained using a modified BESO method to solve the topology optimization problems, and to help understand how its parameters affect the final value of the objective function when designing metamaterials with zero thermal expansion. The BESO methodology used in this work was implemented following the next steps:

1. Defining the initial domain: square base cell full of material 1, where the four elements at the center are filled with material 2.
2. Defining the BESO parameters:
   - Evolutionaty ratio, ER.
   - Addition ratio, AR_{max}.
   - Filter radius $R_{\min}$.
   - Final volume fraction of material 1, V_1^*.
   - Final volume fraction of material 2, V_2^*.
3. Calculate the displacement fields $\boldsymbol{U}$ and $\boldsymbol{\phi}$, usign equations 4 and 5, respectively.
4. Calculate the homogenized thermal expansion coefficients using equations 1 to 3.
5. Calculate the elemental sensitivity numbers using equations 11 to 18.
6. Filter the sensitivity numbers and apply the history averaging (Sigmund and Petersson, 1998; Huang and Xie,2010b) .
7. Calculate the volume target for both materials (Huang and Xie,2010b).
8. Update $\boldsymbol{X}_1$.
9. Repeat steps 3 to 8 until the colume constraint for material 2 is satisfied, when satisfied go to step 10.
10. Update $\boldsymbol{X}_2$. .
11. Repeat steps 3 to 10 until the colume constraint for material 1 and the stop criterion are satisfied.
12. Remove disconected island of solid material using the inverse virtual temperature method (Liu et al, 2015).
13. The final topology is obtained.

PARAMETER ANALYSIS

In this work we focus on the influence of the BESO parameters, ER, $AR_{\max}$, $R_{\min}$ and the volume fraction of both materials, in the final value of the objective function. As the initial topology is almost full of material 1 (Huang and Xie, 2011), the ER represents the percentage of material 1 that is removed from the design domain each iteration until its final volume is reached and the $AR_{\max}$, limits the amount of material 2 that will be turned material 1, and the amount of void that will be turned material 2. The design problem of obtaining a metamaterial with zero thermal expansion was chosen to perform this parameter analysis. Using the methodology presented in section , it is possible to obtain a topology with zero thermal expansion like the one depicted in fig, 1.

The base cell considered in this work is discretized into 100×100 four-node quadrilateral plane stress elements, and the two materials are assumed to be isotropic with Young's modulus $E_1 = E_2 = 1$, isotropic thermal expansion coefficients $\alpha_1 = 10\alpha_2 = 10$ and Poisson's ratio $\nu_1 = \nu_2 = 0.3$. It is considered the dihedral symmetry D_2. The penalization factors $p_1 = q_1 = 1$ and $p_2 = q_2 = 3$ are maintained constant for all cases.

Figure 2 presents the relation between the objective function and each BESO parameter studied. The results shown in figure 2(a) indicate that the algorithm does not converge to the desired property when the addition ratio is greater than 3%. It was found that the objective function does not dependent on the evolutionary ratio considering an absolute error of less than 0.01, as observed in figure 2(b). Another important finding was that the filter radio does not present any influence in the final objective function for values between 0.04 and 0.07 as depicted in figure 2(c). As figure 2(d)

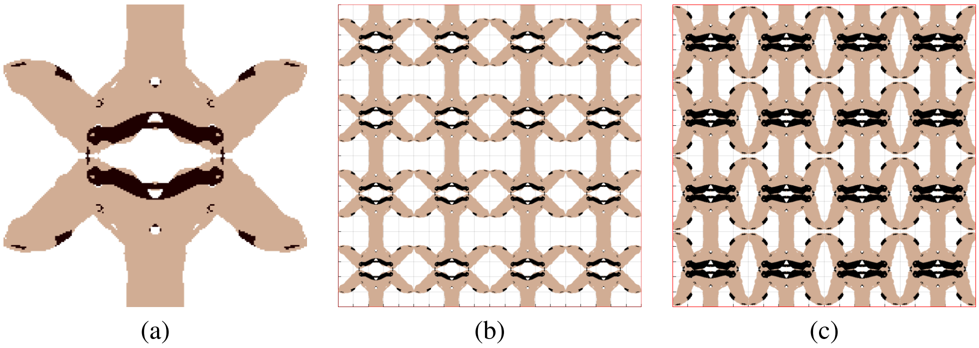

Figure 1 – Final topology for a zero thermal expansion metamaterial design: (a) final topology; (b) 4×4 **undeformed array; (c)** 4×4 **deformed array**

shows, there is a local maximum of the objective function for a value of 20% of material 2 considering 40% of material 1, while considering a constant volume of material 2 of 10% it is observed in figure 2(e) that the final value of the objective function is approximately proportional to the volume percentage of material 1, however, figure 2(e) shows that the best volume percentage for 50% of solid material is 10% of the material with a high thermal expansion coefficient and 40% of the material with a low thermal expansion coefficient.

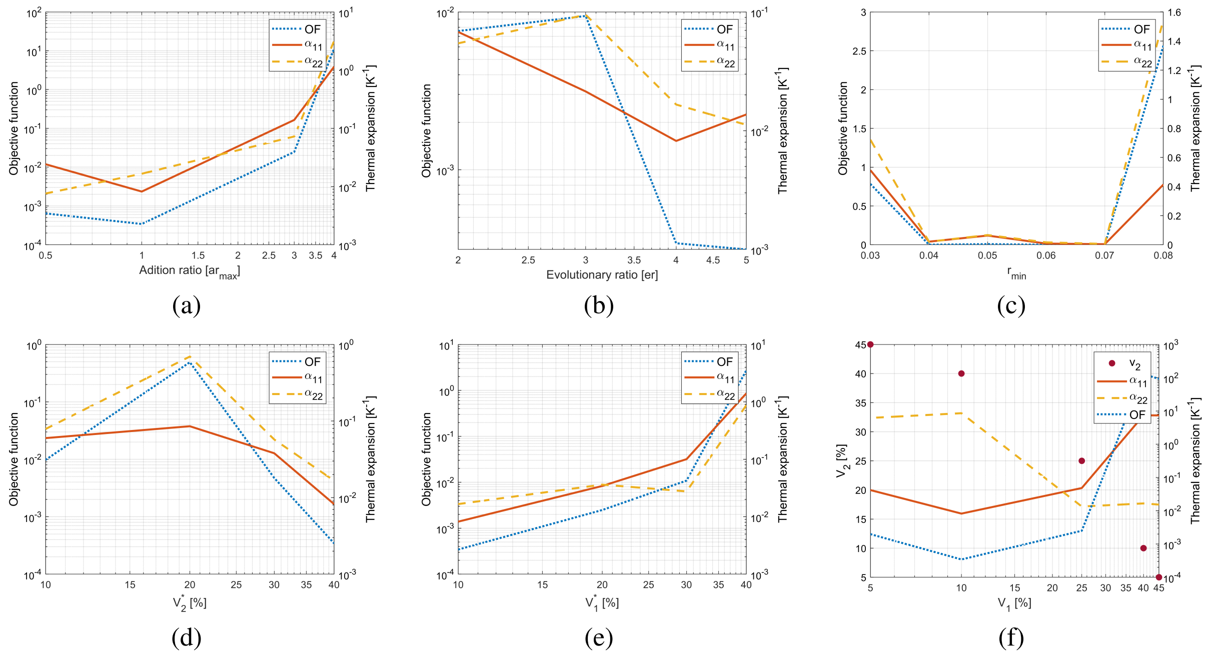

Figure 2 – Graphs of the objective function vs the BESO parameters: (a) Objective function vs addition ration; (b) Objective function vs evolutionary ratio; (c) Objective function vs filter radio; (d) Objective function vs volume percentage of material 2**; (e) Objective function vs Volume percentage of material** 1**; (f) Volume percentage of material** 1 **vs volume percentage of material (2)**

CONCLUSIONS

The present research aimed to examine the dependency of the objective function used to design metamaterials with zero thermal expansion on the BESO parameters. This study has identified that there is no dependency of the final value of the objective function on the evolutionary ratio and the filter radio for values of the last one between 0.04 and 0.07. The research has also shown that the algorithm does not converge when using values of addition ratio greater than 3%. This work has shown that for a final solid volume of 50%, a volume percentage of 10% of material 1 and 40% of material

2 presents the best value of the objective function. The small amount of data did not allow identify the influence of the volume percentage of material 1, when the volume percentage of material 2 is fixed and vice-versa, on the final value of the objective function. It is recommended to run more tests to identify their relationship.

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