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Numerical Analysis of the Effective Thermal Properties and the Stability for NTE Metamaterials Using CAE Fidesys

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Abstract. Metamaterials are composite materials, the properties of which are determined primarily by their geometric cellular microstructure, and not by the properties of the components included in their composition. The article is devoted to the metamaterials with a negative thermal expansion coefficient (NTE). The thermal expansion effective coefficients of such materials are analyzed. Effective thermal expansion is calculated numerically, by solving a boundary value problem of thermoelasticity on the metamaterial's periodicity cell using finite element method. A strain tensor is averaged over the cell. Effective thermal properties are estimated using the averaged solution results. Also, a stability of NTE-metamaterial's cell under thermal loads is analyzed. The article presents a dependency of the metamaterial effective thermal expansion coefficients on various geometric parameters of its cell. Variation of these parameters allows to make the thermal expansion effective coefficient both zero and negative with a large absolute value. A metamaterial is proved to be stable under thermal loads in a wide range of temperatures.

INTRODUCTION

Metamaterials are composite materials, the properties of which are determined primarily by their geometric (cellular [1]) microstructure, and not by the properties of the components included in their composition. Metamaterials may have unique optical, radiophysical, electrical, acoustic and other properties that open broad perspectives for different industrial applications. Such materials have a cellular structure [2] and are manufactured by 3D printing.

This article is devoted to numerical modeling of metamaterials with a negative thermal expansion coefficient [3]. Such materials shrink when heated. Such metamaterials which do not change their sizes when heated or cooled are of practical interest. They can be used in microchip devices, adhesive and dental fillings and high-precision optical or mechanical devices under variable external temperatures. NTE-metamaterials are usually manufactured using 3D printing with two components with various mechanical and thermal properties: a harder one with a smaller thermal expansion coefficient and a softer one with a higher coefficient. It is important to note that both components have positive thermal expansion coefficients.

A size of the metamaterial periodicity cell is about a millimeter. At the same time, products made of a metamaterial may have a size of about 10 cm or even a meter. Therefore while running numerical structural or thermal analysis of a full product or its part made of a metamaterial with a microstructure, it is impossible (and actually not necessary) to simulate the geometry of each cell. To speedup such calculations, a heterogeneous metamaterial is replaced by an anisotropic and homogeneous effective material which mechanical behavior corresponds, on average, to the initial metamaterial. At the same time, the question arises: How to estimate the mechanical and/or thermal properties of this effective material?

The effective properties estimation for heterogeneous material is one of the main problems of the mechanics of composites. In this paper, the effective thermal characteristics of the NTE-metamaterial [4] are estimated by numerical solving a boundary value problem of thermoelasticity on its periodicity cell [5] with periodic boundary

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conditions. The results are averaged over the volume of cell [6]. Finally effective linear thermal expansion coefficients are computed.

NTE metamaterials are intended for using in a wide range of temperatures. This raises the problem of their stability under thermal loads. We present results of bucking analysis of a periodicity cell obtained using FEM.

PROBLEM STATEMENT AND SOLUTION ALGORITHM

First, let us give the definition of effective thermal expansion [7]. We call the effective (averaged) material (in terms of temperature expansion) such a homogeneous material that will satisfy the following condition: if we consider the periodicity cell [6] of the initial metamaterial and fill-in the same volume with the homogeneous material, then the averaged over the volume thermal strains on these cells are equal in case of equal temperature distributions in the volumes. The thermal expansion coefficients of this material will be called effective coefficients of thermal expansion. Using this definition, we describe a method of the estimation of the effective thermal conductivity coefficients of the metamaterial. To estimate the effective coefficient of thermal expansion of the metamaterial, we solve a boundary value problem of elasticity [8] on its periodicity cell V_0 taking the thermal expansion into account:

$$\begin{gathered} \nabla\sigma^{\mathrm{el}} = 0, \\ \sigma^{\mathrm{el}} = \sigma - \sigma^{\mathrm{th}}. \end{gathered} \tag{1}$$

Here σ is total stress tensor, σ^{el} is mechanical (elastic) stress tensor [9], σ^{th} is thermal stress tensor.

The periodic boundary conditions [10] are applied to the cell, and then it is heated at ΔT. Under the influence of a temperature, the cell is deformed. We derive the effective temperature expansion in the form of a linear relation between the thermal strain tensor and ΔT:

$$\varepsilon_{ij}^{\mathrm{th}} = \alpha_{ij}\Delta T. \tag{2}$$

Effective thermal expansion coefficients are calculated from the ratio [7]:

$$\alpha_{ij} = \frac{\varepsilon_{ij}^{\mathrm{e}}}{\Delta T}. \tag{3}$$

Boundary conditions applied to the periodic cell should be discussed in more details (see Fig. 1). The non-periodic boundary conditions in this problem are zero pressure, which allows it to expand freely with increasing temperature. Periodic boundary conditions also allow the volume to expand freely with a limitation: the volume, which was the composite's periodicity cell before the deformation, should remain a periodicity cell after the deformation. For this, a pair of points is fixed (1, 2), the first of which is on the face $x = A$, the second—on the face $x = -A$, and their projections coincide (these may be angular points.). And the corresponding restraint is applied on the displacements of each pair of points $(i, -i)$:

$$u_i - u_{-i} = u_1 - u_2, \tag{4}$$

where u is the displacement vector of a point.

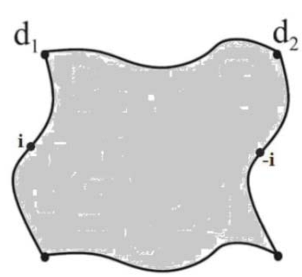

FIGURE 1. Periodic boundary conditions.

FIGURE 2. NTE metamaterial.

We note again that in this equation, a pair of points $(i, -i)$ vary, passing throughout the surface of the faces $x = A$ and $x = -A$; and the pair of points $(1, 2)$ is fixed, the same for all restraints of the equation. Similar restraints are applied on corresponding to each other points from faces $y = B$ and $y = -B$ and from faces $z = C$ and $z = -C$. Such boundary conditions allow the models to freely change their volume, while keeping the shape of a periodicity cell.

RESULTS

In the paper, we simulate the effective thermal properties of the NTE metamaterial and study their dependence on the geometric cell parameters. Calculations are carried out using a software module Fidesys Composite of CAE Fidesys [11]. For constructed periodicity cells, a set of numerical experiments is carried out, in which the effect of the geometric parameters of the model on the metamaterial thermal expansion coefficient is shown. The metamaterial components' properties are described by Young's modulus, Poisson's ratio and thermal expansion coefficient.

The study examines the cell's model with two materials: copper (hard, but with a smaller thermal expansion coefficient) and polymer (soft, but with a large thermal expansion coefficient) with a large number of voids. Figure 2 shows the cell structure of such a metamaterial. Black color corresponds to copper (a more solid component with a smaller thermal expansion coefficient), grey is a polymer (a softer component with a higher thermal expansion coefficient). For this metamaterial model we present dependency of the effective thermal expansion coefficients on geometric parameters—the angle of inclination of polymer rods with respect to the copper contour. These calculations are carried out for different combinations of the original model parameters: the thickness of the cell contour, the thickness of the polymer rod and the thickness of the diagonal copper rods. Also, a buckling analysis of the cell under thermal deformations is carried out. As a result, a temperature range was determined, within which this structure is stable. For a model consisting of two materials: copper and polymer, a dependency of the temperature expansion coefficient on the angle α was analyzed with a fixed thickness of the frame. As a result we may conclude the following terms. Firstly, it's possible to choose the parameters of the cell, for which the metamaterial has a zero effective thermal expansion coefficient—that is, when the temperature changes, it keeps its size. Secondly, with certain combinations of parameters, the effective coefficient is negative, and its module is large enough (equal to the thermal expansion coefficient of the polymer). Figure 3 shows the dependence of thermal expansion coefficient (units of the K^{-1}) on the angle α between the copper contour and the polymer rod. The following notation was introduced on the graph: T is the thickness of the copper contour of the cell, P is the thickness of the polymer rod, C is the thickness of the copper diagonal. Sizes are given in relation to the total cell size.

For a deeper analysis of the properties of the resulting model, the buckling analysis under thermal loads is performed on the cell. The results show that an increase in the thickness of the copper diagonals and the contour allows one to expand the temperature range in which the metamaterial remains stable. The thickness of the polymer rod also influences on the stability: there is some optimal value (depending on the thickness of the contour and the diagonals), at which the temperature range is the widest.

The plots of the dependence of the critical temperatures on the thickness of the contour and the diagonals are shown in Fig. 4. The vertical axis corresponds to the thickness of the contour in the hundredths, the horizontal axis is the temperature axis.

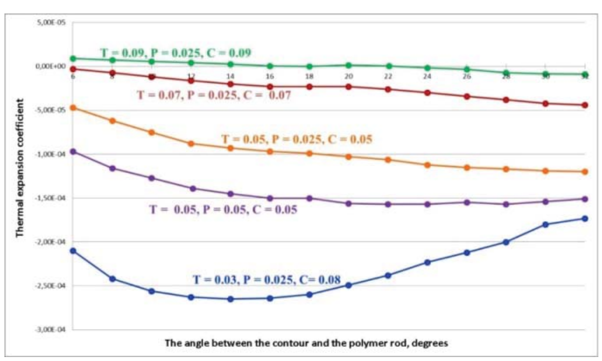

FIGURE 3. An effective thermal expansion coefficient versus an angle between the periodicity cell's contour and the polymer rod.

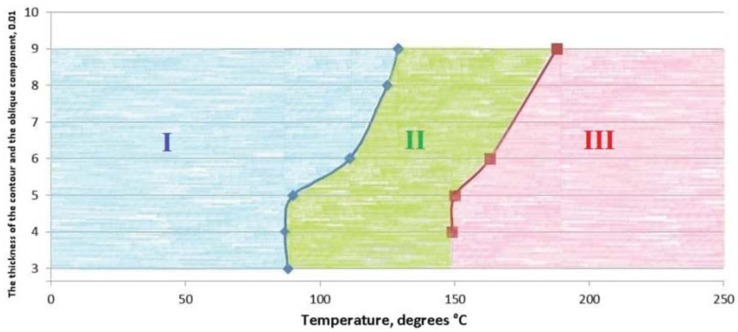

FIGURE 4. Stability areas.

The blue line corresponds to the cell with $P = 0.025$, the red line corresponds to the cell with $P = 0.05$. For the first cell, the area of stability is I. For the second cell, the areas of stability are I and II. The graphs show that the increase of the thickness of the contour and the diagonals causes the non-linear increase of the critical temperature value for the metamaterial.

Finally we perform the buckling analysis for the cell with the smallest effective thermal expansion coefficient (the lower graph in Fig. 3, $T = 0.03$, $P = 0.025$, $C = 0.08$, $\alpha = 14°$) and for the cell with almost zero coefficient (the top graph in Fig. 3, $T = 0.09$, $P = 0.025$, $C = 0.09$, $\alpha = 18°$). The critical temperature is 105ºC for the first cell and 129ºC for the second cell. In indicates that NTE metamaterials with different cell parameters are stable under thermal loading in a wide temperature range.

CONCLUSION

Thus, the results of the calculations demonstrate that a proper choice of the geometric parameters of the periodicity cell of the specified shape allows one to achieve a negative effective coefficient of thermal expansion with a large absolute value or almost zero effective coefficient. At the same time, NTE metamaterials are stable under thermal loading in a wide temperature range.

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