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A NEW METAMATERIAL PLATE WITH TUNABLE THERMAL EXPANSION

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Summary. Homogeneous materials typically expand when heated, leading to dimensional changes and often significant thermal stresses in structures subject to temperature variations. Microstructured periodic materials, also called metamaterials, offer a promising solution for achieving zero, negative, and in general tunable equivalent thermal expansion which is needed to mitigate unwanted mechanical effects of temperature changes. To obtain zero or negative equivalent thermal expansion coefficient at least two different materials must be combined and typically the unit cell is designed in two dimensions, with different parts made of the two constituent materials, and then it is extruded in the out-of-plane direction.

In this work, we propose a novel geometry, with a non-symmetric layered unit cell, that is fully compatible with fabrication processes employed for micro-electro-mechanical systems. Parametric studies show that a proper design of the unit cell allows to achieve the desired coefficient of thermal expansion and to tune (or even cancel) the global thermal-induced deflection due to the asymmetrical layers configuration in the metamaterial plate.

1 INTRODUCTION

The design of all structures subject to significant temperature variations must consider the effects of thermal strains. Most of the materials used in engineering have a positive coefficient of thermal expansion (CTE) and hence they increase in size when heated. This can cause undesired effects beyond dimensional changes, such as thermal stresses or warping. In those cases, materials with negative, zero, or more in general programmable thermal expansion would be useful to control and mitigate the temperature variation effects.

Few natural materials show negative thermal expansion, a recent review of the understood mechanisms has been carried out by Liang et al. [1]. However, those materials are not typically used in engineering and they might not be suitable for actual applications [2].

Metamaterials, i.e. microstructured materials, generally with periodic patterns, have emerged in the last two decades as an alternative to obtain fully tunable thermal expansion. Their main advantage is the possibility to combine many different constituent materials, including typical engineering materials with positive thermal expansion, to obtain the desired, global, effective thermal behaviour through a proper geometrical design. Metamaterials with tunable CTE proposed in the literature can be classified in bending-dominated and stretch-dominated depending on the underlying mechanism allowing to obtain zero or negative CTE [3, 4]. In general, the microstructure results in a non-isotropic equivalent CTE [5], but one can also obtain almost isotropic metamaterials [6], with the same behavior in two orthogonal directions. However, to the best of the authors' knowledge, none of the negative CTE metamaterials proposed so far can be manufactured by the processes of micro-lithography used for micro-electro-mechanical systems (MEMS) [7].

In the present work, we propose a novel bi-layered configuration with a base structure made of one constituent material, and a layer made of the other constituent on top of some parts of the base structure. The periodic in-plane repetition of this cell leads to a metamaterial plate that can exhibit negative in-plane CTE. The arrangement of layers is non-symmetric with respect to the mid-plane of the metamaterial plate, hence in general the plate deflects when heated or cooled. However, also this thermal-induced curvature can be tuned and, if necessary, set to zero by a proper design of the unit cell. The proposed configuration is compatible with micro-lithography fabrication processes used for micro-electro-mechanical systems, thus opening the way for the design of new devices: a patent on a MEMS thermometer has been submitted [8].

The paper is organized as follows. In Section 2 we present a review of the main mechanisms available in the literature to obtain a negative CTE and we propose a new cell geometry for a stretch-dominated metamaterial. In Section 3, the novel non-symmetrical layered metamaterial plate is presented, its effective thermal properties are computed through numerical simulations and the influence of geometric and material parameters on these properties is discussed in detail. Some conclusions are given in Section 4.

2 BASIC MECHANISMS TO ACHIEVE NEGATIVE CTE

2.1 Bending-dominated metamaterials

Bending-dominated metamaterials were first proposed in [9]. They typically exploit bi-material beams which bend when heated due to the different CTE of the two constituent materials. If the beams have curved axes (as in arches) and the material with higher CTE (represented in orange all along this paper) is placed on the side of smaller curvature, the additional thermal-induced curvature shortens the projection of the beams as shown in Figure 1, causing an overall contraction in that direction.

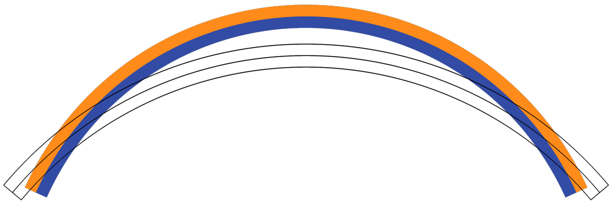


Figure 1: Bi-material arch with horizontal contraction on heating. Initial configuration in black, configuration after heating in color: high-CTE material in orange, low-CTE material in blue.

Figure 2a reports an example of a truss beam proposed in [10] where the insertion of such curved bi-material elements allows to tune the overall thermal expansion. Combining several bi-material arches, one can also obtain a two-dimensional metamaterial with negative thermal expansion, as the one proposed in [11], see Figure 2b. The effective thermal expansion of these geometries can be easily tuned by varying the initial curvature of the arch and the thicknesses of the two materials.

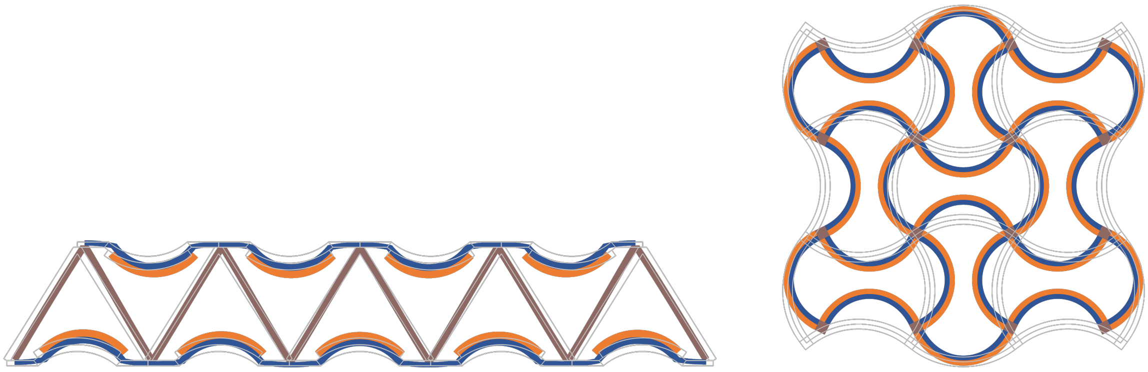

(a) (b)

Figure 2: Examples of bending-dominated metamaterials (initial configuration in gray, configuration after heating in color): (a) 1D truss metabeam proposed in [10]; (b) 2D metamaterial proposed in [11].

2.2 Stretch-dominated metamaterials

The other mechanism of metamaterials with negative CTE is the stretch-dominated one: in this case, there is a larger variety of configurations, with the common characteristic of exploiting the different axial elongation of elements made of different materials to obtain equivalent negative thermal expansion. The simplest geometry showing this effect is a truss triangle such as the one in Figure 3, where the material 2 of the orange bar has a higher CTE α_2 than the one of the blue bars α_1, i.e. $\alpha_2 > \alpha_1$. Upon heating, depending on the actual geometry and the difference between the two thermal expansion coefficients, the base can expand more than the other edges causing the angle θ to increase and the height h to decrease, obtaining negative equivalent thermal expansion in the vertical direction. In this case, the main parameter governing the value of the effective thermal expansion in the vertical direction is the angle θ itself, in addition to the CTE of the two materials α_1 and α_2. The equivalent thermal expansion in the vertical direction for this triangle can be calculated and reads

$$\alpha_v^* = \frac{\mathrm{d}h}{h\ \mathrm{d}T} = \alpha_1 - (\alpha_2 - \alpha_1)\tan^2\theta \tag{1}$$

Therefore for fixed materials composing the truss, i.e. for fixed α_1 and α_2, one can compute the value of the angle to obtain $\alpha_v^* = 0$, namely

$$\theta = \arctan\sqrt{\frac{\alpha_1}{\alpha_2 - \alpha_1}} \tag{2}$$

Figure 4 shows the unit cells of some stretch-dominated materials proposed in the literature to obtain tunable or negative thermal expansion. Even though the bars are not hinged, their slenderness ensures a behavior similar to that described above. The cell in Figure 4a has an equivalent CTE which is positive in the vertical direction and negative in the horizontal one, while the cells in Figures 4b and 4c have the same behavior in the horizontal and vertical direction and hence will be called “with isotropic thermal properties”. It should be noted however that the microstructure is only two dimensional and the out-of-plane CTE is completely different.

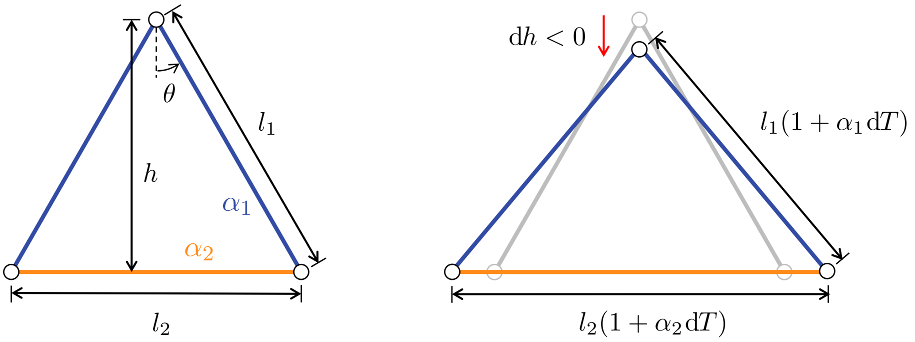
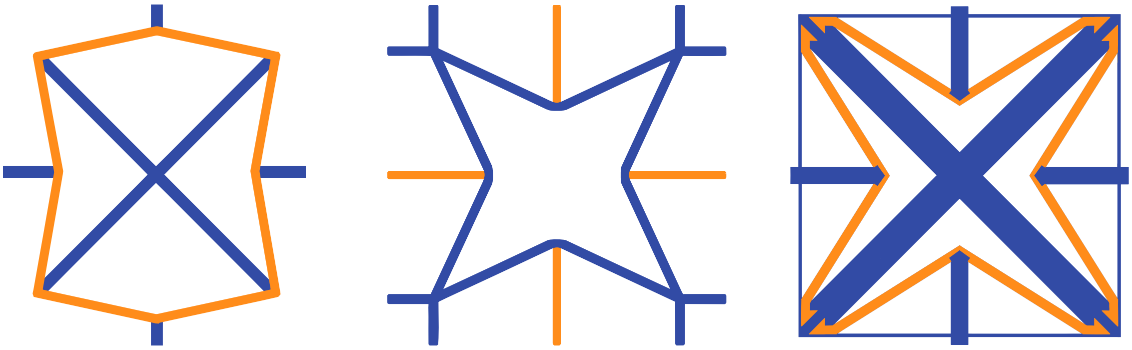


Figure 3: Stretch-dominated triangle and its deformed configuration upon heating in case of negative equivalent vertical CTE.



(a) (b) (c)

Figure 4: Unit cells of stretch-dominated metamaterials with negative CTE proposed in the literature, from: (a) [5], (b) [12] and (c) [13].

In this work, we propose a geometry of a stretch-dominated metamaterial similar to the ones in Figure 4 , modified to have isotropic thermal properties and to simplify manufacturing while obtaining an improved behavior in terms of the minimum thermal expansion achievable. The final geometry of the unit cell proposed in this work is shown in Figure 5, left. The cell is composed of a four-pointed star, made of a high CTE material, with the diagonals made of another low CTE material; the re-entrant corners of the star of two adjacent cells are connected by this second material.

The mechanism that allows obtaining the desired negative thermal expansion can be seen in Figure 5, center. Upon heating, the points of the star are constrained to have the same expansion of the diagonals, which are made of the lower-CTE material, thus the inclined segments (orange) accommodate their additional thermal expansion by moving the vertical and horizontal elements which connect the adjacent cells inward. When the CTE difference between the two materials is large enough, this effect is sufficient to obtain a global negative thermal expansion, as shown in Figure 5, right, for an array of 3×3 cells.

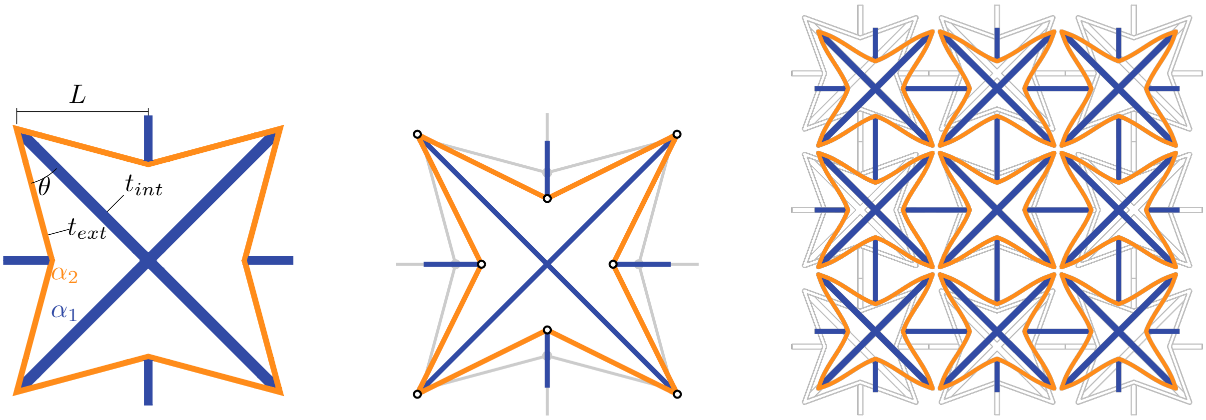


Figure 5: The proposed unit cell: parameters defining its in-plan geometry; its deformed configuration upon heating (assuming elements are pin-jointed) and deformed configuration of a 3×3 metamaterial showing the negative effective thermal expansion (initial configuration in gray, configuration after heating in color).

3 LAYERED METAMATERIAL

The unit cells of two-dimensional metamaterials with negative CTE proposed in the literature and, in particular, those described in the previous section are generally designed in the plane and then extruded in the out-of-plane direction as shown in Figure 6 (left). In this work, we propose a novel configuration based on layered unit cells, as shown in Figure 6 on the right. To obtain the high-CTE four-pointed star inside the cell, the high-CTE material is layered on top of the base structure which is entirely made of a single low-CTE material. The layered structure, like the original one, allows the achievement of a zero or negative equivalent thermal expansion coefficient $\alpha^* \leq 0$. The main advantage of this configuration is being compatible with micro-lithography fabrication processes used, e.g., for micro-electro-mechanical systems (MEMS).

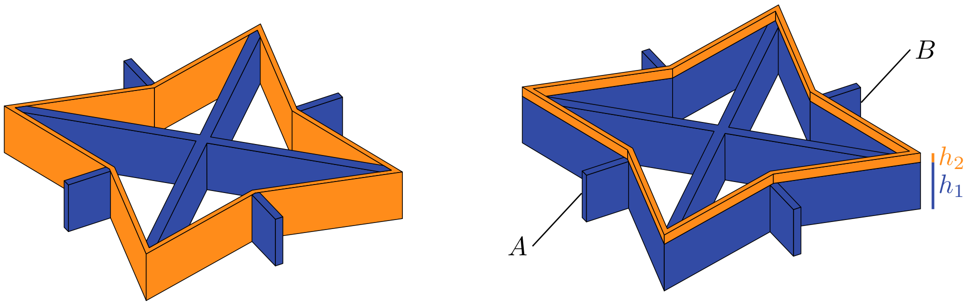


Figure 6: Negative CTE metamaterials: the traditional way of placing materials in a unit cell (left) and the proposed new layered structure of the unit cell (right).

If the layer is placed asymmetrically with respect to the mid-plane, as in Figure 6 (right), the metamaterial in general bends upon a temperature variation. This effect can be useful for some applications, but can also be avoided by a proper design as detailed in Section 3.1. To

Table 1: Material properties at 20 °C from [14].

Material	Young's Modulus [GPa]	Poisson's ratio -	CTE [ppm/°C]
Silicon (Si) (polycristalline)	163	0.22	2.6
Nickel (Ni)	205	0.29	12.6
Silicon oxide (SiO_2)	70	0.17	0.5
Diamond-like carbon (DLC)	1145	0.07	1.0

characterize the metamaterial one has also to compute an equivalent global "thermal curvature" χ^* due to a unit temperature variation. This curvature is here defined as the ratio between the relative rotation of the vertical faces A and B of a cell (see Figure 6, right) and the cell dimension $2L$.

3.1 Influence of geometric parameters

The equivalent thermal properties α^* and χ^* of the new layered metamaterial depend on the thermo-mechanical properties of the constituent materials and on the parameters defining the exact geometry, namely, the in-plane thicknesses t_{int} and t_{ext}, the out-of-plane thicknesses h_1 and h_2, the cell dimension L and the angle θ of the star points, as defined in Figures 5 and 6. To understand the influence of geometric parameters on global properties, several parametric studies have been carried out and are presented in this section.

For these studies, we select silicon as the base, low-CTE, material, and nickel as the top-layer, high-CTE, material, as this is one of the most promising combinations in terms of achievable properties and of practical fabrication in MEMS. Their thermo-mechanical properties are reported in Table 1. It should be noted that to obtain a global behavior with negative α^*, the material used in the top layer should have not only a CTE much larger than the other one but also must be stiffer. These two requirements are met when selecting nickel as material for the layer above silicon.

The contour plots of α^* and χ^* obtained at varying normalized in-plane thicknesses t_{int}/L and t_{ext}/L, having fixed the other geometric parameters, are shown in Figure 7. On both contours, the solid line identifies the couples of thicknesses corresponding to zero equivalent CTE $\alpha^* = 0$, while the dashed line those corresponding to zero equivalent thermal curvature $\chi^* = 0$. Negative values of α^* are obtained by increasing t_{int} with respect to t_{ext}, as this increases the relative stiffness of the diagonals with respect to the star contour. Point A identifies one cell (having $t_{int} = 5.23\ \mu$m and $t_{ext} = 1.80\ \mu$m) with both α^* and χ^* negative ($\alpha^* = -2.88\alpha_1$ and $\chi^* = -...$ m^{-1}K^{-1}), that will be further considered in the following.

Figure 8 shows the contour plots of α^* and χ^* obtained at varying angle θ, defining the sharpness of the points of the star, and of the layer relative thickness h_2/h_1. Continuous and dashed lines correspond again to $\alpha^* = 0$ and $\chi^* = 0$, respectively. Negative values of α^* are obtained by increasing θ and h_2/h_1.

The above parametric analyses show that it is possible to have zero, positive, or negative thermal expansion and curvature. Considering Figure 8 in particular, it is clear that these two properties can be tuned independently, so that different combinations of effective thermal expansion and curvature can be obtained. Figure 8 shows also a combination of parameters

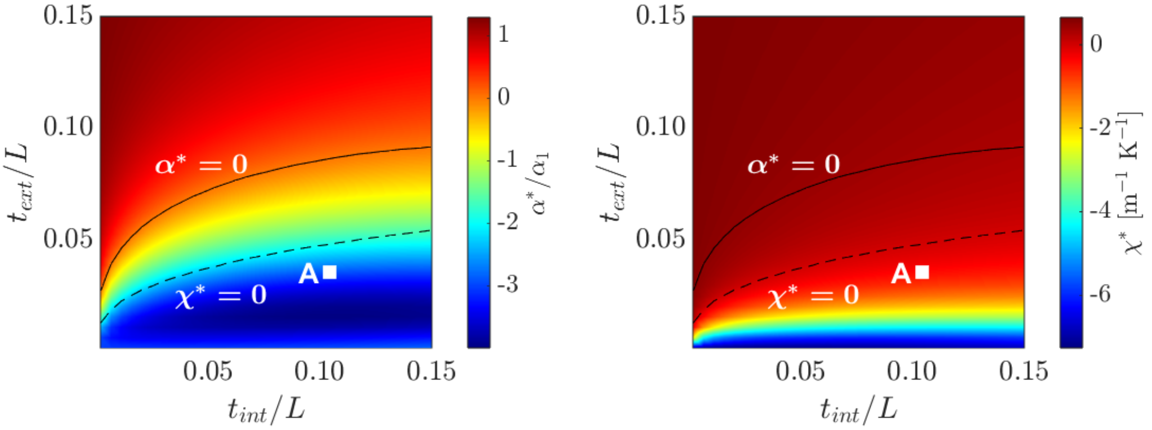


Figure 7: Contour plots of normalized effective thermal expansion α^*/α_1 and curvature χ^* for varying t_{int} and t_{ext} (cell with silicon and nickel; other dimensions: $L = 50\ \mu$m, $h_1 = 10\ \mu$m, $h_2 = 2\ \mu$m, $\theta = 40°$).

that results in a cell having simultaneously zero effective thermal expansion and zero curvature (marked as B on the plot and corresponding to $\theta = 30°$ and $h_2 = 1.13\ \mu$m). Cell C ($\theta = 36.6°$ and $h_2 = 2.95\ \mu$m) instead has negative α^* ($\alpha^* = -0.62\alpha_1$), actually the minimum one achievable with the other fixed parameters ($L = 50\ \mu$m, $t_{int} = 2\ \mu$m, $t_{ext} = 3\ \mu$m, $h_1 = 10\ \mu$m), and positive χ^*.

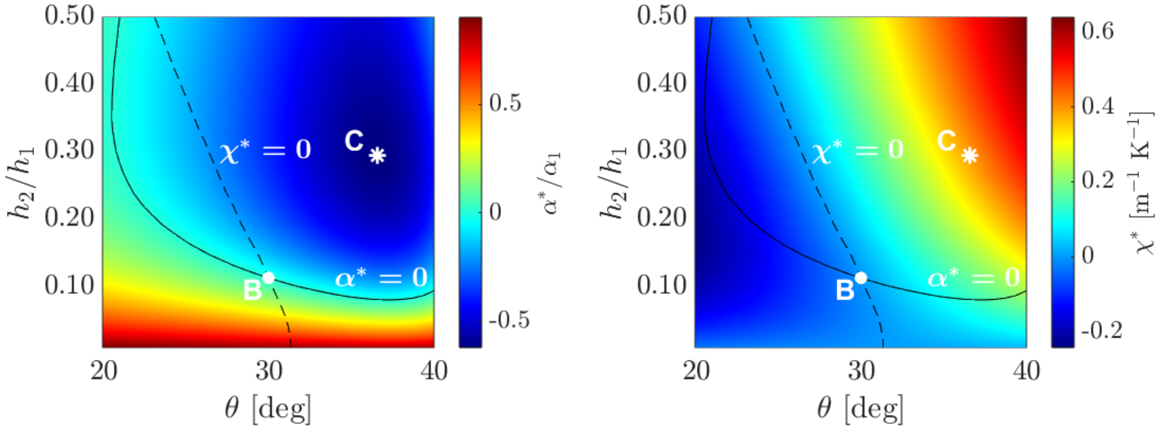


Figure 8: Contour plots of normalized effective thermal expansion α^*/α_1 and curvature χ^* for varying θ and h_2 (cell with silicon and nickel; other fixed dimensions: $L = 50\ \mu$m, $t_{int} = 2\ \mu$m, $t_{ext} = 3\ \mu$m, $h_1 = 10\ \mu$m).

Figure 9 shows the geometry of the unit cells marked as A, B, and C on the contour plots and the deformed configuration due to a temperature increase of a small metaplate made of 5×5 cells. The metaplates composed of cells A and C, which have non-zero curvature, show a significant deflection, while the metaplate composed of cells B remains globally flat despite having small local deflections inside each unit cell.

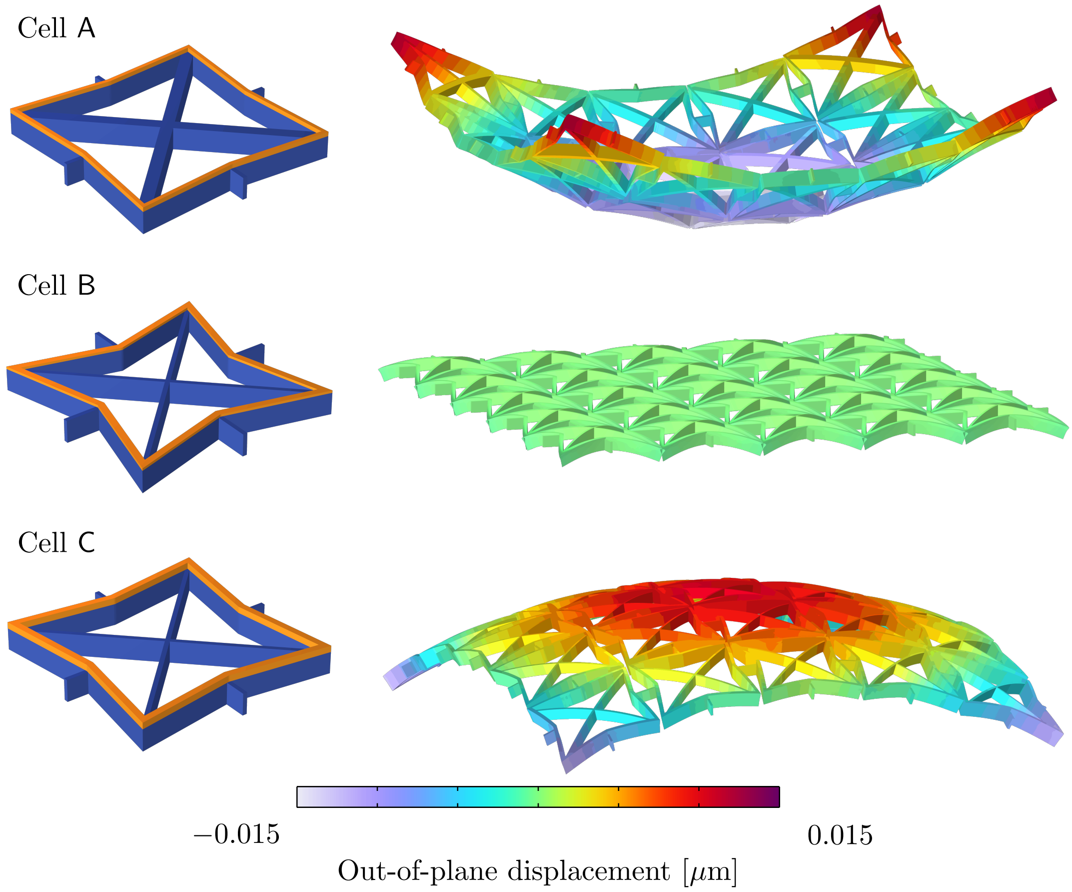


Figure 9: Cells A, B, and C of Figures 7–8: cell geometry and 5×5 metamaterial deformed configuration.

3.2 Influence of temperature-dependent material parameters

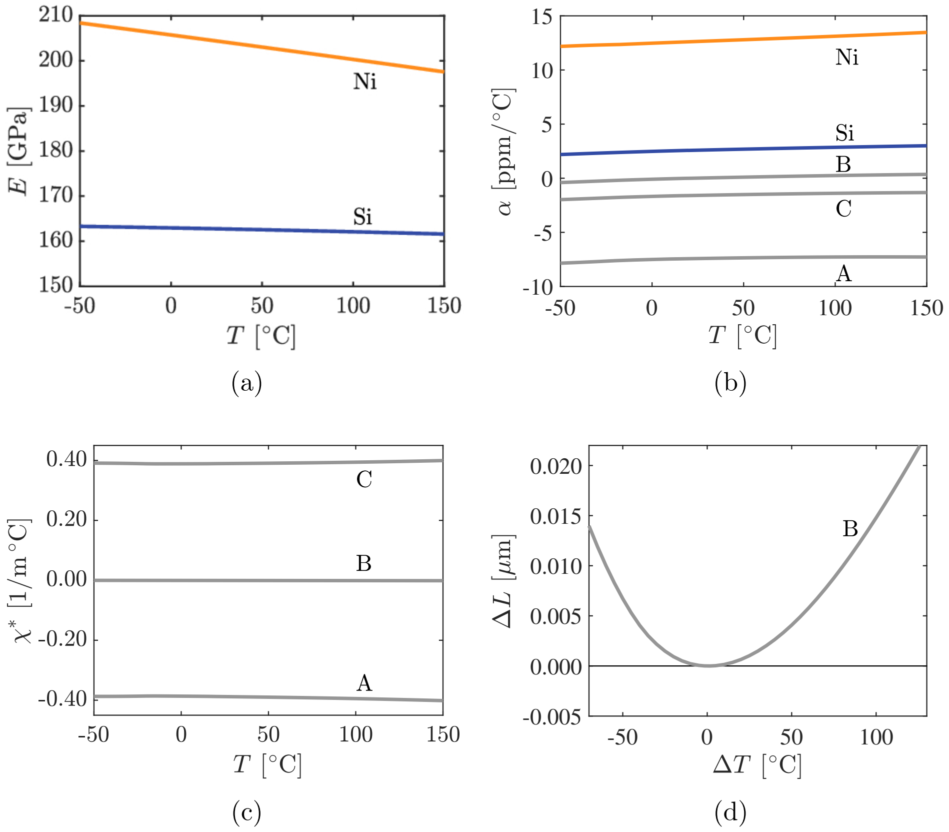
The studies up to now have been carried out considering a 1 °C temperature variation with respect to room temperature (20 °C). However, the constituent materials have properties that show a non-negligible variation with temperature and this should be considered in the design of these metaplates.

Figure 10a shows the variation of the silicon and nickel Young's modulus E with the temperature between −50 °C and 150 °C: for both materials the elastic stiffness decreases with temperature. The CTE of silicon and nickel, along with the effective thermal expansion of the three cells (A, B and C) is plotted in Fig. 10b as a function of the temperature. The increase with temperature of the effective thermal expansion of the cells is very similar to the one of the constituent materials.

Figure 10c shows that the curvature coefficient χ^* is almost constant with temperature, in the range [−50 °C, 150 °C], for the three geometries considered, which means that the out-of-plane deflection of a meta-plate made with cells A or C increases linearly with the temperature variation in the considered range, while the curvature of cell B is almost constantly zero so the corresponding meta-plate remains globally flat for any temperature variation (as shown in

Figure 9).

Figure 10d shows another peculiar behaviour of the metamaterial with cell B: since its effective thermal expansion is tuned to be zero at about room temperature, but it is not perfectly constant with temperature, the effective CTE is slightly negative below that temperature and slightly positive above constituting a case of sign-toggling CTE. This means that, starting from an initial configuration at room temperature, any temperature variation ΔT, both positive or negative, causes expansion ΔL of the metamaterial made of cell B, albeit the effect is rather small.



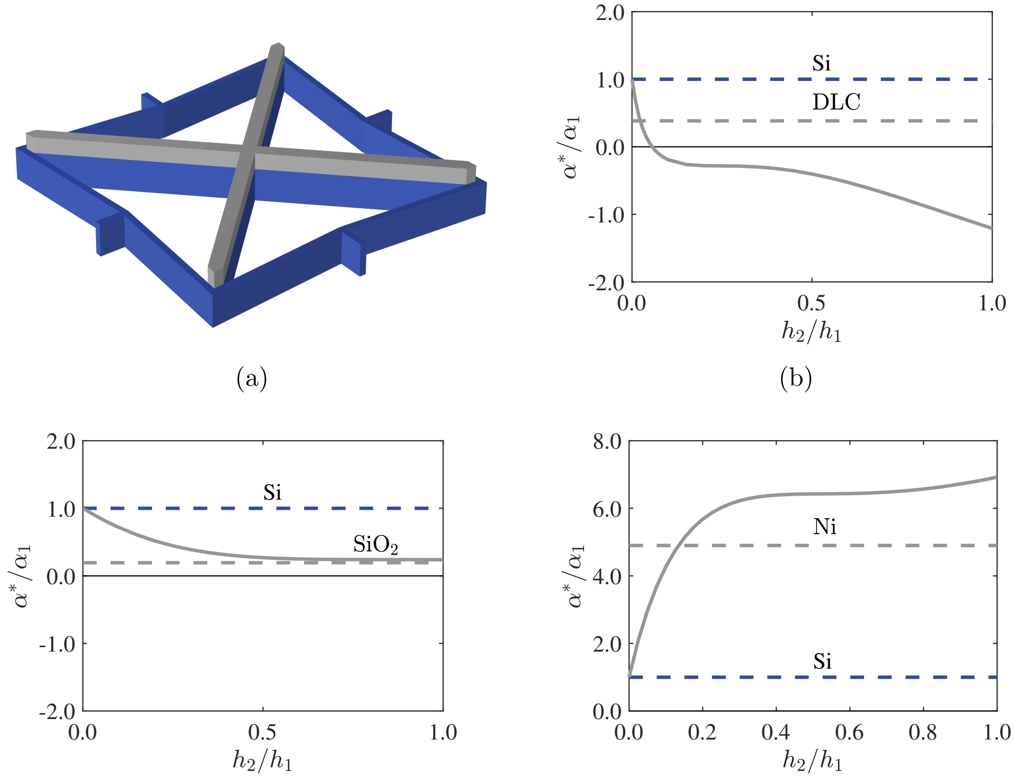
(a) (b)

(c) (d)

Figure 10: Variation with temperature of mechanical and thermal properties: (a) Young's modulus E of constituent materials; (b) coefficient of thermal expansion α of constituent materials and cells of Figures 7–8; (c) curvature coefficient and (d) expansion of a metamaterial made of cell B with side length 500 μm.

3.3 Influence of constituent materials

Other materials can be selected to be layered on silicon to obtain new metamaterials with negative α^*. Selecting a material with a CTE lower than the one of silicon, one can still obtain a global negative CTE by placing the layer on top of the diagonals as shown in Figure 11a. This is the case of a layer made of diamond-like carbon (DLC), its low CTE, together with its high stiffness (cfr Table 1) allows to obtain a metamaterial with negative α^* also using layers of small thickness h_2, as shown in Figure 11b.



(a) (b)

(c) (d)

Figure 11: Metamaterial with layer on the diagonals: unit cell geometry (a), effective thermal expansion α^* as a function of h_2, with DLC (b), SiO_2 (c) and Ni (d) layered on the diagonal. Cell dimensions: $L = 50\ \mu$m, $t_{int} = 2\ \mu$m, $t_{ext} = 1\ \mu$m, $h_1 = 10\ \mu$m, $\theta = 40°$.

When using instead a silicon oxide (SiO_2), even though the CTE is very low, the low stiffness of the layer does not allow to achieve negative equivalent CTE (see Figure 11c). For a layer thickness equal to that of the base structure, and other geometric parameters fixed, α^* tends to the one of silicon oxide.

Finally, with this configuration, if the additional material has a higher CTE than the base material (as it is in the case of nickel with respect to silicon) the effective thermal expansion of the metamaterial increases with respect to the one of the base material and can easily be higher than the one of both constituent materials, see Figure 11d.

At difference from the case with the second layer on the boundary of the star (Figure 6 right), when the second layer is placed on the diagonals, the curvature cannot be canceled: the metamaterial with the higher-CTE material layered on the diagonals shows only positive curvature (and conversely, the other one shows only negative curvature). Moreover, the magnitude of the curvature increases with the layer thickness, hence optimal effective CTE imply larger curvatures.

Remark – By using the geometries proposed in the present work, but with two symmetric layers (on the top and on the bottom of the base structure), one automatically obtains metamaterials with zero thermal curvature. However in the micro-lithography process of MEMS the single layer can be more easily realized, therefore we focus here on the non-symmetric configuration.

4 CONCLUSIONS

In this work, we propose a new metamaterial plate, exhibiting unusual, extreme effective thermal properties, which is made of two materials: one constitutes the base structure of the metaplate while the other one, with a higher CTE, is layered on top of some regions of the first material.

Parametric studies at varying geometric parameters show the versatility of the proposed star-shaped unit cell, which can be properly designed to achieve an in-plane isotropic null or negative CTE. The asymmetrical configuration of the materials induces an out-of-plane deflection when the metaplate is heated or cooled, but this curvature can be properly tuned (upward/downward) or even canceled by a proper geometrical design of the unit cell.

When considering the temperature-dependent behaviour of the constituent material parameters, numerical analyses show that the effective CTE increases in temperature, while the designed thermal-induced curvature is rather independent of temperature.

Finally, when the top layer is made of a material with a lower CTE than the base structure, a different layer configuration can still allow to obtain negative equivalent CTE.

The layered configuration for the metamaterial cell is completely new and has the advantage to be fully compatible with micro-lithography processes. Therefore it can be employed, e.g., in the design of new MEMS devices that are currently under study. The same strategy of layered unit cell could also be convenient for other structural applications at larger scales.

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