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Composites with needle-like inclusions exhibiting negative thermal expansion: A preliminary investigation

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ABSTRACT

In this work a simple cylindrical structure with a stiff needle-like inclusion embedded within a much softer matrix is presented and analysed with the aim of obtaining a system with tunable thermal expansion properties. It is shown that by the correct combination of the thermal and mechanical properties of the matrix and inclusion, it is possible to design a system which can be tailor-made to exhibit particular values of the coefficient of thermal expansion (CTE) in the radial direction and also negative thermal expansion (NTE). In particular an analytical model to quantify the radial strain with changes in temperature is derived and verified through finite element analysis. The model is used to find correct property combinations which lead to particular values of thermal expansion which could also be negative or zero.

1. Introduction

It is a well known fact that most materials which we encounter in everyday life expand on heating and contract when cooled, a property which may be explained by looking at interatomic distances [1–2]. This subject of thermal expansion is one of great practical importance and has been studied for many years since miscalculations of the temperature effects may lead to disastrous consequences.

Expansion in a material may be one of two forms: isotropic or anisotropic. In isotropic expansion, the material expands by the same extent in any direction (isotropically) upon heating whilst if the extent of expansion is dependent on the particular direction where the measurement is taken, then the expansion is referred to as anisotropic expansion. To quantify thermal expansion in some particular direction one may make use of the linear coefficient of thermal expansion, henceforth referred to as CTE which may be defined as α which relates the resultant strain ε as a result of a change in temperature of dT through $\varepsilon = \alpha dT$.

As noted above, in most cases, materials expand when heated, i.e., ε is positive for a positive dT (i.e. as T increases) with the result that the CTE is positive. However, it should be noted that materials which defy common expectation and contract when heated do exist [3–19]. It should also be noted that for anisotropic systems, different values for the CTE will exist, depending on the direction of measurement and it is possible that a system exhibits negative thermal expansion (NTE) in some but not all directions. Over the years, there have been various studies aimed at designing, analysing, manufacturing and/or testing of materials and structures having very particular CTE values, in particular, studies looking at systems, including composites exhibiting NTE [3–21]. Some of these studies have considered the possibility of generating very low or negative thermal expansion in structures constructed from conventional materials. These systems, which are constructible at any lengthscale, include those proposed by Clegg et al. [17–20] and Lakes [21] and have the advantage that they are relatively easy to construct at reasonable costs and thus have excellent potential for commercialisation. Alderson et al. [22] have also proposed a method for achieving these effects using auxetic materials (i.e. materials exhibiting negative Poisson's ratio). Normally, such systems also offer the added advantage that they can be tailor-made to exhibit any desired thermal expansion properties (positive, negative or near zero) through careful choice of the geometric parameters and/or materials used in the construction. Furthermore, such systems are also of interest in view of the fact that they can be engineered to exhibit other interesting macroscopic properties, e.g. negative Poisson's ratio [23–25] with the result that one achieves multifunctional systems with obvious added value.

In this paper we propose and discuss a novel system constructible at any lengthscale including the microscale from conventional components having different mechanical and thermal properties which may be combined to form composite systems which exhibit any desired CTE values, in particular negative ones (NTE).

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2. The concept

For simplicity, to illustrate how systems operating through the proposed mechanism can be designed to exhibit NTE, we shall first consider a simple and basic system and predict the optimal requirements for it to exhibit this effect. The system which is shown in Fig. 1 consists of a cylindrical rod of length l and radius r made of a material B which is embedded inside another cylindrical shell of thickness t made from a material A having different thermal and mechanical properties with all dimensions being measured at a reference temperature T.

Assuming that materials A and B are perfectly bound to each other at the interface and that they are isotropic with respect to their thermal and mechanical properties, when the system is subjected to a change in temperature ΔT, both materials expand or contract in volume accordingly, each at a different rate. Since the materials are bound to each other, they cannot expand freely and as a result, each of them exerts forces on the other. In particular, the material with the higher CTE exerts a tensile force in the longitudinal direction on the material having the lower CTE and conversely the latter exerts a compressive force on the former resulting in a mechanical strain. This strain in turn gives rise to an additional strain in the radial direction, the magnitude of which is dependent on the Poisson's ratio (henceforth referred to as Poisson's effect). This causes a contraction (or an expansion) in this direction and unless the Poisson's ratio of the materials is zero, this Poisson's effect may have significant contributions to the overall radial strain and therefore should not be neglected.

In addition, to further simplify our analysis, we shall also assume that:

(1) the inclusion has a needle shape, i.e. the length is much larger compared to its thickness so that changes in dimension arising from the Poisson's effect due to expansion in the radial direction can be ignored since they are negligible when compared to that resulting from a longitudinal expansion;
(2) Young's modulus of the outer cylinder (i.e. the matrix) is much smaller than that of the inclusion and thus additional mechanical strains in the radial direction arising due to mismatch of the CTEs can be neglected;
(3) no necking effects occur during deformation.

Thus, in the analytical model it is being assumed that the strain at the interface is only dependent on the thermal expansion and Poisson's effect of material B, i.e. the inner circumference of material A expands accordingly to accommodate the changes in the outer circumference of material B thereby satisfying the boundary condition of the interface (and therefore eliminating gaps or unrealistic overlaps).

In this way, it is possible to derive a simple expression for the radial strain by taking into consideration only the radial thermal strain and the additional radial mechanical strain arising from Poisson's effect due to expansion in the longitudinal direction. Taking first the longitudinal strain ε_l into consideration, it can be quantified through the following equation:

$$\varepsilon_l = \alpha_A \mathrm{d}T + \frac{F_A}{a_A E_A} = \alpha_B \mathrm{d}T + \frac{F_B}{a_B E_B} \tag{1}$$

where α is the CTE of the material, E is Young's modulus, a is area, F the force exerted by the other material and the subscript refers to the material (materials A and B). At equilibrium, $F_B = -F_A = F$, so that solving for F, the following expression is obtained:

$$F = \frac{a_A a_B E_A E_B(\alpha_A - \alpha_B)}{a_B E_B + a_A E_A}\mathrm{d}T \tag{2}$$

The mechanical strain on material A arising from this force is therefore:

$$\varepsilon_A^l = \frac{-F}{a_A E_A} = -\frac{a_B E_B(\alpha_A - \alpha_B)}{a_B E_B + a_A E_A}\mathrm{d}T \tag{3}$$

so that the induced radial strain arising from Poisson's effect can be given by:

$$\varepsilon_A^r = \frac{\nu_A a_B E_B(\alpha_A - \alpha_B)}{a_B E_B + a_A E_A}\mathrm{d}T \tag{4}$$

and similarly for material B:

$$\varepsilon_B^r = -\frac{\nu_B a_A E_A(\alpha_A - \alpha_B)}{a_B E_B + a_A E_A}\mathrm{d}T \tag{5}$$

Therefore, the total strain ε_r in the radial direction, taking also into account the thermal expansion of both materials can be given by:

$$\varepsilon_r = \frac{2(t\alpha_A + r\alpha_B)\mathrm{d}T + 2\varepsilon_A^r t + 2\varepsilon_B^r r}{2(r+t)} = \left[\frac{t\alpha_A + r\alpha_B}{(t+r)} + \frac{(\alpha_A - \alpha_B)(t\nu_A a_B E_B - r\nu_B a_A E_A)}{(a_B E_B + a_A E_A)(t+r)}\right]\mathrm{d}T \tag{6}$$

Thus defining α_r as the thermal expansion coefficient in the radial direction, we note that:

$$\alpha_r = \frac{t\alpha_A + r\alpha_B}{(t+r)} + \frac{(\alpha_A - \alpha_B)(t\nu_A a_B E_B - r\nu_B a_A E_A)}{(a_B E_B + a_A E_A)(t+r)} \tag{7}$$

Since a_i, E_i, and r are all positive quantities, it follows that the α_r and the radial strain is negative if:

$$t\frac{\alpha_A}{\alpha_B} + r < \left(1 - \frac{\alpha_A}{\alpha_B}\right)(t\nu_A a_B E_B - r\nu_B a_A E_A) \tag{8}$$

This inequality suggests that for a system with $E_A < E_B$ as in our earlier assumptions the NTE effect can be enhanced by decreasing α_A/α_B. This ensures that thermal expansion in the radial direction of the thicker material is minimal so that the main contribution comes from the Poisson's effect which can be enhanced by using a soft matrix with a high Poisson's ratio and a much stiffer inclusion with a low or negative Poisson's ratio. In this way, the matrix has very little effect on the inclusion, i.e. the degree by which material A is stretched is much higher than that by which B is compressed. This in turn means that the decrease in thickness of A is much larger than the increase in thickness of B (if $\nu_B > 0$) making NTE possible. If the inclusion is auxetic, the change in its radial dimension due to compression will further contribute to a more negative thermal expansion (and also have the additional advantage of a larger pull-out resistance [26,27]). For example for a system with $r = 0.5$ mm, $t = 50$ mm, $E_A = 0.01$ GPa, $E_B = 200$ GPa, $\nu_A = 0.49$, $\nu_B = 0.3$, $\alpha_A = 15 \times 10^{-6}$ K^{-1} and $\alpha_B = 324 \times 10^{-6}$ K^{-1} the strain

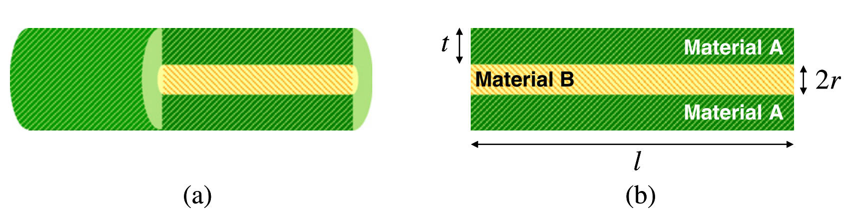

Fig. 1. (a) A cylindrical structure consisting of a needle-like inclusion of material B embedded in a matrix of material A and (b) a cross-section showing its dimensions.

in the radial dimension for a 100 K increase in temperature is predicted to be -8.09×10^{-3} and -8.15×10^{-3} if an auxetic inclusion ($\nu_B = -0.3$) is used. It is also interesting to note that zero thermal expansion is also predicted if $\nu_A = 0.091$.

3. Simulations

In an attempt to obtain further evidence that what is proposed here can indeed result in a method for controlling the thermal expansion in the radial direction which could also lead to NTE, we used the Finite Elements (FE) software package ANSYS Academic Research V. 12.0 to construct this most basic system. In the simulation, we used two elastic materials A and B which were perfectly bonded together and meshed using the 2-D, 8-node, coupled-field PLANE223 plane element with axisymmetric behaviour where the z-axis is the axisymmetric axis while symmetric boundary conditions were applied along the r-axis (Fig. 2). The nodal degrees of freedom (DOF) are translations in the z- and r-directions and temperature where Table 1 lists the nodal constraints. As regards loading, a uniform temperature rise of 100 K was applied on all the nodes.

Two sets of simulations were performed. In the first, this system was solved linearly for the geometry corresponding to $l = 500$ mm, $t = 50$ mm and $r = 0.5$ mm. The material was modelled as perfectly elastic and isotropic with $E_A = 0.01$ GPa, $E_B = 200$ GPa, $\nu_B = 0.3$, $\alpha_A = 15 \times 10^{-6}$ K^{-1} and $\alpha_B = 324 \times 10^{-6}$ K^{-1} while the Poisson's ratio of the matrix (ν_A) was varied from $-1.0 < \nu_A < 0.5$ subjected to a temperature rise of 100 K. In the second set, ν_A was set at 0.49 whilst the thickness t was allowed to vary from $100 > t > 0$ with all the other parameters set as before. It should be emphasised that although the simulations performed here are in the mm range, the effect is scale independent and can also be exhibited at smaller or larger scales.

As post-processing, for both sets of simulations, the radial strain ε_r was recorded as ν_A or t were varied from which we calculated the thermal expansion coefficient α_r in the radial direction as $\alpha_r = \varepsilon_r \Delta T^{-1}$. The results of these two sets of simulations are shown in Figs. 3 and 4 which compare the FE results with those predicted by the analytical model.

These results clearly show that in accordance to what is predicted by the analytical model, the systems presented here can exhibit a wide range of thermal expansion properties which can be varied by varying either the types of materials used (something which may be limited by the availability of materials having the required properties) or the geometric parameters, such as the thickness of the outer material. In particular, the simulations confirm that in the radial direction, the system can indeed exhibit not only negative linear thermal expansion, a property which is exhibited best when the outer material (the matrix) has high positive

Table 1
Translational nodal constraints applied on the nodes lying on the lines shown in Fig. 2, where U_r and U_z denote displacements in the r- and z-directions respectively.

Line	DOFs constraints	
	U_r	U_z
1	0	–
2	–	0
3	Coupled[a]	–
4	–	Coupled[a]
5	–	Coupled[a]

[a] The DOF is equal for all the nodes.

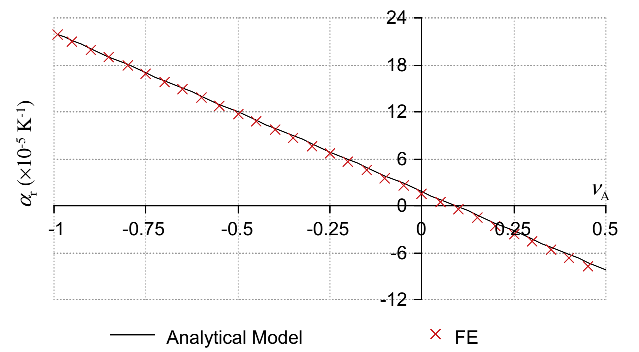

Fig. 3. Plot of the radial CTE α_r versus Poisson's ratio of the matrix ν_A for both the FE and analytical results.

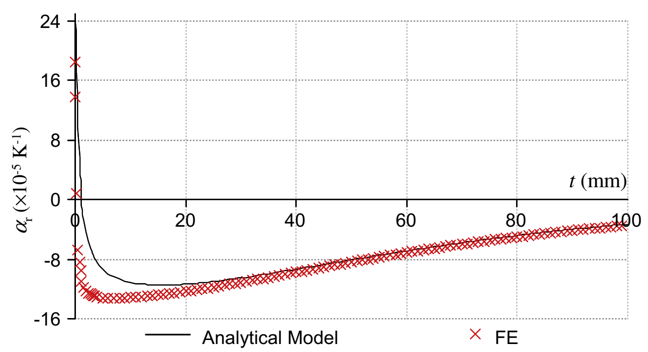

Fig. 4. Plot of the radial CTE α_r versus the matrix thickness t for both the FE and analytical results.

Poisson's ratios but also zero linear thermal expansion. This property is highly desirable in applications where a system has to maintain its structural integrity while subjected to significant changes

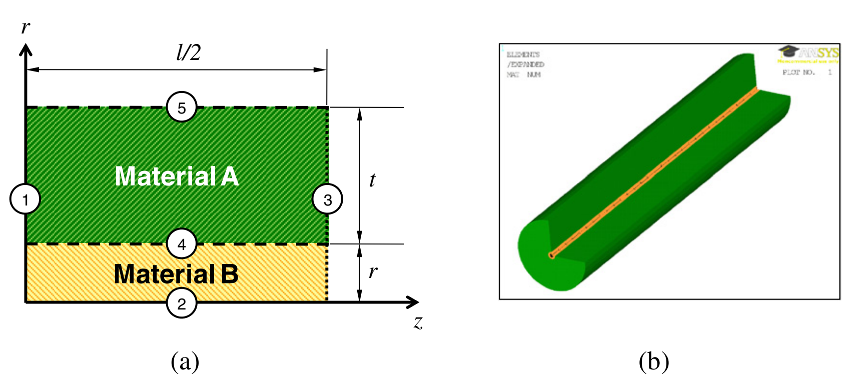

Fig. 2. (a) Line numbers showing the respective nodes. (b) 3/4 of the composite in 3D.

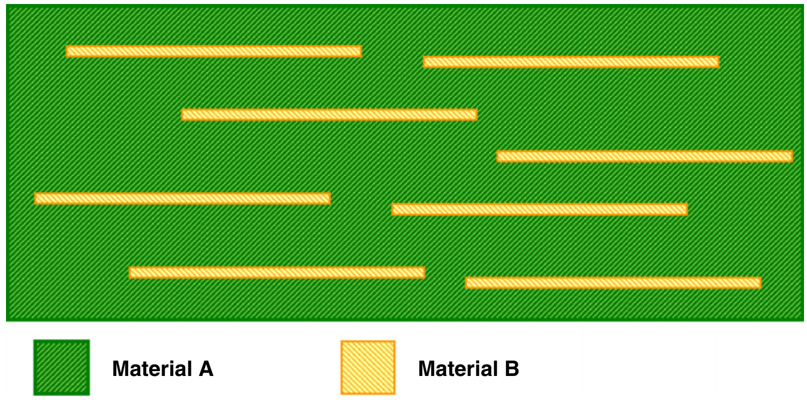

Fig. 5. An example of a realistic but more complex system which can be built to exhibit particular CTE properties using the principles presented here.

in temperature which would otherwise lead to changes in the geometrical features of the structure, for example, in the construction of railway tracks, bridges, Bragg gratings [28] and satellites [29]. It is also interesting to note that when auxetic materials are used, the Poisson's ratio (mechanical properties contribution) makes it possible to get volumetric thermal expansion which is higher than what could have been achieved when one considers only thermal expansion effects. All this is very significant as it confirms that the setup proposed here may indeed be used as a mechanism to achieve any pre-desired thermal expansion properties.

Let us now intercompare the predictions made by the analytical and FE models. Both Figs. 3 and 4 show that the analytical model does indeed predict, to a first approximation, the magnitude of the thermal expansion in the radial direction, thus adding confidence in the analytical model. In particular we note that in cases when $t \gg r$, the analytical model predicts the thermal expansion in the radial direction to a high degree of accuracy. Also interesting to note is that both analytical and FE models suggest a similar profile for the variation of α_r versus t which suggest that there is an optimal thickness t of the outer material (for a fixed inclusion thickness r) which optimises the magnitude of NTE.

The main discrepancies between the analytical and FE models seem to occur at low values of t and these are evident in the plots of α_r against the thickness t of the surrounding material where at low values of t, the analytical model underestimates the extent of NTE. The most likely reason for this underestimation is due to the fact that at small values of t, Poisson's effects as a result of an increase in the thickness r (and hence the circumference) of the needle shaped inclusion are not insignificant. Such increase in the circumference will cause an additional thinning of the outer material, which thinning has not been accounted for in the analytical model. All this suggests that although there is a need to fine-tune the analytical model so as to take into account this effect (something which unfortunately will decrease the simplicity of the analytical model), the analytical model as presented here can already provide a reasonable estimate of the thermal expansion properties of such systems.

Before we conclude, it is important to note that the concepts presented here may be used in the design and manufacture of real composites exhibiting such NTE properties or for controlling the thermal expansion of composites (which may not necessarily have to exhibit NTE). For example, an easily constructible but more complex system based on the same mechanism is illustrated in Fig. 5 which shows a cross-section of a possible composite where the highly expanding and hard needle shaped inclusions are moulded inside the matrix in a random but aligned manner. Other systems which could be modified to exhibit these effects include fibre-reinforced composites which if constructed using the right component materials would also be able to exhibit these unusual properties. In such systems, one would assume that the CTE will also be affected by other factors such as the degree of perfection in the alignment of the needle shaped inclusions and the packing, but the principles which may lead to the unusual thermal effects presented in this paper, including the ability to exhibit NTE, remain the same. It is also important to note that although materials which have the thermal and mechanical properties required to achieve this NTE effect in a very significant manner are not currently in abundance, the effect may be obtained by building micro mechanical systems (e.g. using syringe-like structures filled with a highly expanding fluid embedded within a soft material) or having the components themselves being man-made composites which are tailor-made to have the required properties.

4. Conclusion

This work presented a concept for controlling the thermal expansion through the introduction of highly expanding and hard needle shaped inclusions into a soft matrix. In particular, we derived an analytical model for a simple cylindrical system containing a needle-like inclusion which can be tailor-made to exhibit any pre-desired positive or negative thermal expansion coefficient in radial directions. In fact, the derived expression for the radial strain showed that by the correct combination of the materials' thermal and mechanical properties, NTE and zero thermal expansion in the radial direction are possible, with the NTE effect being further enhanced by the use of auxetic inclusions. The validity of the model under the made assumptions has also been verified using finite element analysis.

We hope that the models presented and discussed here will encourage experimentalists to manufacture and commercialize new materials which can be tailor-made to have properties to fit particular practical applications based on the concepts presented here. Given the simplicity of our systems and their adjustability, we envisage materials based on what is proposed should find extensive use in many practical applications where negative or zero thermal expansion is required, or where the thermal expansion needs to be controlled in a cost-effective manner.

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