Phys. Status Solidi B **250**, No. 10, 2057–2061 (2013) / **DOI** 10.1002/pssb.201384227

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

Modeling of thermal expansion coefficients of composites with disc shaped inclusions and related systems

Brian Ellul and Joseph N. Grima*

Faculty of Science, University of Malta, Msida MSD 2080, Malta

Received 29 June 2012, revised 27 April 2013, accepted 3 August 2013
Published online 4 October 2013

Keywords analytical model, auxetic, negative thermal expansion, Poisson's ratio,

* Corresponding author: e-mail auxetic@um.edu.mt, Web: www.auxetic.info, Phone: +356 2340 2274

The subject of thermal expansion, particularly negative thermal expansion, is a topic of great practical importance in view of its relevance in many everyday applications and the consequences which may arise when the thermal expansion if not controlled. This paper presents a detailed analytical model of a composite system, which enables control of the thermal expansion through the use of the thinning that is observed when a conventional material is mechanically stretched (the Poisson's effect). It is shown that the model can predict the thermal expansion of such systems to an extent comparable to more complex finite element simulations. The proposed model also permits optimization of the system to exhibit maximum negative thermal expansion, or, thermal expansion of a desired magnitude.

1 Introduction Most materials tend to change size when subjected to a temperature change, normally expanding when heated and contracting when cooled [1, 2]. These changes in dimensions are measured through the coefficients of thermal expansion (CTE), which have positive values if the materials behave in the conventional manner, i.e., expand when heated, and negative values (NTE) if the materials shrink when heated (see Fig. 1). In some materials, in particular single crystalline materials, this expansion is anisotropic, i.e., the extent of expansion is dependent on the particular direction where the measurement is taken. In such systems, the thermal expansion is usually measured in terms of the linear thermal expansion coefficient, α_L which relates the strain ε_L in the direction, where the thermal expansion is being measured to ΔT, the change in temperature, through:

$$\varepsilon_L = \alpha_L \Delta T.$$

In recent years there have been various developments in the field of NTE and several materials and structures, which exhibit this property have been discovered or proposed [3–22]. In particular, it has recently been shown that one may obtain very low or negative thermal expansion coefficients in systems constructed from readily available conventional materials by making use of the fact that when a material having conventional positive Poisson's ratio is stretched, then it gets thinner, a property which may be used to counterbalance the increases in dimension that occur due to conventional thermal expansion so as to obtain a system which would exhibit a net negative or low positive thermal expansion in particular directions [23–25]. For example, it was recently proposed by Grima et al. [25] that through this "Poisson's effect," NTE can be achieved by inserting hard coin-shaped, high CTE inclusions in a soft, low CTE, high Poisson's ratio matrix so as to obtain a net negative thermal expansion coefficient in the direction orthogonal to the surface of the coin through the so called "Poisson's effect," see Fig. 2a. This system is in a way similar to idea proposed by Grima et al. [23] who proposed that NTE may be obtained by a sandwich composite having thin hard high CTE skins which sandwich a soft, low CTE, high Poisson's ratio matrix, see Fig. 2b, which system was modeled through finite element (FE) simulations and a basic analytical model.

In this respect, it should be noted that as discussed elsewhere, although the published analytical model for the sandwich system can be used to predict the thermal expansion coefficients of the sandwich structure may give a reasonable prediction for the thermal expansion coefficients for systems having moderate amounts of the soft layer when compared to the hard layer, this model may not be used for

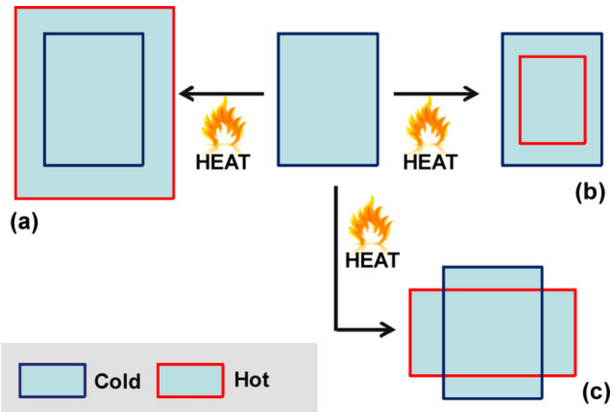

Figure 1 System showing (a) isotropic positive thermal expansion, (b) isotropic negative thermal expansion (NTE), and (c) anisotropic thermal expansion with conventional thermal expansion in the horizontal direction and NTE in the vertical direction.

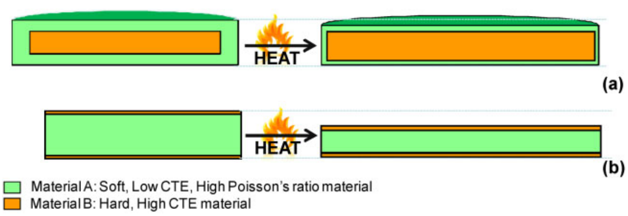

Figure 2 (a) The concept of achieving NTE from a coin-shaped, high-CTE hard inclusion inside a soft low-CTE high Poisson's ratio matrix [25]. (b) The concept of achieving NTE from a sandwich, having high-CTE hard surrounding a soft low-CTE high Poisson's ratio matrix [23].

systems where the properties and/or amount of soft material are such that they offer non-negligible mechanical resistance, as is in practice.

In view of all this, in an attempt to obtain a better understanding of the manner how to adjust the thermal expansion through the Poisson's effect, this work presents a detailed analytical model which corrects the shortcomings of the published analytical model to make it applicable to predict the CTE of the systems with hard coin shaped inclusions in a soft matrix, or of the sandwich panels made from a soft core surrounded by two hard skins.

This new model makes fewer assumptions than the model proposed by Grima et al. [23] and hence it is more general.

2 Analytical model The system to be modeled consists of a "sandwich composite" as shown in Fig. 3a which, without loss of generality, has a cylindrical shape having a core with material B which is sandwiched between two symmetric layers of material A.

The following assumptions are made, namely:

(1) Materials A and B are isotropic with respect to their thermal expansion and mechanical properties and that they are thermally conductive;

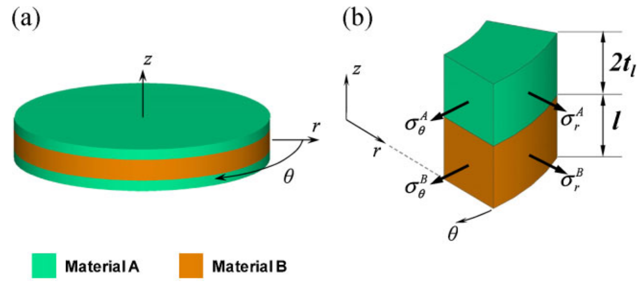

Figure 3 The system modeled and the dimensions used: (a) cylindrical coordinate system and (b) a simplified elemental diagram showing the stresses on each material in the $r\theta$-plane where material A has the overall length ($2t_l$) of both the top and bottom layers in the figure on the right.

(2) there are no stresses in the axial direction throughout the sample including at the interface between material A and material B, i.e., a plane stress structure ($\sigma_z = 0$),as long as the structure can expand freely in the z-direction;

(3) no necking/shearing effects are considered, i.e., after the deformations, the structure still remains perfectly cylindrical in shape.

Considering the elements in Fig. 3b, applying the conditions for in-plane equilibrium one will obtain:

$$l\sigma_{\rm r}^{\rm A} + 2t_l\sigma_{\rm r}^{\rm B} = 0, \tag{1}$$

$$l\sigma_{\theta}^{\rm A} + 2t_l\sigma_{\theta}^{\rm B} = 0, \tag{2}$$

where σ refers to the stress whilst its subscript and superscript refer to the direction and material, respectively. For compatibility of the strains in the $r\theta$-plane, the two materials A and B must expand equally in each respective direction, i.e.,

$$\varepsilon_{\rm r}^{\rm A} = \varepsilon_{\rm r}^{\rm B}, \tag{3}$$

$$\varepsilon_{\theta}^{\rm A} = \varepsilon_{\theta}^{\rm B}, \tag{4}$$

where ε refers to the strain and its subscript and superscript refer to the direction and material, respectively.

From the constitutive equations, i.e., Hooke's law in 3D using polar coordinates [26] for isotropic materials together with plane stress conditions ($\sigma_z^{\rm A} = \sigma_z^{\rm B} = 0$), including the thermal strains $\alpha_{\rm A}\Delta T$ and $\alpha_{\rm B}\Delta T$ of materials A and B, respectively due to a ΔT change in temperature, then:

$$\varepsilon_{\rm r}^{\rm A} = \frac{\sigma_{\rm r}^{\rm A} - \nu_{\rm A}\sigma_{\theta}^{\rm A}}{E_{\rm A}} + \alpha_{\rm A}\Delta T, \tag{5}$$

$$\varepsilon_{\rm r}^{\rm B} = \frac{\sigma_{\rm r}^{\rm B} - \nu_{\rm B}\sigma_{\theta}^{\rm B}}{E_{\rm B}} + \alpha_{\rm B}\Delta T, \tag{6}$$

$$\varepsilon_{\theta}^{\rm A} = \frac{\sigma_{\theta}^{\rm A} - \nu_{\rm A}\sigma_{\rm r}^{\rm A}}{E_{\rm A}} + \alpha_{\rm A}\Delta T, \tag{7}$$

$$\varepsilon_\theta^{\mathrm{B}} = \frac{\sigma_\theta^{\mathrm{B}} - \nu_{\mathrm{B}}\sigma_{\mathrm{r}}^{\mathrm{B}}}{E_{\mathrm{B}}} + \alpha_{\mathrm{B}}\Delta T, \tag{8}$$

$$\varepsilon_z^{\mathrm{A}} = -\frac{\nu_{\mathrm{A}}}{E_{\mathrm{A}}}(\sigma_\theta^{\mathrm{A}} + \sigma_{\mathrm{r}}^{\mathrm{A}}) + \alpha_{\mathrm{A}}\Delta T, \tag{9}$$

$$\varepsilon_z^{\mathrm{B}} = -\frac{\nu_{\mathrm{B}}}{E_{\mathrm{B}}}(\sigma_\theta^{\mathrm{B}} + \sigma_{\mathrm{r}}^{\mathrm{B}}) + \alpha_{\mathrm{B}}\Delta T. \tag{10}$$

Solving equations above for the radial strain and the axial strain, one can find the effective coefficient of thermal expansions α_{r} and α_{a} in the radial and axial directions, respectively where:

$$\alpha_{\mathrm{r}} = \frac{\varepsilon_{\mathrm{r}}^{\mathrm{A}}}{\Delta T} = \frac{\varepsilon_{\mathrm{r}}^{\mathrm{B}}}{\Delta T}, \tag{11}$$

$$\alpha_{\mathrm{a}} = \frac{2t_l\varepsilon_z^{\mathrm{A}} + l\varepsilon_z^{\mathrm{B}}}{\Delta T(l + 2t_l)}. \tag{12}$$

From equations above, the effective coefficient of thermal expansions α_{r} and α_{a} in terms of the material and geometric properties may be written as:

$$\alpha_{\mathrm{r}} = \frac{2\alpha_{\mathrm{A}}t_lE_{\mathrm{A}}(\nu_{\mathrm{B}} - 1) + \alpha_{\mathrm{B}}lE_{\mathrm{B}}(\nu_{\mathrm{A}} - 1)}{2t_lE_{\mathrm{A}}(\nu_{\mathrm{B}} - 1) + lE_{\mathrm{B}}(\nu_{\mathrm{A}} - 1)}, \tag{13}$$

$$\alpha_{\mathrm{a}} = \frac{(2t_l\alpha_{\mathrm{A}} - l\alpha_{\mathrm{B}})(2t_l\nu_{\mathrm{B}}E_{\mathrm{A}} - l\nu_{\mathrm{A}}E_{\mathrm{B}}) - (2t_l\alpha_{\mathrm{A}} + l\alpha_{\mathrm{B}})(2t_lE_{\mathrm{A}} + lE_{\mathrm{B}}) + 4t_ll(\alpha_{\mathrm{B}}\nu_{\mathrm{A}}E_{\mathrm{B}} + \alpha_{\mathrm{A}}\nu_{\mathrm{B}}E_{\mathrm{A}})}{(2t_lE_{\mathrm{A}}(\nu_{\mathrm{B}} - 1) + lE_{\mathrm{B}}(\nu_{\mathrm{A}} - 1))(2t_l + l)}. \tag{14}$$

Table 1 Material properties of materials A and B which are the materials of the matrix and the inclusion, respectively, used in this discussion.

material property	material A	material B
Young's modulus	$E_{\mathrm{A}} = 10\,\mathrm{MPa}$	$E_{\mathrm{B}} = 200\,\mathrm{GPa}$
Poisson's ratio	$\nu_{\mathrm{A}} = 0.49$	$\nu_{\mathrm{B}} = 0.3$
CTE	$\alpha_{\mathrm{A}} = 15 \times 10^{-6}\,\mathrm{K}^{-1}$	$\alpha_{\mathrm{B}} = 324 \times 10^{-6}\,\mathrm{K}^{-1}$

3 Results and discussion

The equations above clearly show that the effective CTE values of these systems are highly dependent not only on the thermal expansion properties of the component materials A and B, but also on their mechanical properties, in particular their Young's moduli and Poisson's ratios, and their relative amounts (i.e., the relative values of t_l and l).

More specifically, the maximum NTE with respect to t_l/l can thus be found by differentiating the expression for α_{a} with respect to t_l/l and solving for t_l/l.

$$\frac{\partial\alpha_{\mathrm{a}}}{\partial(t_l/l)} = 0 \tag{15}$$

from which analysis, if material A and B have the properties in Table 1, i.e., material B is the hard material having a high CTE whilst material A is the soft, low CTE high Poisson's ratio material, it may be shown that the ideal t_l/l ratio which gives the maximum NTE possible in the axial direction occurs at $t_l/l = 74.16$. This corresponds to the value predicted by detailed analytical model as discussed elsewhere thus confirming the validity of this model.

It may also be shown that in the limit when $E_{\mathrm{B}} \gg E_{\mathrm{A}}$ so that E_{A} can be assumed to be zero when compared to E_{B}, then the equation for α_{a} becomes equivalent to that for α_z derived by Grima et al. [23] for the systems illustrated in Fig. 2b.

Let us now discuss and compare the results of the analytical model presented here to the results obtained from the FE simulations for the system with coin shaped inclusions shown in Fig. 2a for $t = 0$ mm, i.e., when the structure resembles the one shown in Fig. 3a. From this analysis (see Fig. 4), it is clear that the effective CTE values of these systems are highly dependent on the properties and relative amounts of materials A and B in a rather complex manner and that the overall thermal expansion of the system may be carefully controlled not only through the choice of the constituent materials, but, more importantly, from their relative amounts. Extremely important from a practical point of view is the fact that a very wide range of thermal expansion values may be manifested, something which confirms the potential of this concept to be used to control the observed thermal expansion. Furthermore, from Fig. 4, it may be shown that there is an excellent agreement between the predictions of the analytical model and the results of the FE simulations, something, which gives confidence to both the analytical model and FE simulations. In particular, the results confirm that for such systems, the NTE effect can indeed occur in the axial direction, the extent of which is dependent on both l and t_l in the manner predicted by the analytical model. These results also show that for materials having the mechanical and thermal expansion properties discussed here, the most interesting systems are those where $l \approx 10$ for $r = 0.5$ (i.e., systems where the inclusion is in the shape of a cylinder having a 1:10 aspect ratio for diameter to length) since such systems will exhibit high negative values of NTE for a very wide range of t_l values.

Also, if one had to compare the results of the earlier model by Grima et al. [23] to the one derived here (see Fig. 5), one would note that the errors resulting from ignoring the effects of E_{A} start to become significant for systems with small values of l, in particular for the systems with $l = 0.10$ and $l = 0.05$ thus confirming the need for this more complex approach (giving less elegant equations) for

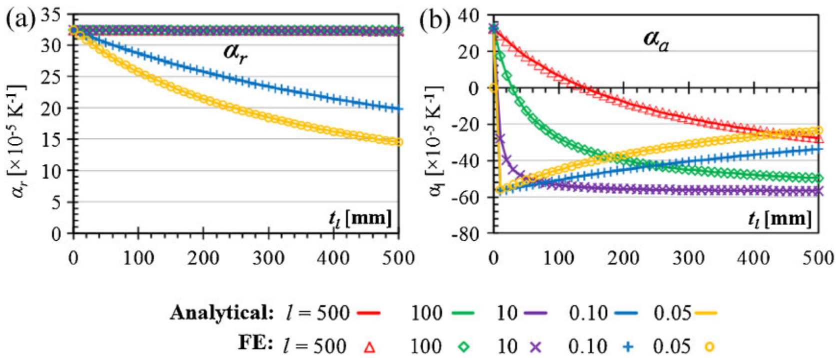

Figure 4 Comparison of the CTE in the (a) radial and (b) axial directions of FE results presented elsewhere [25] with the analytical models derived here. Note that the FE data relates to the system in Fig. 2a for the special case when $t = 0$, i.e., the structure similar to the one shown in Fig. 3a.

modeling these systems. In fact, for these systems, if the predictions were made by the old model, then it would have been erroneously predicted that the NTE would have remained approximately constant for a large range of t_l values, something which is in fact not the case as indicated by the improved analytical model presented here and the FE data. Here it must be emphasized that this new improved model will in fact be better at describing the sandwich NTE systems proposed by Grima et al. [23] when compared to the existent model. Also, it should he highlighted that the new insights provided in this work are very significant, especially in view of the fact that the earlier model had predicted that for maximum NTE, one should aim for very thin amounts of the hard high CTE material (the coin, or the hard skin) when compared to the matrix, a prediction which will not remain valid if the stiffness of the soft component is not negligible, as will normally be the case in real practical situations.

Before concluding, it is important to emphasize that a similar correction should be made for the model of the NTE in the radial direction of the systems with needle like inclusions, and also to make a model that could handle concurrent non-zero t_l and t, something which is beyond the scope of this work. Furthermore, a factor which should not be ignored is the fact that the model presented here has the limitation that what is modeled here is a highly idealistic scenario where the hard inclusions do not permanently deform the softer matrix, something which is likely to happen (unless improvements are made and precautions are taken in the design and manufacture) in systems where the inclusions are similar to a “sharp blade” which could “cut into” and tear the material. The same is likely to apply to the systems with needle shaped inclusion. It would also probably be useful to manufacture the systems with surfaces that prevent slipping/debonding of the inclusion from the matrix. Also, here it should be noted that systems having comparable values of l and r are likely to be less affected by such problems and hence may be more practical to use in the manufacture of such systems, particularly if their edges are rounded so as to avoid stress concentrations in the soft matrix.

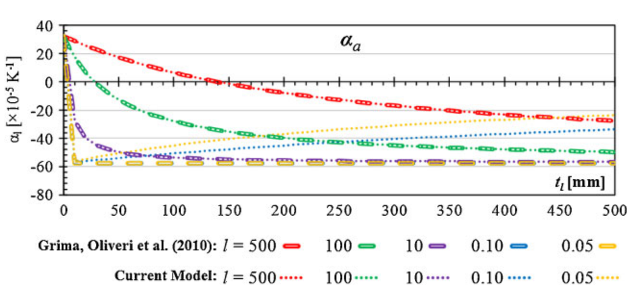

Figure 5 Comparison of the CTE in the axial direction (α_l) between the model presented by Grima et al. [23] and the one presented here. Note that for systems where t_l is small, which are the most interesting systems from a NTE point of view, the deviations are very significant, thus highlighting the importance of the current model.

4 Conclusions This work presents an analytical model, which can be used to aid in the elucidation of the mechanism of how the Poisson’s effect may be used to regulate the thermal expansion of composite systems. It is shown that:

(1) the effective thermal expansion coefficient may be controlled and fine-tuned through the choice of the component materials used, and also their relative amounts;
(2) negative thermal expansion may be obtained if the thermal expansion, the mechanical properties and the relative amounts of the component materials are amenable.

In view of the practical importance of the subject of thermal expansion, particularly its control, it is hoped that this model will aid experimentalists who may wish to synthesize and manufacture real systems based on the model presented here.

Acknowledgements The financial support of the Malta Council for Science and Technology through their 2006 R&I

programme is gratefully acknowledged as is the support of the project coordinator, Inġ. Michael Attard of IMA Engineering Ltd. (Malta).

References

[1] M. A. White, Properties of Materials (Oxford University Press, New York, 2000).
[2] R. E. Taylor, Thermal Expansion of Solids, edited by C. Y. Ho (ASM International, Ohio, 1998).
[3] A. Alderson, K. L. Alderson, G. D. Hudson, and D. E. Skertchly, European Patent EP 1989249 B1 (2009).
[4] G. D. Barrera, J. A. O. Bruno, T. H. K. Barron, and N. L. Allan, J. Phys.: Condens. Matter. **17**(4), R217–R252 (2005).
[5] W. J. Clegg, and A. Kelly, Adv. Eng. Mater. **4**(6), 388–392 (2002).
[6] J. S. O. Evans, J. Chem. Soc. Dalton Trans. **19**, 3317–3326 (1999).
[7] J. N. Grima, V. Zammit, and R. Gatt, Xjenza **11**, 17–29 (2006).
[8] J. N. Grima, P. S. Farrugia, R. Gatt, and V. Zammit, Proc. R. Soc. A **463**(2082), 1585–1596 (2007).
[9] J. N. Grima and K. W. Wojciechowski, Phys. Status Solidi B **245**(11), 2369–2372 (2008).
[10] A. Kelly, L. N. McCartney, W. Clegg, and R. J. Stearn, Compos. Sci. Technol. **65**(1), 47–59 (2005).
[11] A. Kelly, R. J. Stearn, and L. N. McCartney, Compos. Sci. Technol. **66**(2), 154–159 (2006).
[12] R. S. Lakes, J. Mater. Sci. Lett. **15**(6), 475–477 (1996).
[13] M. Landert, A. Kelly, R. J. Stearn, and P. J. Hine, J. Mater. Sci. **39**(11), 3563–3567 (2004).
[14] B. A. Marinkovic, M. Ari, P. M. Jardim, R. R. de Avillez, F. Rizzo, and F. F. Ferreira, Thermochim. Acta **499**, 48–53 (2010).
[15] T. Mary, J. S. O. Evans, T. Vogt, and A. W. Sleight, Science **272**(5258), 90–92 (1996).
[16] W. Miller, D. S. Mackenzie, C. W. Smith, and K. E. Evans, Mech. Mater. **40**(4–5), 351–361 (2008).
[17] G. W. Milton, The Theory of Composites (Cambridge University Press, Cambridge, UK, 2002).
[18] O. Sigmund and S. Torquato, Appl. Phys. Lett. **69**(21), 3203–3205 (1996).
[19] O. Sigmund and S. Torquato, J. Mech. Phys. Solids **45**(6), 1037–1067 (1997).
[20] L. J. Vandeperre and W. J. Clegg, in: Materials and Devices for Smart Systems, MRS Proc., Vol. 785, edited by Y. Furuya, E. Quandt, Q. Zhang, K. Inoue, and M. Shahinpoor (Materials Research Society, Boston, MA, 2003), p. D11.4.
[21] A. W. Sleigh, in: McGraw-Hill Yearbook of Science & Technology 2009 (McGraw Hill Professional, New York, 2009).
[22] C. W. Smith, W. Miller, D. S. Mackenzie, and K. E. Evans, *Mechanism for negative thermal expansion and its links to negative Poisson's ratio*, presented at: Second International Workshop on Auxetic and Related Systems, Poznan, Poland (2005).
[23] J. N. Grima, L. Oliveri, B. Ellul, R. Gatt, D. Attard, G. Cicala, and G. Recca, Phys. Status Solidi RRL **4**(5–6), 133–135 (2010).
[24] J. N. Grima, B. Ellul, D. Attard, R. Gatt, and M. Attard, Compos. Sci. Technol. **70**, 2248–2252 (2010).
[25] J. N. Grima, B. Ellul, R. Gatt, and D. Attard, Phys. Status Solidi B **250**, 2051–2056 (2013), this issue.
[26] S. P. Timoshenko, and J. N. Goodier, Theory of Elasticity (McGraw-Hill Book Company, Inc., New York, 1951).