

Cellular solids with tunable positive or negative thermal expansion of unbounded magnitude

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Material microstructures are presented with a coefficient of thermal expansion larger in magnitude than that of either constituent. Thermal expansion can be large positive, zero, or large negative. Three-dimensional lattices with void space exceed two-phase bounds but obey three-phase bounds; lattices and normal materials have a trend of expansion decreasing with modulus. Two-phase composites with a negative stiffness phase exceed bounds that assume positive strain energy density. The author determined Young's modulus and its relation to thermal expansion. Behavior of these composites is compared with that of homogeneous solids in expansion-modulus maps. © 2007 American Institute of Physics. [DOI: [10.1063/1.2743951](https://doi.org/10.1063/1.2743951)]

Thermal expansion of materials is of practical interest since materials in service may experience temperatures which vary considerably. If dimensional stability is desired in a design, then materials of zero or minimal thermal expansion are of interest. Actuators controlled by temperature changes can make use of materials with large thermal expansion. Thermal expansion is described as follows. The strain ε_{ij} in an isotropic solid depends on stress σ_{ij} (elasticity) and on temperature change ΔT (thermal expansion),

$$\varepsilon_{ij} = \frac{1+\nu}{E} \sigma_{ij} - \left[\frac{\nu}{E} \sigma_{ii} - \alpha \Delta T \right] \delta_{ij}, \quad (1)$$

in which ν is Poisson's ratio, E is Young's modulus, α is the thermal expansion coefficient, and δ_{ij} is Kronecker's delta.¹ Thermal expansion of crystalline solids is attributed to the anharmonicity of the interatomic potential and is therefore considered to be a property intrinsic to each material. In common materials, expansion tends to decrease with elastic modulus. Some materials have negative expansion. Zirconium tungstate, in contrast to other negative expansion solids, has a negative expansion over a temperature range of more than 1000°.²⁻⁴

Analytical bounds on the physical properties of composite materials provide limits on properties attainable with variation of phase geometry. For example, the classical Voigt-Reuss and Hashin-Shtrikman bounds provide limits on the elastic modulus of composites.⁵⁻⁷ Such bounds can be useful in the study of complex synthetic composites or biological tissues in which the structure is so complex that one cannot easily analyze the relation between structure and physical properties. Bounds are known for the thermal expansion coefficient α of composite materials⁸ of two solid phases in terms of constituent expansions α_1 and α_2 . The upper bound is a rule of mixtures

$$\alpha = \alpha_1 V_1 + \alpha_2 [1 - V_1], \quad (2)$$

in which V_1 is the volume fraction of phase 1. In the derivation of these bounds it is assumed that the two phases are perfectly bonded, that there is no porosity, and that each phase has a positive definite strain energy. Relaxation of any of these assumptions permits one to achieve arbitrarily large or small values of expansion, as is shown in the following. Three-phase bounds (which also assume positive definite strain energy)^{9,10} are more general; they allow void space. Lattices presented below, as with common materials, follow a trend of decreasing modulus as expansion increases.

Cellular solids contain void space. If the ribs (struts) in a foam or honeycomb are homogeneous, then the thermal expansion of the cellular solid¹¹ is the same as that of the solid from which it is made. Arbitrarily high thermal expansions can be achieved in composites containing two solid phases and void space.¹² Given this concept, it becomes possible to design composites with the aid of topology optimization.¹³ Dense composites with slip interfaces can also exhibit extreme values of expansion.¹⁴ These solids contain rib elements of composite microstructure. Each rib element is a bilayer made of two bonded layers of differing thermal expansion coefficient. Curved rib elements of this type undergo a length change in response to temperature change. This length change gives rise to the thermal expansion of the lattice as a whole. Several hexagonal cell structures based on this concept are shown in Fig. 1. Figure 1(a) depicts a regular hexagonal cell with curved ribs, each of which consists of two dissimilar materials with different thermal expansion coefficients. The center of curvature is not in general at the center of the cell. Figure 1(b) depicts an inverted reentrant cell of a negative Poisson's ratio honeycomb. Figure 1(c) depicts a hexagonal cell with nested rib elements. The nested elements can fill the entire space; void space opens up upon expansion. If the lattice is to be capable of contraction, there must be some initial void space. As for three-dimensional foam lattices, we envisage a lattice cell with bimaterial ribs, as shown in Fig. 2. This cell is of tetrakaidecahedral shape, similar to the cell shape in open cell foams.

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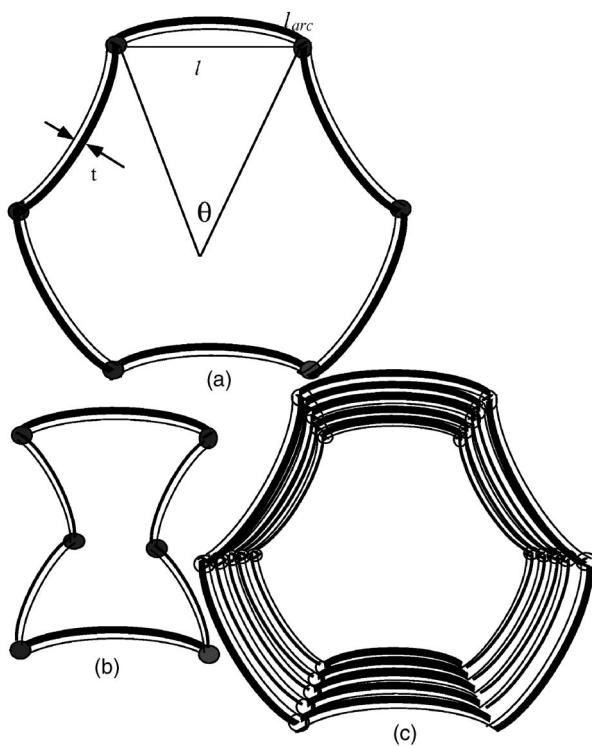


FIG. 1. Hexagonal lattice cells with curved bimaterial ribs: (a) regular hexagonal cell, (b) inverted hexagonal cell for negative Poisson's ratio, and (c) nested lattice cell.

The thermal expansion is determined as follows. A single rib element containing two dissimilar materials of different thermal expansions α_1, α_2 and thicknesses h_1, h_2 will curve in response to a temperature change.¹⁵ The change of length of an initially curved rib element of arc length l_{arc} gives rise to an effective thermal expansion in terms of the included angle θ , a measure of rib curvature, in which the layers are of equal thickness and of equal elastic modulus

$$\alpha = (\alpha_2 - \alpha_1) \frac{l_{\text{arc}}}{(h_1 + h_2)} \left[\frac{1}{2} \cot \frac{\theta}{2} - \frac{1}{\theta} \right]. \quad (3)$$

This expansion is positive if the material on the inner (concave) portion of the curve has the higher value of expansion,

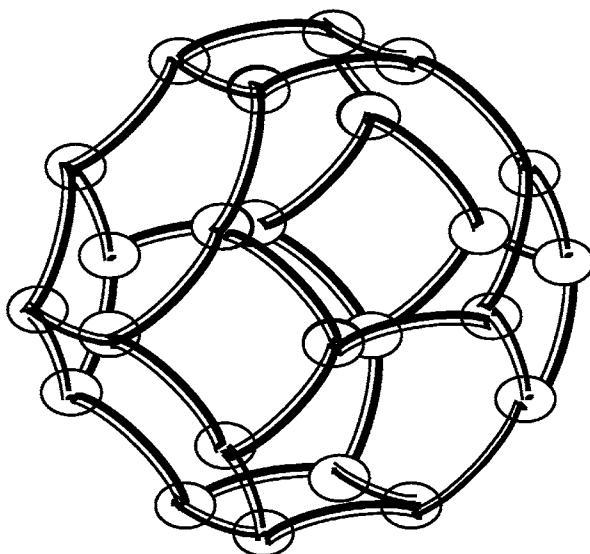


FIG. 2. Tetrakaidecahedral foam cell.

since an increase in temperature will cause the rib to straighten. By contrast, if the constituent with the higher thermal expansion coefficient is on its outer or convex side, an increase in temperature will cause the rib to curve more and become shorter, giving rise to a negative thermal expansion coefficient. If the angle is not too large, this expression assumes a simpler form, with $t=h_1+h_2$,

$$\alpha = (l/t)(\alpha_1 - \alpha_2)(\theta/12). \quad (4)$$

The elastic modulus E for honeycomb (a two-dimensional lattice) with hexagonal cells of material with modulus E_s of thickness t and length l is governed by rib bending and is determined via¹¹

$$E/E_s = 2.3(t/l)^3. \quad (5)$$

The ribs of a three-dimensional lattice containing curved bimaterial rib elements give rise to a thermal expansion following Eq. (3). The elastic modulus is given by¹⁶

$$E/E_s = 0.76\rho^2(1 + 1.09\rho)^{-1}, \quad (6)$$

in which the relative density is $\rho=0.46(t/l)^2$.

Thermal expansion of these lattices is plotted versus elastic modulus E in Fig. 3(a). For the rib materials, a Young's modulus of 200 GPa is assumed, corresponding to steel, and an expansion difference of 10^{-5} is assumed, corresponding to a steel-Invar based rib; the angle θ is one radian. For comparison, the behavior of several known solid materials¹⁷ is also plotted. As shown in Fig. 3(a), one can increase the expansion by making the ribs more slender (a smaller aspect ratio t/l); doing so reduces the modulus. The expansion can be reduced by reducing the rib curvature; rib stiffness hence modulus is relatively insensitive to curvature. Zero expansion is possible. Therefore the region to the left of and below the diagonal line representing each lattice is accessible. A portion of the region to the right, corresponding to a higher modulus, is accessible via nested lattices. A lattice with slender ribs can be nested to a greater degree than a lattice with thick ribs. These hexagonal cells are elastically isotropic in plane in contrast to the cubic cells¹⁴ considered earlier. The hexagonal lattice is anisotropic in the third direction so isotropic bounds do not apply to it. Expansion of the foam is less in magnitude than the isotropic three-dimensional three-phase bound⁹ as shown.

Negative thermal expansion can be easily achieved in the lattices by placing the material of higher expansion on the outer portion of the curve. Negative expansion is not connected with negative Poisson's ratio which can occur in honeycombs or foams with uniform, rather than bimaterial, ribs.¹⁸ Behavior of lattices and other materials in this regime is shown in Fig. 3(b). Few homogeneous materials are available for comparison. Zirconium tungstate is of greatest interest in this context^{3,19} since it exhibits negative expansion over a wide temperature range.

Controllable thermal expansion can also be achieved in two-phase composites with inclusions of negative stiffness²⁰ and no void content. Such composites have been made in the laboratory and shown to have extremely high damping capacity,²¹ too, extreme Young's modulus²² exceeding that of diamond. The composite thermal expansion α_c is related to the bulk modulus K and expansion α of phases 1 and 2 as follows, with K_c as the bulk modulus of the composite⁹

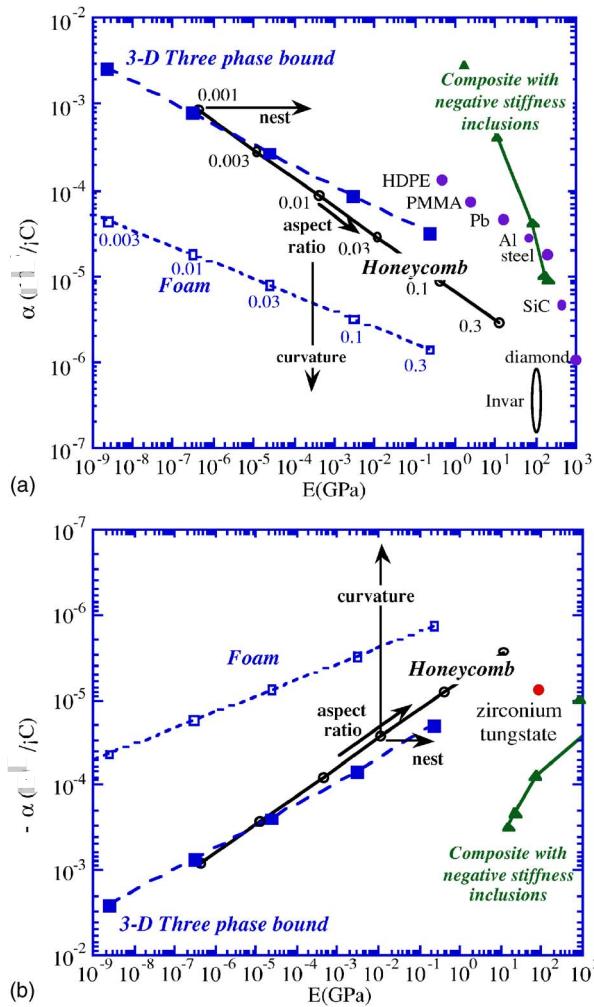


FIG. 3. (Color online) Expansion-modulus maps of lattices and known materials: (a) positive expansion and (b) negative expansion. Numbers refer to aspect ratio t/l . Solid circles ●, homogeneous materials; open circles ○, honeycomb; open squares □, foam; solid triangles ▲, composite with negative stiffness inclusions; and solid squares ■, three-dimensional isotropic three-phase bound.

$$\alpha_c = \alpha_1 + \frac{\alpha_1 - \alpha_2}{1/K_2 - 1/K_1} \left(\frac{1}{K_c} - \frac{1}{K_1} \right). \quad (7)$$

Assuming a matrix Young's modulus of 200 GPa and expansion 10^{-5} , and allowing inclusions 10% by volume with negative bulk modulus, the expansion and Young's modulus

are calculated for a Hashin-Shtrikman composite²³ and plotted in Fig. 3. These composites allow both positive and negative thermal expansions combined with large magnitudes of elastic modulus. The temperature range is likely to be narrow if these materials are based on phase-transforming inclusions. These composites can be stabilized,²⁴ so it may be possible to achieve such composites in other ways.

To conclude, large regions of the expansion-modulus map have been made accessible via two- and three-dimensional cellular solids and by composites in which one phase has a negative bulk modulus. Positive or negative expansion values of arbitrarily large magnitude or zero are possible.

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