Dense solid microstructures with unbounded thermal expansion

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Abstract

Analytical bounds on the physical properties of multiphase media provide limits on properties attainable with variation of phase geometry. We present examples which substantially exceed the bounds for thermal expansion of a two-phase composite, by allowing slip at interfaces between phases. New classes of materials with extreme properties are envisaged, based on slip interfaces.

Microstructure in multiphase materials such as composites and biological tissues may be so complex that theoretical prediction of aggregate physical properties from constituent properties becomes difficult or impossible. Consequently, it is useful to develop analytical bounds upon properties in order to constrain the range of properties which may be expected. Bounds are useful in relating the properties of macroscopic polycrystalline materials to those of single crystals [1], in guiding the pursuit of optimal microstructure in composites [2], and in understanding biological composites such as bone [3,4]. Early work on bounds dealt with stiffness [5-7]. More recently other physical properties have been considered.

For example, bounds have been developed for the thermal expansion coefficient α of composite materials of two solid phases in terms of constituent expansion coefficients α_1 and α_2 [8,9]. The upper bound is a rule of mixtures $\alpha = \alpha_1 V_1 + \alpha_2(1 - V_1)$, in which V_1 is the volume fraction of the first phase. In deriving these bounds it was tacitly assumed that the two phases are perfectly bonded and with zero void content. We show that arbitrarily high thermal expansions can be achieved in composites with interfaces which allow slip.

To that end, envisage rib elements of composite microstructure, each of which is a bi-layer made of two bonded layers of differing thermal expansion coefficient α. The layers have Young's moduli (stiffness) E_1 and E_2, thermal expansion coefficients α_1 and α_2; and thicknesses h_1 and h_2. The bi-layer bends in response to temperature changes. The curvature κ (the inverse of the radius of curvature ρ) of such an unconstrained thin elastic bi-layer is given in terms of the temperature change ΔT by [10].

$$\kappa = 6\Delta T \frac{(\alpha_2 - \alpha_1)}{(h_1 + h_2)} \left\{ \frac{(1 + \frac{h_1}{h_2})^2}{3[(1 + \frac{h_1}{h_2})^2] + (1 + \frac{h_1}{h_2}\frac{E_1}{E_2})\left[(\frac{h_1}{h_2})^2 + \frac{h_2 E_2}{h_1 E_1}\right]} \right\}. \tag{1}$$

The quantity in the {} brackets is defined here as Γ. Such rib elements can be assembled into a lattice or honeycomb in which there is no constraint on rib bend. The thermal expansion α of such a cellular solid due to longitudinal displacement of initially curved rib elements of arc length l_{arc}, and included angle θ, is [11]:

$$\alpha = 6(\alpha_2 - \alpha_1) \frac{l_{arc}}{(h_1 + h_2)} \Gamma \left[\frac{1}{2} \mathrm{ctn} \frac{\theta}{2} - \frac{1}{\theta}\right] \quad (2)$$

Expansion due to rib bending depends on each constituent having a different expansion coefficient. Expansion α becomes large as bi-layers become slender, $l_{arc}/(h_1 + h_2) >> 1$ and as the included angle θ becomes large. The thermal expansion coefficient α of a cellular solid structure based on these bi-layers is therefore unbounded [11]. It can be made much larger in magnitude than the thermal expansion coefficient of either solid constituent.

Inclusion of void space of appropriate shape in a composite microstructure can give rise to unusual mechanical properties such as a negative Poisson's ratio [12]. Void space is not, however a necessary condition to achieve negative Poisson's ratio; a hierarchical laminate with dissimilar constituents also has this property [13]. A common aspect is non-affine or inhomogeneous deformation [14].

For unbounded thermal expansion a cellular solid structure is not necessary either; it is sufficient that the composite contain interfaces which can undergo slip. A simple two-dimensional illustration is shown in Fig. 1, which shows an anisotropic laminate of curved bi-layers with slipping interfaces between bi-layers. One phase is represented by white, the other by black. The thermal expansion in the horizontal direction follows the relation for individual bi-layers, Eq. 2, since, with slip, there is no constraint on the expansion of each bi-layer. As horizontal expansion occurs, the corresponding volume is accommodated from undulations on the top and bottom surfaces as the bi-layers straighten.

High expansion in two directions can be achieved in several dense structures containing bi-layer elements. Fig. 2 shows an example with multiple length scales. Each bi-layer is assumed to have the same included angle θ. Since l_{arc} is proportional to the radial distance from the center of the pattern, a constant expansion strain ε may be achieved by shaping the bi-layers so that the bi-layer thickness $h_1 + h_2$ is proportional to the radial distance from the center of the pattern. As with the structure in Fig. 1, volume change occurs by surface undulations rather than internally. Fig. 3 shows an example of a random two-dimensional structure with multiple size scales, in which slip during expansion causes microscopic voids to open within the structure, giving rise to expansion with volume change. Rib expansion is fully unconstrained in this case only if there is a compliant interphase boundary between inclusions; this could be a microporous layer of one phase. Other examples are possible as well, including hexagonal structures which are mechanically isotropic.

The sign of the thermal expansion coefficient of layered composites is governed by the placement of the constituents within each bi-layer. Specifically, if the constituent with the higher thermal expansion coefficient is on the concave side of each bi-layer, composite thermal expansion is positive since an increase in temperature will cause each bi-layer to straighten. Negative thermal expansion coefficients will occur if the higher expansion constituent is on the convex side of each bi-layer. We remark that molecular design of materials with moderate values of negative linear and volumetric thermal expansion has been conducted [15].

Dense two-dimensional microstructures could be produced by a co-extrusion process, by progressive lamination, or by lithography. One may also envisage three-dimensional microstructures containing graded onion-like laminations, though manufacture may prove challenging.

Use of slip type interfaces or void space to exceed the conventional bounds is applicable to cross properties in materials which exhibit coupled field phenomena. In the present example, thermal expansion couples the mechanical (strain and stress) and thermal (temperature and entropy) fields. Other coupled field phenomena include piezoelectricity, pyroelectricity, electro-optics, stress-induced fluid flow in porous media, and swelling or shrinkage due to hydration changes. By contrast, stiffness, a direct property, is the ratio of stress to strain. In a material with cracks as a type of slip interface, stiffness is reduced [7,16,17]. Effects of the slip interfaces considered here are entirely distinct from effects, due to resonant phenomena [18], of "homeopathic" (arbitrarily small) concentrations of a third phase on dielectric properties.

The present model structures illustrate the importance of assumptions in the demonstration of bounds. Since inclusion of slip interfaces can have a large effect on composite material properties, we envisage new classes of materials with extreme physical properties.

References

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Figures

Fig. 1 Orthotropic dense laminate with a thermal expansion which becomes unbounded as the strip thickness becomes small. One phase is represented by white, the other by black.

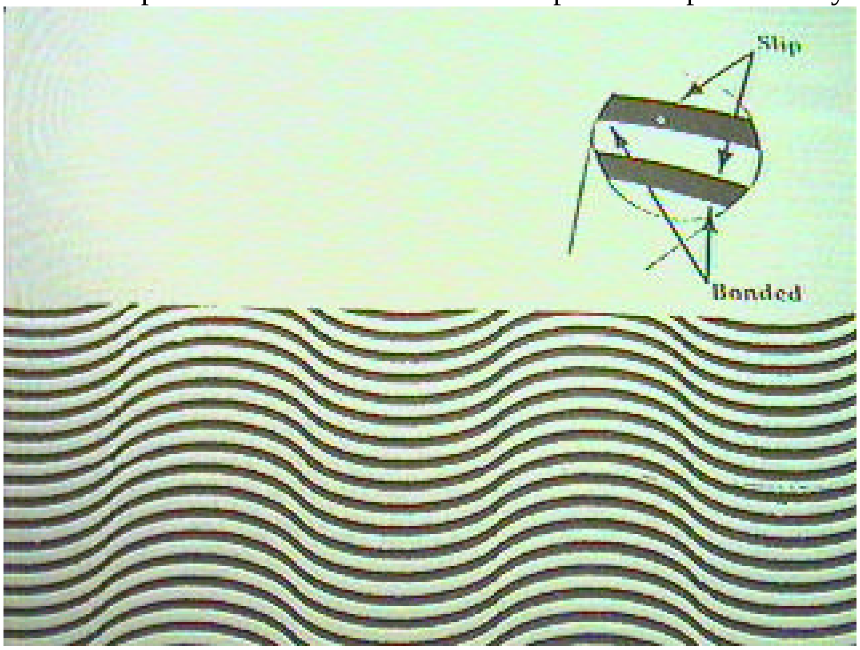

Fig. 2 Cubic dense laminate with a thermal expansion which becomes unbounded as the strip thickness becomes small. The ribs become arbitrarily thin as the center of each cell, therefore the center is not shown.

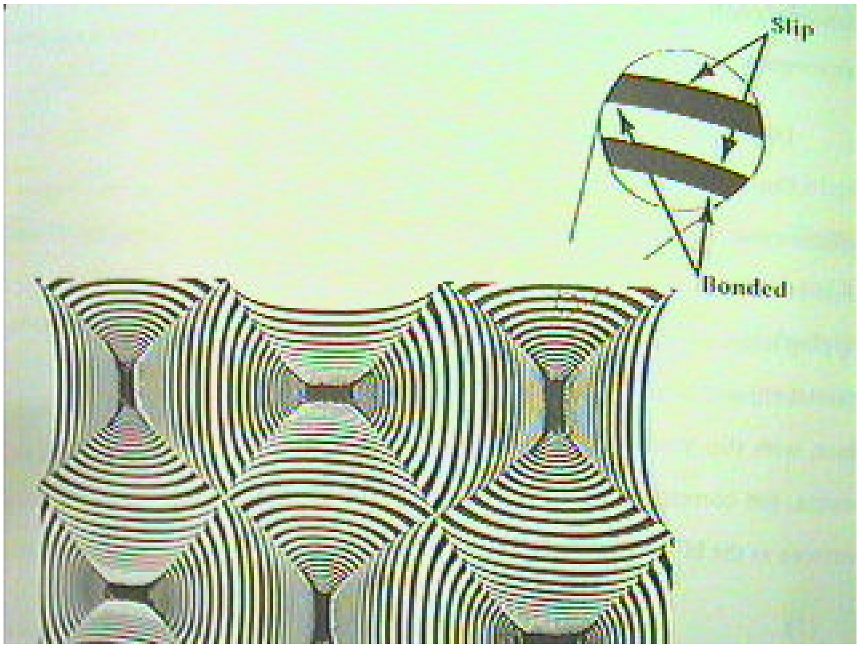

Fig. 3 Random dense structure with laminated inclusions of different size. Curved laminae are alternately bonded and free to slip as in Fig. 1 and 2.