

## Anisotropic and negative thermal expansion behavior in a cellular microstructure

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It is a well-known fact that not all materials possess positive coefficient of thermal expansion. A very common example is that of ice, which experiences volumetric contraction as it melts. Recent reports on negative thermal expansion include (CdMnMg)Te [1], glass fiber/polypropylene composite laminates [2], face-centered-cubic cesium [3], zirconium molybdate and hafnium molybdate [4],  $\text{Sc}_2(\text{WO}_4)_3$  [5] and  $\text{ZrW}_2\text{O}_8$  [6–9]. Literature on negative thermal expansion is too numerous to be listed (e.g. [10–16]). As such, interested readers may refer to the general reviews by Evans *et al.* [17, 18] and Sleight [19]. Here, we are concerned with a special class of material behavior that exhibits anisotropic thermal expansion, with emphasis on a combination of both positive and negative thermal expansion along its principal axes—hence leading to large thermally induced shearing. In recent years the concept of Poisson-shearing material property has been introduced whereby prescription of out-of-plane strain (direction-3) gives a positive and negative principal strains in direction-1 and direction-2 respectively, thereby leading to large shearing in the 1–2 plane [20–23]. As an extension to these works, the present paper replaces the out-of-plane loading with the change in temperature as the driving force for large shearing. A cellular microstructure with its corresponding analytical model is proposed herein which exhibits positive and negative thermal expansions in two perpendicular directions.

Consider a cellular microstructure shown in Fig. 1 and its idealized representative volume element (RVE), as depicted in Fig. 2a, which consists of thermally inexpandible rod elements (thick lines) and thermally expandible rod elements (thin lines). The sides of the RVE remain mutually orthogonal under thermal loading such that the RVE does not undergo a distortion leading to repeat-cell angles departing from  $90^\circ$  in the plane. However, unequal principal normal strains lead to maximum shearing that can be observed for an element rotated by  $45^\circ$  from the principal axes. We let the inexpandible rod be rigidly fixed at the central junction (that is,  $\theta_3$  and  $\theta_4$  being constant). The assumption of rigid rods at the central junction is highly essential to ensure that point C in Fig. 2a remains fixed to enable RVE contraction with increase in temperature—hence a negative thermal expansion—when both  $\theta_1$  and  $\theta_2$  are less than  $\pi/4$ . The magnitude of negative thermal expansion is greatly reduced when the central junction angles and rods are rotatable and expandible respectively.

The mechanistic link between the RVE considered herein and the negative Poisson's ratio material, as shown in Fig. 2b, is the rod subtended by an angle  $\theta_1$ . A consequence of  $\theta_1 < (\pi/4)$  is negative thermal expansion and negative Poisson's ratio in direction  $x_1$  corresponding to Figs 2a and b respectively. However the RVE considered herein, as shown in Fig. 2a, does not exhibit negative Poisson's ratio due to the existence of rigid central rods and junction, which are essential in ensuring negative thermal expansion.

Given the relationship between the coefficient of thermal expansion,  $\alpha$ , of the thermally expandible rods and their corresponding thermal strain as

$$\varepsilon = \alpha \Delta T \quad (1)$$

where  $\Delta T$  refers to the change in temperature, then the effective relationship for the entire RVE can be written as

$$\varepsilon_{\text{eff}} = \alpha_{\text{eff}} \Delta T \quad (2)$$

such that the effective property is obtained by considering the geometry of the RVE and every elements contained therein. The effective shear strain for the RVE as a result of temperature change can be written in a form analogous to Equation 2, that is

$$\gamma = \beta \Delta T \quad (3)$$

where  $\beta$  is herein defined as the coefficient of thermal shearing. The following analysis expresses the shear strain in terms of temperature induced geometrical alteration of the proposed RVE.

With reference to Equation 1, the new lengths of  $l_1$  and  $l_2$  are

$$l'_i = l_i(1 + \alpha \Delta T); \quad (i = 1, 2) \quad (4)$$

with a change in environmental temperature by  $\Delta T$ , as depicted in Fig. 3. Taking equal projected length, we have the new angles of  $\theta_1$  and  $\theta_2$  as

$$\theta'_1 = \sin^{-1} \left( \frac{\sin \theta_1}{1 + \alpha \Delta T} \right). \quad (5)$$

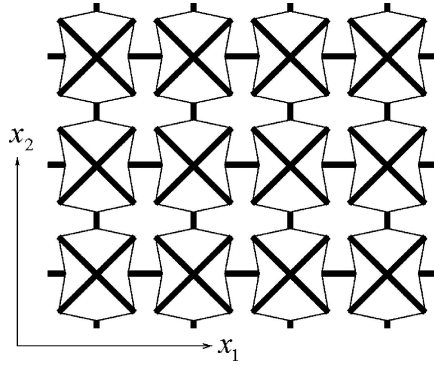
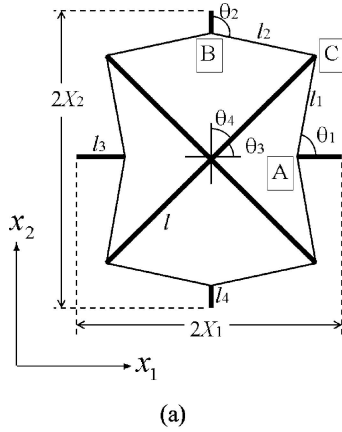
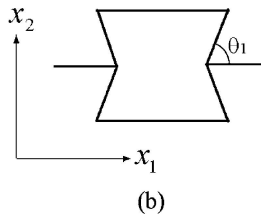


Figure 1 An idealized microstructure showing 12 representative volume elements (RVE).



(a)



(b)

Figure 2 Geometrical properties of one RVE: (a) anisotropic thermal expansion, and (b) negative Poisson's ratio via re-entrant structure.

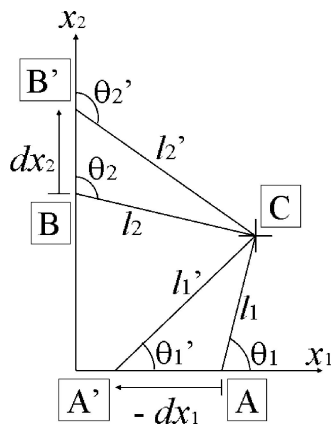


Figure 3 Changes in lengths and angles in one quarter of RVE.

This gives the displacements of points A and B as

$$dx_1 = l_1 \cos \theta_1 - l_1 (1 + \alpha \Delta T) \times \cos \left[ \sin^{-1} \left( \frac{\sin \theta_1}{1 + \alpha \Delta T} \right) \right] \quad (6)$$

along axes  $x_1$  and  $x_2$  respectively. Perusal to Fig. 2 shows that the half widths of the RVE are

$$X_i = l \cos \theta_{i+2} - l_i \cos \theta_i + l_{i+2}. \quad (7)$$

such that the principal strains are

$$\varepsilon_i = \frac{dx_i}{X_i}. \quad (8)$$

Since the relationship between the inexpandible and expandible rods of lengths  $l$  and  $l_i (i = 1, 2)$  respectively is

$$\frac{l}{l_i} = \frac{\sin \theta_i}{\sin \theta_{i+2}}, \quad (9)$$

the coefficient of thermal shearing is therefore

$$\beta = \frac{1}{\Delta T} (\varepsilon_1 - \varepsilon_2) \quad (10)$$

where the principal strains for the RVE are

$$\varepsilon_i = \frac{\cos \theta_i - (1 + \alpha \Delta T) \cos[\sin^{-1}((1 + \alpha \Delta T)^{-1} \sin \theta_i)]}{(\sin \theta_i / \tan \theta_{i+2}) - \cos \theta_i + (l_{i+2}/l_i)}. \quad (11)$$

For illustration purposes, we consider a special case whereby the criss-cross inexpandible rod element is symmetrical about diagonal axes

$$\theta_3 = \theta_4 = \frac{\pi}{4}, \quad (12)$$

the extendible rod elements are of equal length

$$l_1 = l_2, \quad (13)$$

the RVE is a square

$$X_1 = X_2, \quad (14)$$

the angles  $\theta_{1,2} = 90^\circ \mp \phi$  such that

$$\theta_1 + \theta_2 = \pi \quad (15)$$

and that the length  $l_4$  is minimized to a zero

$$l_4 = 0. \quad (16)$$

For such a geometry, the principal thermal strains and the coefficient of thermal shearing reduce to

$$\varepsilon_1 = -\varepsilon_2 = \frac{\cos \theta_2 - (1 + \alpha \Delta T) \cos[\sin^{-1}((1 + \alpha \Delta T)^{-1} \sin \theta_2)]}{\sin \theta_2 - \cos \theta_2} \quad (17)$$

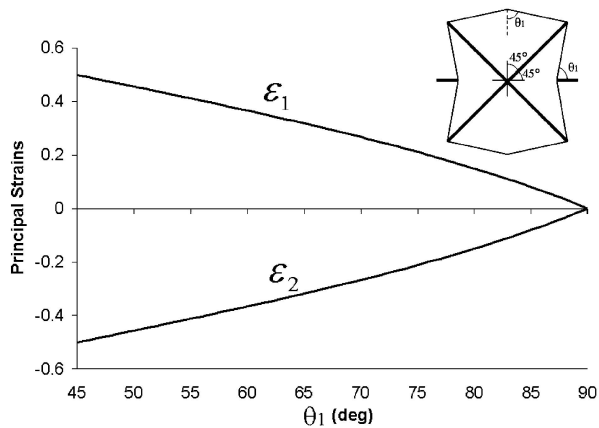


Figure 4 Effect of special case RVE geometry on the thermally induced principal strains.

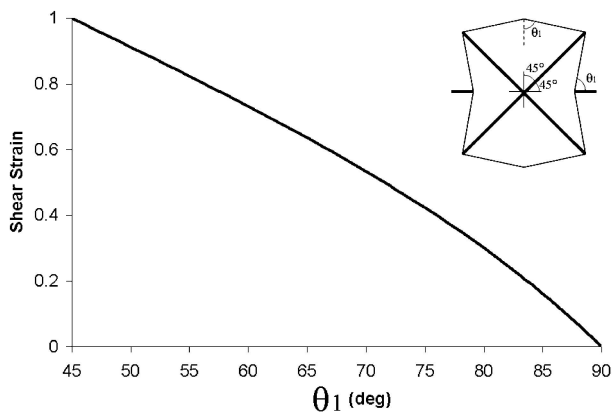


Figure 5 Influence of special case RVE geometry on the thermally induced shear strain.

and

$$\beta = \frac{2}{\Delta T} \left[ \frac{(-1)^{i+1} \cos \theta_i}{\sin \theta_i + (-1)^{i+1} \cos \theta_i} \right] \quad (18)$$

respectively, where  $i = 1$  or  $i = 2$ . Plots of principal strains ( $\varepsilon_1, \varepsilon_2$ ) and shear strain  $\gamma = \beta \Delta T$  versus  $\theta_1$  are furnished in Figs 4 and 5 respectively to demonstrate the influence of microstructural geometry on the thermally induced shear strain.

In concluding, the concept of thermal shearing coefficient has been defined and an idealized RVE proposed

for analytical purposes. In the special case considered herein, it was demonstrated that the coefficient of thermal shearing is dependent on microstructural geometry and the change in temperature, but independent from the coefficient of thermal expansion.

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