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Negative linear compressibility of hexagonal honeycombs and related systems

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Materials exhibiting negative linear compressibility display the very unusual and unexpected property of expanding in at least one direction when placed under compressive hydrostatic stress. Here, it is shown that this property may be manifested by systems having high positive Poisson's ratios (non-auxetic), including non re-entrant hexagonal honeycombs and wine-rack models where deformation primarily involves changes in the angles between the ribs of the structures.

Keywords: Honeycomb structure; Elastic behaviour; Analytical methods; Modelling; Negative compressibility

When a material is subjected to a hydrostatic stress it usually contracts in all directions. However, there are occasional reports of materials and structures that behave in a different fashion [1–14], i.e. exhibit negative compressibility, meaning that they possess the unusual property of expanding in one or more directions when hydrostatically compressed. Such materials are predicted to have a number of applications ranging from extremely sensitive pressure detectors, telecommunication line systems, to optical materials with very high refractive index [1].

So far, very few materials have been reported to exhibit negative linear compressibility (i.e. expand in one direction when compressed hydrostatically). The ones identified so far include methanol monohydrate [2], a hypothetical carbon-based system [1] caesium dihydrogen phosphate [4], lanthanum niobate [5], $Ag_3[Co(CN)_6]$ [6] and orthorhombic high-pressure paratellurite (TeO_2) phase [7]. Structures which exhibit negative linear, area and volume compressibility on a macrolevel have also been reported [8–10]. These include structures assembled from triangular building blocks [8] or chiral units constructed from bimaterial strips [9]. In the case of triangular units, in the idealized scenario, the mechanism requires triangles constructed from three pin-jointed rods where the base rod is made from a different and softer material than the other two. When such a triangle is placed in an atmosphere of positive (tensile) hydrostatic stress, the base rod expands to a larger extent than the other two, pulling them apart so that overall, the triangle gets shorter, i.e. exhibits negative linear compressibility in the direction perpendicular to the base. In the case of the chiral units, the mechanism requires the use of bimaterial ligaments made up of two materials having dissimilar mechanical properties, bonded together, which can curve when placed under pressure [11]. These ligaments must be connected together in such a way that the cooperative curving of the ligaments will result in an overall expansion of the system when this is placed in a medium of negative (compressive) hydrostatic stress. As shown elsewhere [8,9], such mechanisms can be employed to exhibit not only negative linear compressibility, but also an overall area or volumetric compressibility. However, for these two mechanisms to operate, the material must be porous so as to ensure that the fluid which is exerting the hydrostatic stress on the system can freely penetrate inside the system so as to permit the uneven contraction or expansions of the different components in the system. In addition to these systems, other structures which have also been reported to exhibit negative compressibility include systems operating through a wine-rack-type mechanism which can be used to explain the experimentally measured or predicted negative linear compressibility at the molecular level [1]. In this respect, it should be noted that although it is now obvious that such mechanisms have a very important role in generating negative linear compressibility,

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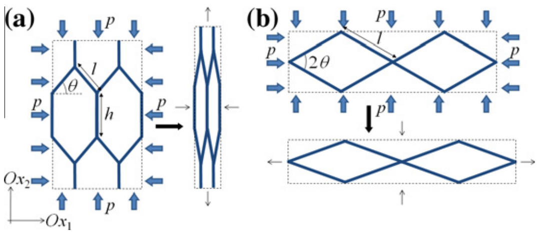

Figure 1. The proposed (a) hexagonal honeycomb and (b) wine-rack model which may exhibit negative linear compressibility when placed under a hydrostatic stress p.

no rigorous treatment of such systems has been presented so far to explain the necessary conditions for achieving negative linear compressibility. In view of this, here we will examine in detail through analytical modelling the possibility of achieving negative linear compressibility by non re-entrant hexagonal (when θ in Fig. 1 is positive) and wine-rack-type honeycombs; we will show that, under the right conditions, both systems may exhibit negative linear compressibility.

The on-axis linear and area compressibility of a two-dimensional (planar) system can be related to the compliance coefficients s_{ij}, more specifically to its on-axis Poisson's ratios ν_{ij} and Young's moduli E_i since:

$$\beta_{11} = s_{11} + s_{12} = \frac{1}{E_1} - \frac{\nu_{21}}{E_2} \quad (1)$$

$$\beta_{22} = s_{21} + s_{22} = \frac{1}{E_2} - \frac{\nu_{12}}{E_1} \quad (2)$$

These expressions clearly suggest that the on-axis linear compressibilities may assume negative values in cases when the Poisson's ratio is high and positive so that $\nu_{ij} > E_i/E_j$. Such conditions are not impossible to achieve, and as shown below they are indeed possible for hexagonal honeycombs deforming through changes in the angle between the ribs of the honeycomb (idealized hinging model). Hexagonal honeycombs have been extensively studied [15–18] in view of the ability of their re-entrant versions to achieve negative Poisson's ratios (auxetic behaviour). In particular, it has been shown that they can deform through three non-mutually exclusive deformation mechanisms, including flexure [15,16], stretching of the ribs and/or hinging of the ribs [17,18], where the on-axis Poisson's ratios ν^h_{ij} in the $Ox_i - Ox_j$ and Young's moduli E^h_i for loading in the Ox_i direction for the idealized hinging model are given by:

$$\nu^h_{12} = (\nu^h_{21})^{-1} = \frac{\cos^2(\theta)}{(h/l + \sin(\theta))\sin(\theta)} \quad (3)$$

$$E^h_1 = \frac{K_h\cos(\theta)}{b\sin^2(\theta)(h/l + \sin(\theta))} \qquad E^h_2 = \frac{K_h(h/l + \sin(\theta))}{b\cos^3(\theta)} \quad (4)$$

where, as shown in Figure 1a, h and l are the lengths of the vertical and inclined ribs, respectively; θ is the angle that the inclined ribs make with the horizontal (negative for re-entrant honeycombs and positive for non re-entrant honeycombs); b is the out-of-plane thickness of the honeycomb; and K_h is the hinging force constant.

It has also been shown that if such honeycombs deform solely through stretching of the ribs (idealized stretching model), the corresponding Poisson's ratios ν^s_{ij} and Young's moduli E^s_i are given by:

$$\nu^s_{12} = -\frac{\sin(\theta)}{h/l + \sin(\theta)} \qquad \nu^s_{21} = -\frac{\sin(\theta)(h/l + \sin(\theta))}{2h/l + \sin^2(\theta)} \quad (5)$$

$$E^s_1 = \frac{K_s}{b\cos(\theta)(h/l + \sin(\theta))}$$
$$E^s_2 = \frac{K_s(h/l + \sin(\theta))}{b\cos(\theta)(2h/l + \sin^2(\theta))} \quad (6)$$

where K_s is the stretching force constant, whilst for a honeycomb which deforms through concurrent hinging and stretching, the two single-mode models can be combined to obtain the resulting Poisson's ratios ν^{h+s}_{ij} and Young's moduli E^{h+s}_i since:

$$E^{h+s}_i = \left(\frac{1}{E^h_i} + \frac{1}{E^s_i}\right)^{-1}, \quad \nu^{h+s}_{ij} = E^{h+s}_i\left(\frac{\nu^h_{ij}}{E^h_i} + \frac{\nu^s_{ij}}{E^s_i}\right) \quad (7)$$

Using these equations, the on-axis linear compressibilities β_{11} and β_{22} in the Ox_1 and Ox_2 directions for the idealized hinging model become:

$$\beta^h_{11} = \frac{(h\sin(\theta) - l\cos(2\theta))b\tan(\theta)}{K_h l}$$
$$\beta^h_{22} = \frac{b\cos(\theta)(l\cos(2\theta) - h\sin(\theta))}{K_h(l\sin(\theta) + h)} \quad (8)$$

where in the range $-90° < \theta < 90°$, β^h_{11} is negative if $h/l < \cos(2\theta)/\sin(\theta)$, β^h_{22} is negative if $h/l > \cos(2\theta)/\sin(\theta)$ with $\beta^h_{11} = \beta^h_{22} = 0$ when $h/l = \cos(2\theta)/\sin(\theta)$. Note that the special case when $h = 0$, the system becomes equivalent to a wine-rack-type structure (Fig. 1b) and the compressibility expressions simplify to:

$$\beta^h_{11} = \frac{b}{K_h}\cos(2\theta)\tan(\theta) \qquad \beta^h_{22} = \frac{b}{K_h}\cos(2\theta)\cot(\theta) \quad (9)$$

where the sign of the compressibility is now simply dependent on θ where β^h_{11} is negative if $0 < \theta < 45°$, β^h_{22} is negative if $45° < \theta < 90°$ with $\beta^h_{11} = \beta^h_{22} = 0$ when $\theta = 45°$.

In the case of the idealized stretching model, the on-axis compressibilities are always positive and in the case of hexagonal honeycombs are given by:

$$\beta^s_{11} = \frac{b\cos(\theta)(2l\sin(\theta) + h)}{lK_s}$$
$$\beta^s_{22} = \frac{b\cos(\theta)(2l\sin^2(\theta) + h\sin(\theta) + 2h)}{K_s(l\sin(\theta) + h)} \quad (10)$$

whilst in case of the concurrent hinging and stretching models, the on-axis compressibilities may assume both positive or negative values and are given by:

$$\beta^{h+s}_{11} = \frac{b}{l}\left[\frac{(h\sin(\theta) - l\cos(2\theta))\tan(\theta)}{K_h} + \frac{(2l\sin(\theta) + h)\cos(\theta)}{K_s}\right] \quad (11)$$