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Three-dimensional metamaterials with a negative Poisson's ratio and a non-positive coefficient of thermal expansion

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ABSTRACT

Four types of three-dimensional (3-D) metallic metamaterials with tailorable thermo-mechanical properties are designed. For the first three types, the structure-property relations are studied by adjusting design parameters including two length parameters, one angle parameter and two material combinations. For the fourth type, one additional angle parameter is involved. It is shown that each of the four types of metamaterials designed exhibits the cubic symmetry and thus needs three independent elastic constants to characterize its elastic behavior and one coefficient of thermal expansion to describe its isotropic thermal expansion. The effects of the design parameters on the effective Poisson's ratio (PR), coefficient of thermal expansion (CTE), Young's modulus, shear modulus and the relative density are systematically investigated for each of the four types of designed metamaterials by using unit cell-based finite element simulations that incorporate periodic boundary conditions. It is found that 3-D metallic metamaterials with positive, near-zero or negative PR and CTE can be obtained by tailoring the bi-material lattice structures and material combinations. Also, it is revealed that metamaterial # 1 can achieve both a negative PR and a non-positive CTE while maintaining a high stiffness and a low relative density (and thus a lightweight). The good tunability of thermo-mechanical properties of the four types of metamaterials provides an avenue of enabling the expansion of Ashby's material chart to produce more material options for engineering applications.

1. Introduction

Metamaterials are architected materials exhibiting exotic properties that are not attainable by natural or traditional materials (e.g., [55]). A growing number of studies have been devoted to exploring such materials (e.g., [2,3,8,11,15,39,44,50]).

Mechanical metamaterials that have been explored include those with a negative Poisson's ratio (PR) or a non-positive coefficient of thermal expansion (CTE).

Metamaterials with negative PRs, also called auxetic materials, have been designed and manufactured for over 30 years (e.g., [6,12,16,20,21,24,30,31,34,47,52,60]). Such materials can find applications in sports equipment, protective helmets, body armor, sensors, deployable structures, morphing airfoils, jounce bumpers, and knee prosthetics (e.g., [26,40,51,53,61]).

Metamaterials with a zero or negative CTE have been developed using lattice structures (e.g., [10,23,32,33,43,45,59,62,65,66]), which can be used in temperature-sensitive structures or devices such as precision instruments, satellite antennas, thermal sensors, and bridges to ensure measurement accuracy and mitigate thermomechanical stresses.

For auxetic materials with negative Poisson's ratios, both two-dimensional (2-D) and three-dimensional (3-D) architectures have been developed (e.g., [16,30,34,49,52,60]). However, for metamaterials displaying non-positive CTEs, most micro-architectures proposed are two-dimensional (e.g., [22,23,28,29,32,33,43,62]). Only a few 3-D microstructures have been developed for such metamaterials. Wu et al. [63] designed 3-D anti-chiral structures using bi-material strips made from polymeric materials to achieve a negative CTE. However, the stiffness issue was not addressed in their study. Wang et al. [59] extended the original 2-D design of Hopkins et al. [28] to 3-D microstructures. A large negative CTE was obtained in their study, but variations in the stiffness were not considered. Xu and Pasini [65] introduced octet lattices and compared isooctet and anisooctet lattice structures with the structures designed by Wang et al. [59] and Miller et al. [43]. Although anisooctet structures can achieve a negative CTE with a superior structure efficiency in a prescribed direction, such structures do not display isotropic thermal expansion. More recently, Qu et al. [48] developed a 3-D lattice composed of two different constituent materials and showed that a negative effective CTE can be achieved. But the stiffness of the proposed lattice structure was not considered in their work.

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Metamaterials exhibiting both negative PRs and negative CTEs have also been explored (e.g., [22,25,54]). Such metamaterials have the potential to be utilized in dental fillings, which normally experience temperature variations from different food and drink intake and need to resist chewing forces as well. Deployable space structures such as antennas and solar panels, which are required to maintain thermal stability in the cryogenic environment in space, can also be designed using metamaterials with tunable thermal expansion and Poisson's ratio. Furthermore, sensors and filters can be devised by employing such metamaterials that can be tailored to be responsive to both temperature changes and mechanical forces.

Recently, a systematic study of 2-D lattice-based metamaterials with negative PRs and non-positive CTEs was conducted by Ai and Gao [2]. However, such studies are still lacking for 3-D metamaterials displaying negative PRs and CTEs simultaneously.

In the current work, four types of 3-D bi-material lattice metamaterials with both negative PRs and non-positive CTEs are designed by extending the 2-D re-entrant lattice structures proposed in Ai and Gao [2] and modifying one micro-architecture provided in Wang et al. [59]. It is shown that each of the four types of metamaterials designed herein exhibits the cubic symmetry and thus needs three independent elastic constants to characterize its elastic behavior and one coefficient of thermal expansion to describe its isotropic thermal expansion. The effective thermo-mechanical properties are evaluated, and structure-property relations are explored for each of the four types of metamaterials with aluminum-Invar and stainless steel-Invar material combinations.

2. Newly designed 3-D metamaterials

One mechanism of obtaining a negative effective CTE for a lattice structure is to employ two families of struts with different CTEs (e.g., [23]), in which the mismatch of thermal expansion of the two materials can lead to contraction of the structure for a temperature increase or expansion of the structure for a temperature decrease. On the other hand, re-entrant structures can result in auxetic properties (e.g., [16,31,52,57]). Hence, re-entrant structures and bi-material struts can be combined to generate metamaterials with both negative PRs and negative CTEs. 2-D metamaterials with negative PRs and CTEs have recently been designed in Ai and Gao [2] using this combined approach. Four types of 3-D metamaterials are proposed herein by extending the micro-architectures for 2-D metamaterials provided in Ai and Gao [2], which are shown in Fig. 1.

As described in Ai and Gao [2], among the four types of 2-D metamaterials, the first one can possess a negative PR and a negative CTE at the same time without significantly comprising its load-carrying capability. Hence, the unit cell for 2-D metamaterial # 1 proposed in Ai and Gao [2] is chosen herein as the basic construction unit in order to extend the 2-D design of metamaterials with negative PRs and CTEs to 3-D configurations.

Three types of 3-D metamaterials are designed by extending the unit cell for 2-D metamaterial # 1 using different spatial tessellations, as displayed in Fig. 1(a)-(c). In each case, the red and blue struts represent the materials with the higher and lower CTEs, respectively. All struts have a square cross section with an edge length t. Through respectively positioning three 2-D unit cells on three perpendicular coordinate planes and making the center for each 2-D unit cell coincide, 3-D metamaterial # 1 (unit cell) can be obtained, as shown in Fig. 1(a). Metamaterial # 2, depicted in Fig. 1(b) in its unit cell, is generated through packing six 2-D unit cells, in which each 2-D unit cell is placed on one of the six surface planes of a 3-D cubic unit cell. The proposed metamaterial # 3, displayed in Fig. 1(c), is produced by modifying the micro-architecture of 3-D metamaterial # 1 through connecting each corner point of the cubic unit cell to the three nearest joints of the three re-entrant units.

On the other hand, metamaterial # 4, illustrated in Fig. 1(d), is modified from the micro-architecture designed in Wang et al. [59] by letting the outmost four struts near each of the six cubic cell surfaces protrude inward. These outmost struts can be characterized using one additional angle parameter θ_0, as displayed in Fig. 1. Note that θ describes the positions of the re-entrant struts (red) with the higher CTE, while θ_0 defines the positions of the re-entrant struts (blue) with the lower CTE, which are in addition to those located near the center of the cubic unit cell. When θ_0 is set to zero, the micro-architecture of metamaterial # 4 proposed here in Fig. 1(d) will be reduced to the original one presented in Wang et al. [59]. Note that the geometrical constraint $\theta_0 < \theta$ is imposed in the current work for simplicity. These four proposed unit cells shown in Fig. 1(a)-(d) can be tessellated in the x-, y- and z-directions to obtain periodic lattice-based metamaterials, as displayed in Fig. 1(e)-(h), each containing $2 \times 2 \times 2$ unit cells.

From the unit cells illustrated in Fig. 1(a)-(c), it is observed that the first three 3-D metamaterials can be described using three geometrical parameters: two lengths H_1 and H_2 and one angle θ. For metamaterial # 4 shown in Fig. 1(d), it has one additional angle parameter θ_0.

Three materials chosen for the struts are the same as those used in Ai and Gao [2] for the 2-D metamaterials, some of which have been fabricated using a robotized laser powder-feed metal additive manufacturing system [13,14]. Based on these three materials (i.e., aluminum (Al) 7075, stainless steel (St) 431 and Invar), two material combinations, Al-Invar and St-Invar, are adopted in the present simulations. The properties for the three materials are summarized in Ai and Gao [2].

The formula for the relative density ρ_r, defined as $\rho_r = \rho/\rho_L$, for each of the four types of the metamaterials is listed in Table 1, where ρ_L is the density of the strut material with the lower CTE (Invar for both the material combinations), and ρ is defined as $\rho = m/V_c$, with m being the mass of the unit cell and V_c being the volume of the cube bounding the unit cell. These formulas are obtained directly from the unit cells shown in Fig. 1. Note that the strut overlapping near joints is not considered in deriving the formulas for ρ_r given in Table 1.

3. Finite element modeling

3.1. Periodic boundary conditions

The four types of metamaterials proposed in Section 2 are periodic lattice structures. Hence, they can be simulated using the unit cells shown in Fig. 1(a)-(d) subject to periodic boundary conditions (PBCs), which ensure the displacement and rotation continuity across boundaries of neighboring cells.

To illustrate how the PBCs are enforced in the present 3-D unit cell models, metamaterial # 1 is analyzed as an example here. Fig. 2 shows the unit cell of 3-D metamaterial # 1 with identified boundary nodes. Due to the periodic nature, each node on one side (e.g., A^+) has a matched node on the opposite side (e.g., A^-) of the unit cell. Note that for simplicity, only two pairs of the matched boundary nodes in each direction are illustrated.

The periodic boundary conditions for a specimen subjected to a prescribed strain $\bar{\varepsilon}_{ij}$ are given by (e.g., [37,38,64])

$$u_i^{k+} - u_i^{k-} = \bar{\varepsilon}_{ij}\left(x_j^{k+} - x_j^{k-}\right),\ \ \varphi_i^{k+} - \varphi_i^{k-} = 0, \quad i, j \in \{1, 2, 3\}, \tag{1}$$

where x_j^{k+} and x_j^{k-} are, respectively, the coordinates of the matched nodes k^+ and k^- on the specimen boundary along the $\mathbf{e}_j$-direction ($j = 1$, 2, 3), u_i^{k+} and u_i^{k-} are, respectively, the displacement components of k^+ and k^-, and φ_i^{k+} and φ_i^{k-} are, respectively, the rotation components of k^+ and k^-.

For the uniaxial loading in the y-direction with a prescribed strain

$$\bar{\varepsilon}_{ij} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{2}$$