Phys. Status Solidi B **250**, No. 10, 2051–2056 (2013) / **DOI** 10.1002/pssb.201384226

physica status solidi b
www.pss-b.com
basic solid state physics

Negative thermal expansion from disc, cylindrical, and needle shaped inclusions

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Received 27 April 2012, revised 1 May 2012, accepted 2 April 2013
Published online 2 July 2013

Keywords auxetic, finite elements modeling, negative thermal expansion, Poisson's ratio

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The concept of reducing the thermal expansion of composites by exploiting the thinning that is observed when a conventional material is mechanically stretched (the Poisson's effect) is explored through finite elements (FE) simulations with the scope of assessing the potential of such systems to exhibit negative thermal expansion (NTE). It is shown that systems made from hard highly expanding needle, cylindrical or coin shaped inclusions embedded within a soft matrix with a high positive Poisson's ratio having low coefficients of thermal expansion may exhibit NTE under certain conditions. In the case of the coin-shaped inclusions, the NTE is maximum in the direction orthogonal to the surface of the coins and in the case of systems with needle-shaped inclusions, the NTE is maximum in the direction orthogonal to the length of the needles.

1 Introduction Most materials tend to expand on heating and contract when cooled, a property, which may be explained by looking at interatomic potentials [1]. Such an expansion may be either isotropic, i.e. the material expands by the same extent in any direction upon heating, or anisotropic, i.e. the extent of expansion is dependent on the particular direction where the measurement is taken. 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, a property which relates a change in temperature of ΔT to the resultant strain ε through $\varepsilon = \alpha \times \Delta T$.

Although as noted above, most materials expand when heated (i.e. have positive CTE), some systems defy common expectation and contract when the temperature is increased [2]. Also, for anisotropic systems, different values for the CTE may exist, depending on the direction of measurement. In particular, it may be 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, analyzing, manufacturing, and/or testing of materials and structures having very particular CTE values, in particular, studies looking at systems exhibiting NTE [2–21]. Some of these studies have considered the possibility of generating very low or NTE in structures constructed from readily available conventional materials with the obvious advantage that they may be constructed at reasonable costs [5, 8, 12]. More recently, Alderson et al. [3] have also proposed a method for achieving these effects using materials exhibiting negative Poisson's ratio (auxetics). It has also been proposed that many of the man-made NTE systems can be modified so as 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.

It was recently proposed by Grima et al. [22, 23] that NTE can be achieved at any length scale 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). In particular, referring to Fig. 1 which consists of a cylindrical rod/needle of length l and radius r made of a material B which is embedded inside and perfectly bonded to another cylindrical shell of thickness t made from a material A having thermal and mechanical properties different from material B (material B is much stiffer than material A and has a higher positive thermal expansion coefficient), then when the system is subjected to a change in temperature ΔT, both materials change size at a different rate. Since materials A and B are bound to each other, they cannot expand freely when a uniform positive temperature change is applied and

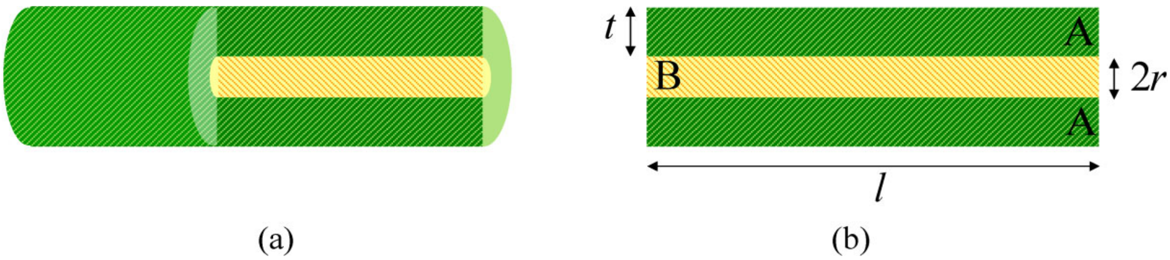


Figure 1 (a) The cylindrical structure proposed by Grima et al. [22, 23] consisting of a needle-like inclusion of material B embedded in a matrix of material A and (b) a cross-section showing its dimensions. All dimensions being measured at a reference temperature *T*.

due to strain compatibility, each of them will exert a force on each other. In particular, when the temperature is increased, 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 the Poisson's effect). If the soft material A has a high positive Poisson's ratio, this Poisson's effect may have significant contributions to the overall radial strain and therefore should not be neglected, as it may even be larger than the strains due to the thermal expansion and thus result in an effective NTE in the radial direction.

In an attempt to obtain a better understanding of the manner how to adjust the thermal expansion from the use of hard inclusions (Material B) which expand more when heated than the surrounding soft matrix (Material A), this work presents the results of finite elements (FE) simulations where the shape of the inclusion was made to vary from an needle to a coin shaped inclusion so as to assess how the effective thermal expansion coefficients may be adjusted by changing the shape of the inclusion.

2 Simulations In an attempt to assess the effect on the effective thermal expansion of having different shaped inclusions embedded in a soft matrix, simulations were performed using the finite elements software package ANSYS Academic Research v. 12.0.

In the simulation, the model in Fig. 2 was constructed using two different elastic materials A and B which were perfectly bonded together and meshed using the two-dimensional, 8-node, coupled-field PLANE223 plane element with axisymmetric behavior about the *z*-axis (Fig. 2). The nodal constraints used in the simulations are listed in Fig. 3 and as regards loading, a uniform temperature rise of 100 K was applied on all the nodes.

In the simulations it was assumed that materials A and B are isotropic where Material A (the matrix) has a Young's modulus of $E_A = 10$ MPa, a Poisson's ratio of $\nu_A = 0.49$ and a CTE of $\alpha_A = 15 \times 10^{-6}$ K^{-1} whilst Material B (the inclusion) has a Young's modulus of 200GPa, a Poisson's ratio of $\nu_B = 0.3$ and a CTE of $\alpha_B = 324 \times 10^{-6}$ K^{-1}. Note that these properties correspond to a soft rubber-like matrix having low values of the thermal expansion (Material A) and a hard inclusion having a high thermal expansion (Material B) where the stiffness of material B is about 2×10^5 higher than that of material A and the thermal expansion coefficient of material B is about 20× higher than that of material A.

Two sets of simulations were performed. In the first set of simulations, the geometric variables were set as $r = 0.5$mm, $l \in \{500, 250, 100, 10, 1, 0.01\}$, $t_l \in \{0,10,25, 50, 250, 500\}$ and *t* was varied in small increments between 0 and 100. In the second set, *r* and *l* were once again given values of $r = 0.5$ mm, $l \in \{500, 250, 100, 10, 1, 0.01\}$ whilst *t* was chosen from the set $t \in \{0,0.01,0.1,0.5,1,2, 3.5, 5\}$ whilst t_l was varied in small increments between 0 and 500 in small increments. Note that simulations were *l* is large would correspond to inclusion which are needle-like whilst simulations where *l* is small would correspond to systems which are coin shaped. Systems where $l \approx r$,

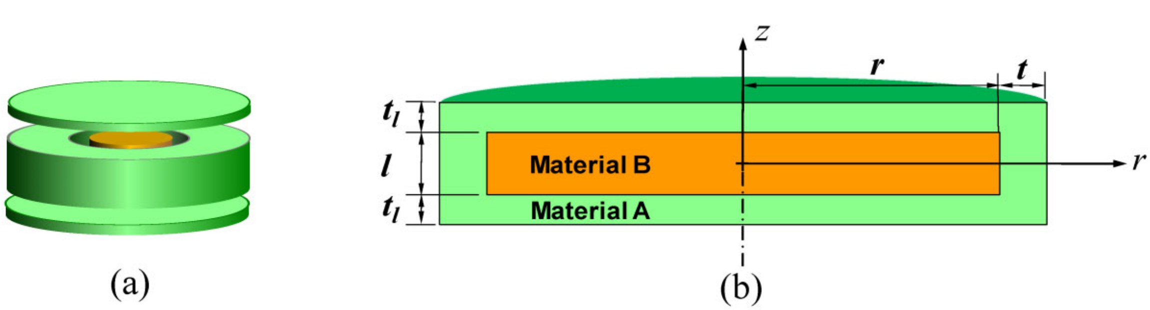
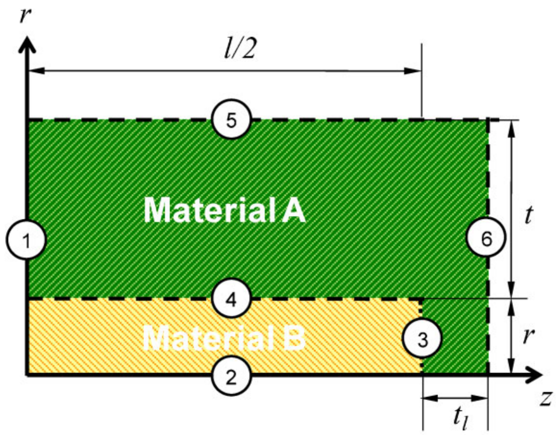


Figure 2 (a) The system modeled, i.e. a cylindrical structure (orange) consisting of an inclusion of material B embedded in a matrix (green) of material A. (b) A cross-section showing its dimensions.



Line	DOFs Constraints	
	U_r	U_z
1	0	-
2	-	0
3	Coupled	-
4	-	Coupled
5	-	Coupled
6	Coupled	-

Figure 3 The boundary conditions applied: U_r and U_z denote displacements in the *r*- and *z*-directions respectively. Translational nodal constraints applied on the nodes lying on the lines shown in the figure. "Coupled" DOFs means that the nodes lying on the respective line have the same displacement normal to the line.

would correspond to stubby shaped inclusions. Note that the simulation were $t_l = 0$ with $l = 500$ would approximately correspond to the simulations reported by Grima et al. [22]. Also, it should be emphasized 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 and the axial strain ε_a were recorded from which the thermal expansion coefficients α_r and α_a in the radial and axial directions respectively were calculated as $\alpha_r = \varepsilon_r \times \Delta T^{-1}$ and $\alpha_a = \varepsilon_a \times \Delta T^{-1}$.

3 Results and discussion The results of these simulations are summarized in the graphs illustrated in Fig. 4 and clearly show that both coin shaped inclusions and needle shaped inclusions have a potential for NTE with the difference that the systems with needle shaped inclusions exhibit NTE primarily in the radial directions whilst coin shaped inclusions exhibit NTE primarily in the axial directions.

In fact, in the systems with coin shaped inclusion, the only system which exhibited NTE in the radial direction was the one where $t_l = 0$ which in some aspects is unrealistic unless one is aiming to manufacture a sheet of NTE material which exhibits the NTE in the plane of the sheet (radial direction), see Fig. 5. On the other hand, most systems with coin-shaped inclusions exhibit NTE in the axial direction. Here, it should be noted that such systems may be considered to be similar to those discussed in Grima et al. [23] for composites with a soft low CTE matrix surrounded by thin hard skins having high CTE.

Going back to the results shown in the graphs in Fig. 4, one may observe that the systems with large values of *l* tend to exhibit NTE in the radial direction unless *t* is very low, as expected from the discussion in the previous section above. Once again here one may note that some systems with needle shaped inclusions do exhibit NTE in the axial directions but this is limited to systems which have very low values of *t* but high values of t_l as illustrated in Fig. 4a(ii) and Fig. 4a(iv). In fact, when one looks at the set of graphs (ii) one will note that in these systems, NTE in the axial direction is exhibited for systems in the lower range of *t*-values where the range of *t*-values which can generate NTE increases as the inclusion becomes less needle like and more coin-shaped as one can clearly see when comparing Fig. 4a(ii) with Fig. 4f(ii). Obviously, systems having $t_l = 0$ cannot exhibit NTE in the axial direction since the material which actually gets thinner as a result of pulling when the system is heated (i.e. the soft material A) is not present in the axial direction.

As systems start to have inclusions where *r* and *l* become of comparable magnitude (see system where $2r = l = 1$), the values of the thermal expansion coefficient are mostly observed to be negative in the axial direction for small values of *t* or in the radial direction for small values of t_l. This feature highlights the fact that in all systems modeled, the amount of soft material in the radial direction reduces the negative CTE in the axial direction, and *vice versa*, a property which may be explained through the images Fig. 6 below where the boundary conditions were changed so as to permit a better visualization of what would have happened in these systems had they to be modeled as a single system (i.e. a system with just one coin) rather as a component in a bulk (i.e. a system which would have required the application of boundary conditions where the surfaces remain "flat"). (These images which correspond to structures having $r = 0.5$, $l = 0.1$, $t_l = 1$ and in the case of the system in Fig. 6a, $t = 0.2$, whilst $t = 1$ in the system in Fig. 6b). The image in Fig. 6b clearly shows that the portion on the left, i.e. the part above the inclusion, is getting thinner axially as a result of the stretching of soft, high

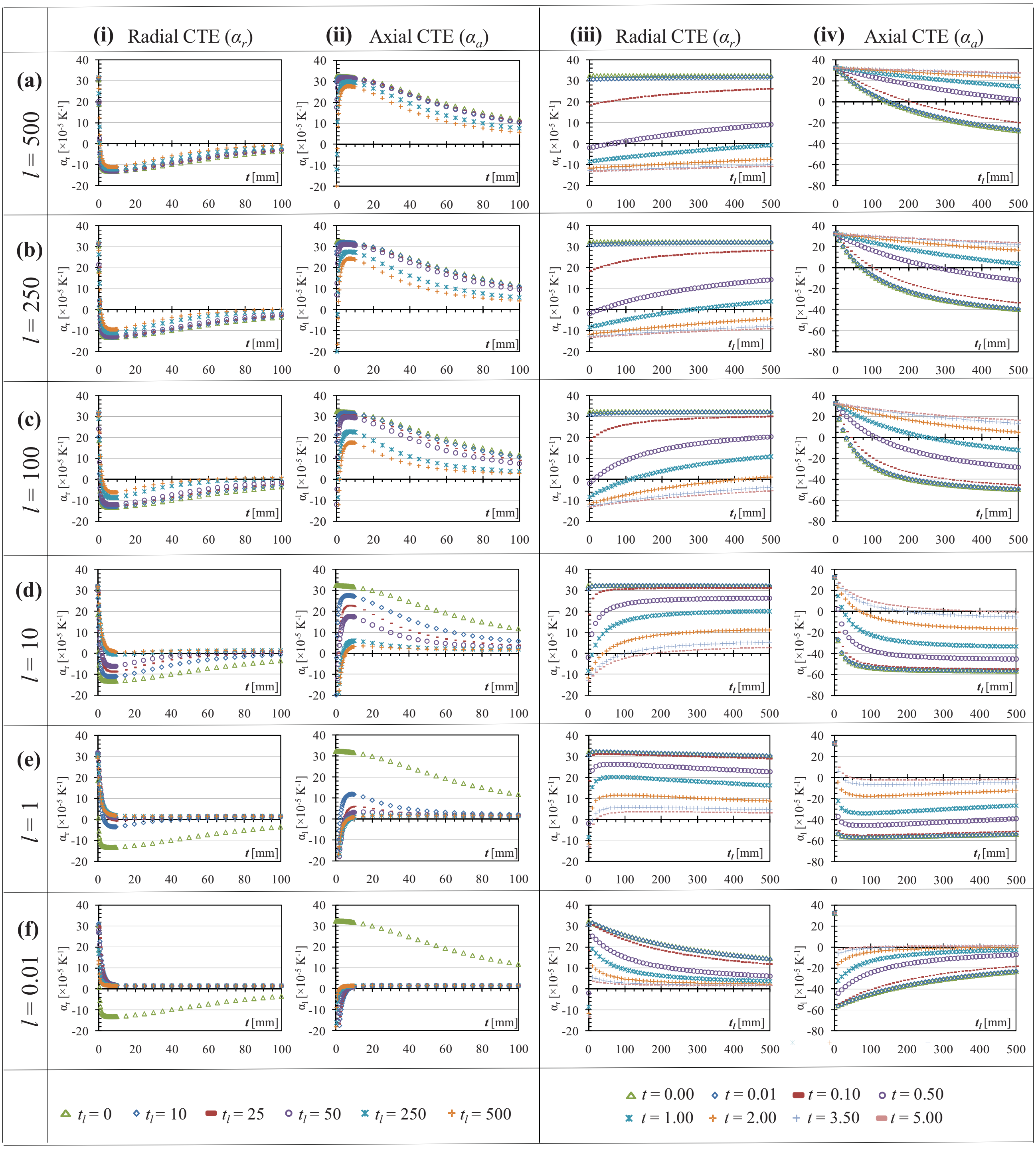


Figure 4 The results of the simulations.

Poisson's ratio and low CTE matrix caused by the expansion of the inner stiff, CTE high stiffness inclusion, as expected from the mechanism being proposed here. However, the portion on the right (i.e. the "t_l part") corresponds to a portion of the system which is not being stretched out by the surface of the coin, with the result that it does not get thinner axially when heated but instead simply expands as a result of the positive thermal expansion of the matrix, something which in that portion of the sample results in conventional thermal expansion. Thus, the average coefficient of thermal expansion in the axial direction of the system in Fig. 6b would have been greatly increased (i.e. made less negative)

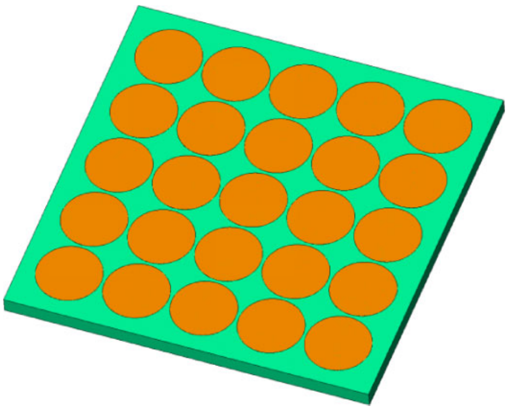


Figure 5 An example of a system which may exhibit NTE in the plane of the sheet (radial direction).

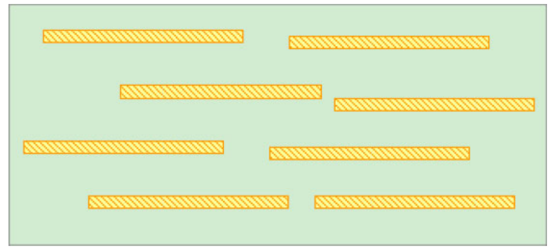


Figure 7 An example of a realistic but more complex system which can be built to exhibit particular CTE properties using the principles presented here.

compared to that in Fig. 6a which has a lower value of t_l. Similar effects would have been observed in the radial direction for equivalent systems having large t_l compared to those having low t_l as illustrated by the fact that the graphs in Fig. 4(iii) show that the radial NTE decreases as t_l increases. On the other hand, if one considers the graphs in Fig. 4(iv), as t_l increases, the NTE effect increases for geometries resembling a needle shape while for systems with small values of l (evident in the graphs for systems with $l < 2r$), the effect is reversed. In fact, the turning point, i.e. when the NTE effect starts to decrease, occurs at around $t_l/l \approx 70$ as shown in Fig. 4(iv).

Before concluding this discussion, it is important to note that as stated above, the idea that NTE can be obtained for systems with coin shaped inclusions in the axial direction could in theory be explained through the model published by Grima et al. [22] for sandwich composite structures designed to exhibit NTE. However, here some caution should be made since in the preliminary model published by Grima et al. [23], one of the assumptions made was that the soft material does not offer any resistance to the growth of the hard material. This assumption may be valid for systems were $E_B/E_A \rightarrow 0$, or systems with very small values of the thickness t_l. However, in real situations, this assumption may lead to significant errors and thus a more realistic model needs to be produced. Also, it is important to highlight 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. 7 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 filled elastomer 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 overall CTE will also be affected by other factors such as the degree of perfection in the alignment of the needle shaped inclusions, the packing, etc., but the principles which may lead to the unusual thermal effects presented in this work, including the potential to exhibit NTE, remain the same.

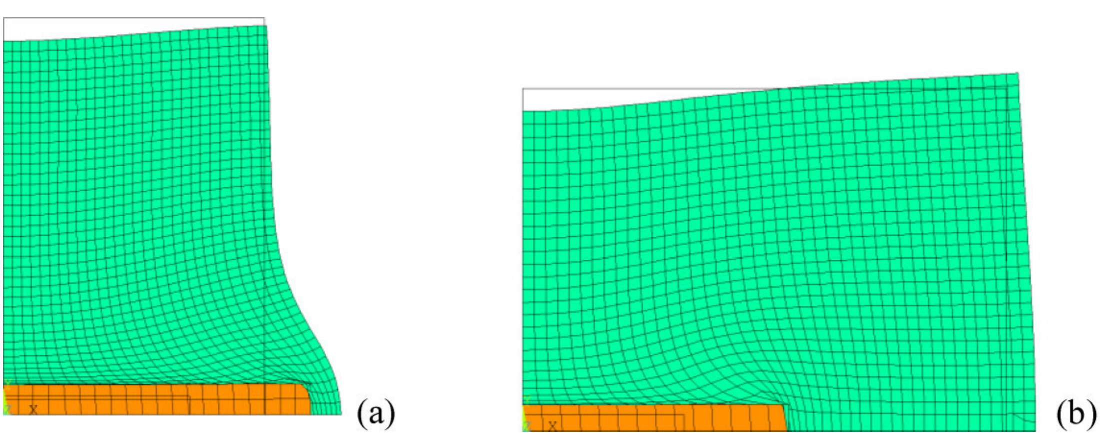


Figure 6 Deformed shapes (magnified 20×) of finite structures, i.e. the edges can deform freely for an inclusion having a coin shaped aspect ratio $l/r = 0.2$ with a surrounding matrix having: (a) $t = 0.2$, $t_l = 1$ and (b) $t = 1$, $t_l = 1$. Note that these systems were obtained using a different set of boundary conditions than the one in Fig. 3 since no coupling of any DOF is imposed.

It is also very important to note that the study presented in this paper is only a preliminary one and to attain a full understanding of the system considered here it is essential that additional aspects are also taken into account. For instance, in addition to the thermal properties, one should also calculate the averaged elastic properties of the composites as well as perform further studies to consider systems where the inclusions are not perfectly aligned with each other. It would also be useful to study systems where there is non-perfect adhesion between the inclusions and the surrounding matrix, as is most likely to happen in real situations.

4 Conclusions This work discussed the concept of controlling the thermal expansion through the introduction of highly expanding and hard coin, cylindrical, or needle shaped inclusions into a soft matrix. In particular, typical examples of such systems were simulated using FE techniques, which confirmed the potential of such concept to control and fine-tune the thermal expansion coefficients, and even exhibit NTE.

It is hoped 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 control in a cost-effective manner.

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