Chapter 2
Micromechanical Models for Auxetic Materials

Abstract This chapter provides a survey of micromechanical models that seek to predict and explain auxetic behavior, based on re-entrant microstructures, nodule-fibril microstructure, 3D tethered-nodule model, rotating squares, rectangles, triangles and tetrahedrals models, hard cyclic hexamers model, missing rib models, chiral and anti-chiral models, interlocking hexagon model, and the “egg rack” model. All the micromechanical models exhibit a common trait—auxeticity is highly dependent on the microstructural geometry. In some of the micromechanical geometries, comparisons between analytical results have been made with experimental or computational results.

Keywords Analytical models • Computational models • Effective elastic properties • Geometrical models • Micromechanics

2.1 Introduction

Figure 1.3.2 summarizes a few typical models which have been adopted to explain auxetic behavior. This chapter explores the micromechanics for some of these models in greater detail, with special emphasis on the adopted geometrical models and the analytical closed-form solutions.

2.2 Re-entrant Open-Cell Microstructure

Masters and Evans (1996) proposed an auxetic behavior based on the traditional 2D re-entrant structure shown in Fig. 2.2.1a, which is a hexagonal array of honeycomb structure (Gibson and Ashby 1988). With reference to Fig. 2.2.1b, the honeycomb is auxetic if $\theta$ is positive (unit cell possesses re-entrant shape) and conventional if $\theta$
Fig. 2.2.1  a A 2D re-entrant structure, b geometry used by Smith et al. (2000), and a molecular re-entrant structure introduced by Evans et al. (1991)

is negative (unit cell possesses hexagonal shape), with the Poisson’s ratio and Young’s modulus in the direction of loading given by Smith et al. (2000)

\[ v_{12} = \frac{\sin \theta (h/l + \sin \theta)}{\cos^2 \theta} \quad (2.2.1) \]

and

\[ E_1 = k \frac{(h/l) + \sin \theta}{b \cos^3 \theta} \quad (2.2.2) \]
where the \( h \) is the half length of the horizontal rib, \( l \) is the length of the inclined rib, and \( t \) is the thickness of the rib, as shown in Fig. 2.2.1b, while \( b \) is the depth of the cell ribs not shown in Fig. 2.2.1b. The parameter \( k \) has been given as

\[
k = E_s b \left( \frac{t}{l} \right)^3
\]

(2.2.3)

where \( E_s \) is the Young’s modulus of the rib material. Results of this model are presented in Sect. 2.9 together with the missing rib model. It is also of interest to note that a similar structure has been introduced by Evans et al. (1991), as shown in Fig. 2.2.1c.

Based on the idealized re-entrant unit cell shown in Fig. 2.2.2a, Choi and Lakes (1995) proposed the corresponding geometry shown in Fig. 2.2.2b for analysis. The resultant Poisson’s ratio at infinitesimal strain is

\[
v_{\text{elastic}} = -\frac{\sin(\phi - \pi/4)}{\cos(\phi - \pi/4)}
\]

(2.2.4)

where the angle \( \phi \) is defined in Fig. 2.2.2b, while the Poisson’s ratio at large strain after plastic hinge formation is given as

\[
v_{\text{plastic}} = \frac{\cos(\phi - \pi/4) - \cos(\phi - \pi/4 - \theta)}{\sin(\phi - \pi/4) - \sin(\phi - \pi/4 - \theta)}
\]

(2.2.5)

where \( \theta \) refers to the clockwise angular rotation of cell rib BC.

The Poisson’s ratio variation upon strain during elastic-plastic deformation was given by Choi and Lakes (1995) as

\[
v_{\text{elasto-plastic}} = v_y - \varepsilon_{\text{ex}} \frac{1 - \cos \eta}{2\varepsilon_x}
\]

(2.2.6)

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Fig. 2.2.2  a An idealized re-entrant unit cell, and b a zoomed-in view of the geometry adopted by Choi and Lakes (1995). Reprinted by permission of SAGE
in which

\[ \varepsilon_x = \frac{1}{\sqrt{2}} \frac{\sin(\varphi - \pi/4) - \sin(\varphi - \pi/4 - \theta)}{1 + \sin(\pi/2 - \varphi)} = \frac{\varepsilon_{ex} \delta}{\delta_e} \tag{2.2.7} \]

and

\[ \eta = \frac{P_e}{P} \left( 3 - \frac{P}{P_e} - 2\sqrt{3 - 2\frac{P}{P_e}} \right) \tag{2.2.8} \]

where \( v_y \) is the Poisson’s ratio at initial yielding, \( \varepsilon_x \) is the strain in the x-direction, \( \varepsilon_{ex} \) is the x-component of strain at initial yielding, \( \delta \) is the deflection, \( \delta_e \) is the deflection at initial yielding, \( P \) is the load, and \( P_e \) is the load at initial yielding. A comparison between the predicted and measured Poisson’s ratio versus strain for copper foam is shown in Fig. 2.2.3 based on the assumption of \( \varepsilon_{ex} = 1 \% \).

### 2.3 Nodule Fibril Microstructure—Hinging, Flexure and Stretching Modes of Fibrils

The nodule-fibril microstructural model proposed by Alderson and Evans (1995) considers deformation by fibril hinging mode, fibril flexure mode and fibril stretching mode separately. With reference to Fig. 2.3.1, the idealized nodule takes
Fig. 2.3.1  Schematic diagram of the nodule-fibril (NF) model, showing a general parameters in a partially extended network, b fully densified network with $l = b/2$, $\alpha_0 = 90^\circ$, and undeformed, partially open networks resulting from c $l < b/2$ with nodules in contact in $x$ direction, d $l > b/2$ with nodules in contact in $y$ direction, and e negative fibril angle (Alderson and Evans 1995, 1997). (With kind permission from Springer Science+Business Media)
a rectangular shape with major axis length \( a \) and minor axis length \( b \), with the fibril geometry defined by its length \( l \) inclined at an angle \( \alpha \) to the \( x \)-axis. Under tensile stress in the \( x \)-direction, the fibrils hinge, thereby reducing the angle of \( \alpha \) until a minimum of \( \alpha = 0^\circ \).

Schematic diagrams for analyzing deformation by the fibril hinging mode under tension in the \( x \) direction and under compression in the \( y \) direction are shown in Fig. 2.3.2a, b respectively. Based on this analysis by Alderson and Evans (1995), the Poisson’s ratio and Young’s moduli due to fibril hinging were obtained as

\[
v_{xy} = -\frac{\cos \alpha (a + l \cos \alpha)}{\sin \alpha (b - l \sin \alpha)} = \frac{1}{v_{yx}}
\]

\[
E_x = \frac{K_h}{l^2 \sin^2 \alpha} \left( \frac{a + l \cos \alpha}{b - l \sin \alpha} \right)
\]

\[
E_y = \frac{K_h}{l^2 \cos^2 \alpha} \left( \frac{b - l \sin \alpha}{a + l \cos \alpha} \right)
\]

while the engineering Poisson’s ratio and engineering Young’s moduli were obtained as

\[
v_{xy}^e = -\frac{\cos \alpha (a + l \cos \alpha_0)}{\sin \alpha (b - l \sin \alpha_0)} = \frac{1}{v_{yx}^e}
\]
\[ E_x = \frac{K_h}{l^2 \sin^2 \alpha} \left( \frac{a + l \cos \alpha_0}{b - l \sin \alpha_0} \right) \quad (2.3.5) \]
\[ E_y = \frac{K_h}{l^2 \cos^2 \alpha} \left( \frac{b - l \sin \alpha_0}{a + l \cos \alpha_0} \right) \quad (2.3.6) \]

where the hinge force coefficient is defined from

\[ l \Delta F = K_h \Delta \alpha \quad (2.3.7) \]

for an angular change \( \Delta \alpha \) in response to a change in force \( \Delta F \) while \( \alpha_0 \) is the initial angle.

With reference to Fig. 2.3.2c, d, the analysis by Alderson and Evans (1995) based on fibril flexure gave the same expression of Poisson’s ratio arising from fibril hinging as described in Eqs. (2.3.1) and (2.3.4). The Young’s moduli due to fibril flexure were obtained as

\[ E_x = \frac{3K_f}{l^2 \sin^2 \alpha} \left( \frac{a + l \cos \alpha}{b - l \sin \alpha} \right) \quad (2.3.8) \]
\[ E_y = \frac{3K_f}{l^2 \cos^2 \alpha} \left( \frac{b - l \sin \alpha_0}{a + l \cos \alpha_0} \right) \quad (2.3.9) \]

while the engineering Young’s moduli were obtained as

\[ E_x^e = \frac{3K_f}{l^2 \sin^2 \alpha} \left( \frac{a + l \cos \alpha_0}{b - l \sin \alpha_0} \right) \quad (2.3.10) \]
\[ E_y^e = \frac{3K_f}{l^2 \cos^2 \alpha} \left( \frac{b - l \sin \alpha_0}{a + l \cos \alpha_0} \right) \quad (2.3.11) \]

where the flexure force coefficient is defined from

\[ K_f \Delta \theta = \Delta M = \frac{l \Delta F}{2} \quad (2.3.12) \]

and \( \Delta \theta \) is the small change (i.e. \( \Delta \theta = \tan \Delta \theta \)) in the slope of the midpoint of the fibril with reference to the fibril orientation, as indicated in Fig. 2.3.2c, d.

Figure 2.3.3 illustrates the fibril stretching mode of deformation. Based on this nomenclature, Alderson and Evans (1995) derived the Poisson’s ratio and Young’s moduli as follows

\[ v_{xy} = \frac{\sin \alpha(a + l \cos \alpha)}{\cos \alpha(b - l \sin \alpha)} = \frac{1}{v_{yx}} \quad (2.3.13) \]
Fig. 2.3.3 Fibril extension under tension of the nodule-fibril network in the x direction (Alderson and Evans 1995). With kind permission from Springer Science+Business Media

\[
E_x = \frac{K_s}{\cos^2 \alpha} \left( \frac{a + l \cos \alpha}{b - l \sin \alpha} \right) \\
E_y = \frac{K_s}{\sin^2 \alpha} \left( \frac{b - l \sin \alpha}{a + l \cos \alpha} \right)
\]  

(2.3.14)  

(2.3.15)

while the corresponding engineering Poisson’s ratio and Young’s moduli were obtained as

\[
\nu_{xy} = \frac{\sin \alpha (a + l \cos \alpha_0)}{\cos \alpha (b - l \sin \alpha_0)} = \frac{1}{\nu_{yx}} \\
E_{x}^e = \frac{K_s}{\cos^2 \alpha} \left( \frac{a + l \cos \alpha_0}{b - l \sin \alpha_0} \right) \\
E_{y}^e = \frac{K_s}{\sin^2 \alpha} \left( \frac{b - l \sin \alpha_0}{a + l \cos \alpha_0} \right)
\]  

(2.3.16)  

(2.3.17)  

(2.3.18)

where the stretching force coefficient is defined as

\[
K_s = \frac{\Delta F}{\Delta s}
\]  

(2.3.19)

for an extension of \(\Delta s\) in response to \(\Delta F\).

Comparison between the analytical models and experimental results are shown in Figs. 2.3.4 and 2.3.5a, b for polytetrafluoroethylene (PTFE), and Fig. 2.3.5c for ultra-high molecular weight polyethylene (UHMWPE). Observation of Alderson and Evans (1995) noted that as \(\alpha\) approaches \(0^\circ\) fibril stretching will become increasingly dominant, and this will have two effects: (a) the transition strain between the predominantly hinging and stretching modes will occur at a higher value of strain as a result of the increase in fibril length, and (b) the transition itself will become smeared over a range of strain.
The analysis by Alderson and Evans (1995) considers fibril hinging, flexure, and stretching separately, and found that fibril flexure and hinging result in exactly the same Poisson’s ratio values and Young’s modulus trends. Following up on this work, Alderson and Evans (1997) considered concurrent hinging and stretching deformation mechanisms to give the following properties based on loading in the x-direction

$$v_{xy} = \frac{[1 - l^2(K_s/K_h)]}{l^2(K_s/K_h) \sin^2 \alpha + \cos^2 \alpha} \sin \alpha \cos \alpha \left( \frac{a + l \cos \alpha}{b - l \sin \alpha} \right)$$ (2.3.20)

$$v'_{xy} = \frac{[1 - l^2(K_s/K_h)]}{l^2(K_s/K_h) \sin^2 \alpha + \cos^2 \alpha} \sin \alpha \cos \alpha \left( \frac{a + l_0 \cos \alpha}{b - l_0 \sin \alpha} \right)$$ (2.3.21)

$$E_x = \left( \frac{l^2 \sin^2 \alpha}{K_h} + \frac{\cos^2 \alpha}{K_s} \right)^{-1} \frac{a + l \cos \alpha}{b - l \sin \alpha}$$ (2.3.22)

$$E'_x = \left( \frac{l^2 \sin^2 \alpha}{K_h} + \frac{\cos^2 \alpha}{K_s} \right)^{-1} \frac{a + l_0 \cos \alpha}{b - l_0 \sin \alpha}$$ (2.3.23)

as well as in the y-direction

$$v_{yx} = \frac{[1 - l^2(K_s/K_h)]}{l^2(K_s/K_h) \cos^2 \alpha + \sin^2 \alpha} \sin \alpha \cos \alpha \left( \frac{b - l \sin \alpha}{a + l \cos \alpha} \right)$$ (2.3.24)

$$v'_{yx} = \frac{[1 - l^2(K_s/K_h)]}{l^2(K_s/K_h) \cos^2 \alpha + \sin^2 \alpha} \sin \alpha \cos \alpha \left( \frac{b - l_0 \sin \alpha}{a + l_0 \cos \alpha} \right)$$ (2.3.25)
Fig. 2.3.5  

(a) Experimental $v_{xy}$ versus $\varepsilon_x$ data (filled circle) for PTFE. Also shown are NF (hinging-plus-stretching) model calculations for $bla = 0.25$, $l = b/2$ and $\vartheta_0 = 90^\circ$. Fit to the $v_{xy}$ data (solid curve), fit to the $E^e_x$ data (dashed curve).

(b) Experimental $E^e_x$ versus $\varepsilon_x$ data (filled circle) for PTFE. NF model calculations for $bla = 0.25$, $l = 0.16a$ and $\vartheta_0 = 90^\circ$. Fit to the $E^e_x$ data (dotted curve). All NF model $E^e_x$ predictions were normalized to the peak experimental $E^e_x$ value of $E^e_x = 0.15$ GPa.

(c) Experimental $v_{yx}$ versus $\varepsilon_y$ data for UHMWPE by Alderson and Neale (1994) (filled circle). Also shown are NF (hinging-plus-stretching) model calculations for $a = b$ and $\vartheta_0 = 40^\circ$ for $l = 0.095b$ (dashed curve) (Alderson and Evans 1995). With kind permission from Springer Science+Business Media.
\[ E_y = \left( \frac{l^2 \cos^2 \alpha}{K_h} + \frac{\sin^2 \alpha}{K_s} \right)^{-1} \frac{b - l \sin \alpha}{a + l \cos \alpha} \] (2.3.26)

\[ E'_y = \left( \frac{l^2 \cos^2 \alpha}{K_h} + \frac{\sin^2 \alpha}{K_s} \right)^{-1} \frac{b - l_0 \sin \alpha_0}{a + l_0 \cos \alpha_0} \] (2.3.27)

For convenience Alderson and Evans (1997) defined an effective hinging force coefficient as

\[ K_{\text{eff}}^h = \frac{K_h}{l^2}. \] (2.3.28)

The elastic moduli were calculated for an arbitrary initial standard parameter set of \( b/a = 1, l = 0.25a, K_s/K_{\text{eff}}^h = 10, \alpha = 45^\circ \) and \( \alpha_0 = 45^\circ \). The effect of varying any one parameter on the behavior of the elastic moduli while keeping the others constant was examined. The effect of varying the force coefficients ratio, \( K_s/K_{\text{eff}}^h \), is shown in Fig. 2.3.6 for the Poisson’s ratio and Young’s modulus due to loading in the \( x \)-direction. The Young’s moduli data were normalized to the data calculated at \( \alpha = 45^\circ \), i.e.

\[ E'_x = \frac{E_x}{E_x(\alpha = 45^\circ)} \] (2.3.29)

because at \( \alpha = 45^\circ \) the Young’s modulus due to hinging is equal to that due to stretching when \( K_s = K_{\text{eff}}^h \).

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**Fig. 2.3.6** a \( v_{xy} \) versus \( \alpha \) for the NF model employing concurrent fibril hinging and stretching mechanisms; b Normalized Young’s modulus data \( E'_x \) versus \( \alpha \) for the NF model employing concurrent fibril hinging and stretching mechanisms; for each curve the data are normalized to the calculated value at \( \alpha = 45^\circ \), i.e. \( E'_x = E_x/E_x(\alpha = 45^\circ) \). For (a) and (b), curves are for \( K_s/K_{\text{eff}}^h = 0.01, 0.1, 1, 10, 100 \) with stretching and hinging mechanisms acting independently, and calculations were performed with \( b/a = 1 \) and \( l = 0.25a \) (Alderson and Evans 1997). With kind permission from Springer Science+Business Media
The effect of varying the geometrical parameters is illustrated in Fig. 2.3.7a. Figure 2.3.7b shows the variation of strain, in loading direction, with $\alpha$, $l_0/a$ and $\alpha_0$, with a critical angle, $\alpha_c$, as indicated in Fig. 2.3.1d, being defined as

![Graphs showing variation of strain with geometrical parameters](image)

**Fig. 2.3.7** a $v_{xy}$ trends for the NF model employing concurrent fibril hinging and stretching mechanisms calculated for a standard parameter set of $b/a = 1$, $K_s/K_{sh}^{eff} = 10$, $l = 0.25a$ and $\alpha = 45^\circ$. $v_{xy}$ versus $l/a$ (top), $v_{xy}$ versus $b/a$ (middle), and $v_{xy}$ versus $\alpha$ (bottom). b $\varepsilon_x$ trends under an $x$-directed load for the NF model employing concurrent fibril hinging and stretching mechanisms calculated for a standard parameter set of $b/a = 1$, $l_0 = 0.25a$, $\alpha_0 = 45^\circ$, $\alpha = 45^\circ$ and $K_s/K_{sh}^{eff} = 10$. $\varepsilon_x$ versus $\alpha$ with $K_s/K_{sh}^{eff} = 0.01, 0.1, 1, 10, 100$ and $\infty$ (hinging) (top), $\varepsilon_x$ versus $l_0/a$ with $\alpha = 60^\circ$ (middle), $\varepsilon_x$ versus $\alpha_0$ (bottom). Alderson and Evans (1997). With kind permission from Springer Science+Business Media.
\[
\sin \alpha_c = \frac{1}{2} \left( \frac{b}{l} \right).
\]  

(2.3.30)

From the plotted results, Alderson and Evans (1997) identified both the geometry and force coefficients involved in the deformation of the network microstructure as the determining factors of the elastic moduli.

Figure 2.3.8a shows that the elastic to plastic transition occurs when the fibril length has increased by 50% of the initial value. The curves also show the same

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**Fig. 2.3.8**  
(a) \(v_{xy}\) versus \(e_x\) for the NF model employing concurrent fibril hinging and stretching mechanisms. \(b/a = 1, \ l_0 = 0.25a, \ \alpha_0 = 90^\circ\), and \(K_s/K_h^{\text{eff}} = 2\) and \(20\) when \(l \leq 1.5l_0\), and \(K_s/K_h^{\text{eff}} = 0.5\) when \(l \geq 1.5l_0\).  
(b) \(v_{xy}\) versus \(e_x\) for the NF model employing fibril hinging (dashed curve) and concurrent fibril hinging and stretching (solid curves) mechanisms. Curves are for: “a” \(b = 0.25a, \ l = 0.125a, \ K_s/K_h^{\text{eff}} = 20\) (elastic) and \(K_s/K_h^{\text{eff}} = 1\) (plastic); “b” \(b = 0.4a, \ l = 0.14a, \ K_s/K_h^{\text{eff}} = 10\) (elastic) and \(K_s/K_h^{\text{eff}} = 0.65\) (plastic)). In all cases \(\alpha_0 = 90^\circ\) and \(K_s/K_h^{\text{eff}}\) is constant at the elastic or plastic value. Transition from elastic to plastic fibril extension was set to occur at \(l = 0.24a\). Experimental \(v_{xy}\) data for PTFE by Caddock and Evans (1989) are also shown (crosses).  
(c) \(E^e_x\) versus \(e_x\) for the NF model employing concurrent fibril hinging and stretching mechanisms. Model parameters as for (b). Experimental \(E^e_x\) data for PTFE are also shown (crosses). Model \(E^e_x\) data normalized to peak experimental value of \(E^e_x = 0.15\) GPa.  
(d) \(v_{xy}\) versus compressive strain \(\epsilon^c_x = -\epsilon_x\) for the NF model employing concurrent fibril hinging and stretching mechanisms (solid curve). Calculations are for \(b = a, \ l_0 = 0.09a\), and \(\alpha_0 = 40^\circ\). \(K_s/K_h^{\text{eff}} = 1.000\) throughout. Experimental \(v_{xy}\) data for UHMWPE are also shown (crosses). Alderson and Evans (1997). With kind permission from Springer Science+Business Media.
general trends, $v_{xy}$ becoming increasingly negative (from an initial value of zero at zero strain) as the strain increases, peaking at a strain of $e_x/C_25 = \alpha_0$ before decreasing towards $v_{xy} \approx 0$ as $e_x$ increases further. Comparison with experimental results of PTFE by Caddock and Evans (1989) are shown in Fig. 2.3.8b, c for $v_{xy}$ and $E_x^c$, respectively, while a comparison with experimental results of UHMWPE by Neale et al. (1993) and Alderson et al. (1997) is given in Fig. 2.3.8d (Alderson and Evans 1997). With kind permission from Springer Science+Business Media.

![Fig. 2.3.9](image)

**Fig. 2.3.9** a $\varepsilon_y$ versus $\varepsilon_x$ for the NF model employing concurrent fibril hinging and stretching mechanisms under an $x$-directed load. Calculations are for $b = 0.25a$, $l_0 = 0.125a$, $\alpha_0 = 90^\circ$ and $K_s/K_h^{\text{eff}} = 200$, 20, 10 and 5. Dashed curve corresponds to $K_s/K_h^{\text{eff}}$ arbitrarily decreasing from $K_s/K_h^{\text{eff}} = 20$ as $\varepsilon_x$ increases from $\varepsilon_x \approx 0.10$. 

b $\varepsilon_x^c$ versus $\varepsilon_y^c$ for the NF model employing concurrent fibril hinging and stretching mechanisms under a $y$-directed load. Calculations are for $b = a$, $l_0 = 0.09a$, $\alpha_0 = 40^\circ$ and $K_s/K_h^{\text{eff}} = 1,000$, 100, 20, 5 and 2. The dashed curve illustrates the effect of decreasing $K_s/K_h^{\text{eff}}$ from 1,000 to 2 in the strain range $0.036 < \varepsilon_x^c < 0.05$ (Alderson and Evans 1997).

2.4 Generalized 3D Tethered-Nodule Model

Based on the 3D tethered nodule, Gaspar et al. (2011) set up the following elastic property equations on the basis of idealized stretching model, the idealized $\phi$ hinging model, and the idealized $\theta$ hinging model. With reference to Fig. 2.4.1a, b, the projections along the $x_i$ directions (for $i = 1, 2, 3$) are $X_1$, $X_2$ and $X_3$ respectively, with the connecting rods possessing equal length $l$ while $\phi$ is the angle between the rods and the $x_3$ direction and $\theta$ is the angle that the projection of the rod in the $x_1 - x_2$ plane makes with the $x_1$ direction.

For an incremental force of $dF_i$, $dF_\theta$ and $dF_\phi$ that causes an incremental change of $dl$, $d\theta$ and $d\phi$ respectively, the stiffness $k_i$, $k_\theta$ and $k_\phi$ are defined as
Gaspar et al. (2011) obtained the following elastic moduli

\[ k_l = \frac{dF_l}{dl} \]  
\[ k_\theta = \frac{dM_\theta}{d\theta} = \frac{ldF_\theta}{d\theta} \]  
\[ k_\phi = \frac{dM_\phi}{d\phi} = \frac{ldF_\phi}{d\phi} \]

respectively. Gaspar et al. (2011) obtained the following elastic moduli

\[ E_1' = \frac{2k_l}{\cos^2 \theta \sin^2 \phi} \left( \frac{X_1}{X_2 X_3} \right) \]
\[ E'_2 = \frac{2k_j}{\sin^2 \theta \sin^2 \phi} \left( \frac{X_2}{X_1 X_3} \right) \]  
(2.4.5)

\[ E'_3 = \frac{2k_j}{\cos^2 \phi} \left( \frac{X_3}{X_1 X_2} \right) \]  
(2.4.6)

\[ v'_{31} = (v'_{13})^{-1} = -\cos \theta \tan \phi \left( \frac{X_3}{X_1} \right) \]  
(2.4.7)

\[ v'_{32} = (v'_{23})^{-1} = -\sin \theta \tan \phi \left( \frac{X_3}{X_2} \right) \]  
(2.4.8)

\[ v'_{12} = (v'_{21})^{-1} = -\tan \phi \left( \frac{X_1}{X_2} \right) \]  
(2.4.9)

Based on idealized stretching model, the following elastic moduli

\[ E_1^\phi = \frac{2k_\phi}{l^2 \cos^2 \theta \cos^2 \phi} \left( \frac{X_1}{X_2 X_3} \right) \]  
(2.4.10)

\[ E_2^\phi = \frac{2k_\phi}{l^2 \sin^2 \theta \cos^2 \phi} \left( \frac{X_2}{X_1 X_3} \right) \]  
(2.4.11)

\[ E_3^\phi = \frac{2k_\phi}{l^2 \sin^2 \phi} \left( \frac{X_3}{X_1 X_2} \right) \]  
(2.4.12)

\[ v_{31}^\phi = (v_{13}^\phi)^{-1} = \cos \theta \cos \phi \left( \frac{X_3}{X_1} \right) \]  
(2.4.13)

\[ v_{32}^\phi = (v_{23}^\phi)^{-1} = \sin \theta \cos \phi \left( \frac{X_3}{X_2} \right) \]  
(2.4.14)

\[ v_{12}^\phi = (v_{21}^\phi)^{-1} = -\tan \phi \left( \frac{X_1}{X_2} \right) \]  
(2.4.15)

Based on idealized \( \phi \) hinging model, and the following elastic moduli

\[ E_1^\theta = \frac{2k_\theta}{l^2 \sin^2 \theta \sin \phi} \left( \frac{X_1}{X_2 X_3} \right) \]  
(2.4.16)

\[ E_2^\theta = \frac{2k_\theta}{l^2 \cos^2 \theta \sin \phi} \left( \frac{X_2}{X_1 X_3} \right) \]  
(2.4.17)

\[ v_{12}^\theta = (v_{21}^\theta)^{-1} = \cot \phi \left( \frac{X_1}{X_2} \right) \]  
(2.4.18)

Based on idealized \( \theta \) hinging model (Fig. 2.4.2).
Fig. 2.4.2 Phase diagrams showing regions of negative Poisson’s ratio: a for fibril stretching only, b for $\phi$-deformation only, and c for $\theta$-bending only by Gaspar et al. (2011). With kind permission from Springer Science+Business Media
The elastic moduli, taking into consideration all three modes of deformation are therefore given by Gaspar et al. (2011) as

\[
\begin{align*}
\frac{1}{E_1} &= \frac{X_2 X_3}{2X_1} \left( \frac{\cos^2 \theta \sin^2 \phi}{k_l} + \frac{l^2 \cos^2 \theta \cos^2 \phi}{k_\phi} + \frac{l^2 \sin^2 \theta \sin \phi}{k_\theta} \right) \\
\frac{1}{E_2} &= \frac{X_1 X_3}{2X_2} \left( \frac{\sin^2 \theta \sin^2 \phi}{k_l} + \frac{l^2 \sin^2 \theta \cos^2 \phi}{k_\phi} + \frac{l^2 \cos^2 \theta \sin \phi}{k_\theta} \right) \\
\frac{1}{E_3} &= \frac{X_1 X_2}{2X_3} \left( \frac{\cos^2 \phi}{k_l} + \frac{l^2 \sin^2 \phi}{k_\phi} \right)
\end{align*}
\] (2.4.19) (2.4.20) (2.4.21)

\[
\begin{align*}
\nu_{12} &= \frac{X_1}{X_2} \frac{\sin \theta \sin \phi}{k_l} + \frac{l^2 \sin \theta \cos \phi \cot \phi}{k_\phi} - \frac{l^2 \sin \theta}{k_\theta} \\
\nu_{21} &= \frac{X_2}{X_1} \frac{\cos \theta \sin \phi}{k_l} + \frac{l^2 \cos \theta \cos \phi \cot \phi}{k_\phi} + \frac{l^2 \cos \theta}{k_\theta} \\
\nu_{13} &= \frac{X_1}{X_3} \frac{\cos \phi}{k_l} - \frac{l^2 \cos \phi}{k_\phi} \\
\nu_{23} &= \frac{X_2}{X_3} \frac{\cos \theta \sin \phi}{k_l} + \frac{l^2 \cos \theta \cos \phi \cot \phi}{k_\phi} + \frac{l^2 \cos \theta \tan \theta}{k_\theta} \\
\nu_{31} &= \frac{X_3}{X_1} \frac{\cos \theta \sin \phi}{k_l} + \frac{l^2 \cos \theta \sin \phi}{k_\phi} \\
\nu_{32} &= \frac{X_3}{X_2} \frac{\sin \theta \sin \phi}{k_l} - \frac{l^2 \sin \theta \sin \phi}{k_\phi}.
\end{align*}
\] (2.4.22) (2.4.23) (2.4.24) (2.4.25) (2.4.26) (2.4.27)

### 2.5 Rotating Squares and Rectangles Models

An early account on auxetic behavior arising from the rotation of connected squares was given by Grima and Evans (2000), which exhibits \( \nu = -1 \). Using the geometrical model displayed in Fig. 2.5.1a, they obtained a stress strain relationship in 2D
In general, the compliance matrix in Eq. (2.5.1) is expressed as

\[
\begin{bmatrix}
\varepsilon_1 \\
\varepsilon_2 \\
\gamma_{12}
\end{bmatrix} = 
\begin{bmatrix}
s_{11} & s_{12} & s_{13} \\
s_{21} & s_{22} & s_{23} \\
s_{31} & s_{32} & s_{33}
\end{bmatrix}
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\tau_{12}
\end{bmatrix}.
\]

(2.5.1)

For the particular case of rigid rotating squares of sides \( l \) and rotational stiffness constant of the hinge \( K_h \), Grima and Evans (2000) gave the corresponding compliance matrix

\[
S = \begin{bmatrix}
\frac{1}{E_1} & -\frac{\nu_{12}}{E_1} & \frac{\eta_{12}}{G_{12}} \\
-\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & \frac{\eta_{12}}{G_{12}} \\
\frac{\eta_{12}}{G_{12}} & \frac{\eta_{12}}{G_{12}} & \frac{1}{G_{12}}
\end{bmatrix}
\]

(2.5.2a)

where \( \eta_{ij} \) are the shear coupling coefficients. The effective Young’s modulus is

\[
E = \frac{8K_h}{z l^2 (1 - \sin \theta)}
\]

(2.5.3)

in which \( \theta \) is the angle defined in Fig. 2.5.1b and \( z \) is the thickness of the squares. Extending on this early work, Grima et al. (2007) investigated the auxetic behavior of semi-rigid rotating squares as shown in Fig. 2.5.2.
The analytical model for the on-axis elastic moduli were obtained by Grima et al. (2007) as

\[ v_{12} = v_{21} = -\cot\left(\frac{\psi_1}{2}\right) \tan\left(\frac{\psi_2}{2}\right) \left[ 1 + 4\left(\frac{k_{\psi}}{k_{\phi}}\right)\right]^{-1} \]  

\[ E_1 = E_2 = \frac{8k_{\psi}(k_{\phi} + 2k_{\psi})}{l_{d}^2 z(k_{\phi} + 4k_{\psi})} \frac{\sin\left(\frac{\psi_2}{2}\right)}{\sin\left(\frac{\psi_1}{2}\right) \cos^2\left(\frac{\psi_2}{2}\right)} \]  

\[ G_{12} = \frac{k_{\phi}}{\frac{1}{l_{d}^2 z} \sin\left(\frac{\psi_1}{2}\right) \sin\left(\frac{\psi_2}{2}\right) \sin \phi_1} \]  

where \( l_d \) is the diagonal length of the square (i.e. AC or BD in Fig. 2.5.2), while \( k_{\psi} \) and \( k_{\phi} \) are the rotational stiffness constants that restrain changes to the angles \( \psi \) and \( \phi \), respectively, and \( z \) is the thickness of the squares. At zero strain (i.e. \( \psi_1 = \psi_2 = \psi \)) and initial angle of \( \phi = \pi/2 \), the elastic moduli expressions simplify to

\[ v_{12} = v_{21} = -\left[ 1 + 4\left(\frac{k_{\psi}}{k_{\phi}}\right)\right]^{-1} \]  

\[ E_1 = E_2 = \frac{8k_{\psi}(k_{\phi} + 2k_{\psi})}{l_{d}^2 z(k_{\phi} + 4k_{\psi})} \sec^2\left(\frac{\psi}{2}\right) \]  

\[ (*) \text{ For analytical model:} \]

\[ |AC| = |BD| = L_d \]

\[ \psi_1 = \psi_3, \; \psi_2 = \psi_4, \; \phi_1 = \phi_3 \text{ and } \phi_2 = \phi_4. \]
\[ G_{12} = \frac{k_{\phi}}{E_d} \left[ \sin^2 \left( \frac{\Psi}{2} \right) \right]^{-1}. \] 

The off-axis elastic moduli at an angle \( \zeta \) around the third direction are given by Grima et al. (2007) as

\[ \frac{1}{E'_1} = \frac{m^4}{E_1} + \frac{n^4}{E_2} - m^2 n^2 \left( 2 \frac{v_{12}}{E_1} - \frac{1}{G_{12}} \right) \]  

(2.5.10)

\[ v_{12}' = E_1' \left[ (m^4 + n^4) \frac{v_{12}}{E_1} - m^2 n^2 \left( \frac{1}{E_1} + \frac{1}{E_2} - \frac{1}{G_{12}} \right) \right] \]  

(2.5.11)

\[ \frac{1}{G_{12}'} = \frac{m^4 + n^4}{G_{12}} + 2m^2 n^2 \left( \frac{2}{E_1} + \frac{4v_{12}}{E_1} + \frac{1}{G_{12}} \right) \]  

(2.5.12)

where \( m = \cos(\zeta) \) and \( n = \sin(\zeta) \). Figure 2.5.3 shows the effect of \( k_{\psi} \) and \( k_{\phi} \) in influencing the off-axis Poisson’s ratio \( v_{12}' \), while Fig. 2.5.4 compares the results of \( v_{12}' \) based on analytical model and molecular modeling results.

While the deformation by Grima et al. (2007) considers a change in the shape of the rotating squares, an alternate mode of deformation was later proposed by Grima et al. (2008) which deform solely through changes in length of the sides of the squares, i.e., the squares change their side lengths to become rectangles or squares of different sizes without changing the angles in the system. For this analysis, two possible orientations have been identified, as furnished in Fig. 2.5.5.

Fig. 2.5.3  Off-axis plots for various combinations of \( k_{\psi} \) and \( k_{\phi} \) at \( \psi = 145^\circ \) (Grima et al. 2007). With kind permission from John Wiley & Sons
Fig. 2.5.4 A comparison of the off-axis Poisson’s ratios $\nu^{\zeta}_{12}$ for THO as predicted by molecular modeling (MM) using the Burchart force-field and the analytical model (AM) by Grima et al. (2007). With kind permission from John Wiley & Sons.

Fig. 2.5.5 The unit cells used to derive the mechanical properties of the ‘stretching squares’ model for a Orientation I and b Orientation II. c The geometric relation between the two orientations (Grima et al. 2008). With kind permission from Springer Science+Business Media.
Suppose $k_s$ is the stretching force constant per unit length of the “beam”, which is a side of a square, and $z$ is the thickness of the square, then with reference to Fig. 2.5.6, the elastic moduli have been given by Grima et al. (2008) as

\begin{align}
\nu_{12}^I &= \nu_{21}^I = -\sin \theta \\
E_1^I &= E_2^I = \frac{2k_s}{z} \\
G_{12}^I &= \frac{k_s}{z(1 + \sin \theta)}
\end{align}

for on-axis Orientation I, and

---

**Fig. 2.5.6** One-fourth of an Orientation I unit cell showing dimensions (top left) and forces (top right), as well as an Orientation II unit cell showing dimensions (bottom left) and forces (bottom right) by Grima et al. (2008). With kind permission from Springer Science+Business Media.
\[ \nu_{12}^{II} = \nu_{21}^{II} = 0 \quad (2.5.16) \]
\[ E_1^{II} = E_2^{II} = \frac{2k_s}{z(1 + \sin \theta)} \quad (2.5.17) \]
\[ G_{12}^{II} = \frac{k_s}{z(1 - \sin \theta)} \quad (2.5.18) \]

for on-axis Orientation 2.

Results for the elastic moduli on both orientations are shown in Fig. 2.5.7 at \( k_s = 1 \) and \( z = 1 \). From Eqs. (2.5.13) to (2.5.18), Grima et al. (2008) summarized the elastic properties in terms of compliance matrices as

\[
S^I = \frac{z}{2k_s} \begin{bmatrix}
1 & \sin \theta & 0 \\
\sin \theta & 1 & 0 \\
0 & 0 & 2 + 2 \sin \theta
\end{bmatrix} \quad (2.5.19)
\]

for Orientation I, and

\[
S^{II} = \frac{z}{2k_s} \begin{bmatrix}
1 + \sin \theta & 0 & 0 \\
0 & 1 + \sin \theta & 0 \\
0 & 0 & 2 - 2 \sin \theta
\end{bmatrix} \quad (2.5.20)
\]

for Orientation II.

**Fig. 2.5.7** The variation of the Poisson’s ratios, Young’s moduli and shear moduli with the angle between the squares \( \theta \) when the system is loaded in **a** Orientation I and **b** Orientation II. It is assumed that \( k_s = 1 \) and \( z = 1 \) (Grima et al. 2008). With kind permission from Springer Science+Business Media
The off-axis elastic moduli were also given by Grima et al. (2008) as

\[ v_{12}^{\gamma} = -\frac{\cos^2(2\zeta) \sin \theta}{1 + \sin^2(2\zeta) \sin \theta} \]  

(2.5.21)

\[ E_1^{\gamma} = -\frac{2k_s}{z[1 + \sin^2(2\zeta) \sin \theta]} \]  

(2.5.22)

\[ G_{12}^{\gamma} = -\frac{k_s}{z[1 + \cos(4\zeta) \sin \theta]} \]  

(2.5.23)

where \( \zeta = 0^\circ \) and \( \zeta = 45^\circ \) correspond to Orientations I and II respectively. Figure 2.5.8 shows the off-axis elastic moduli plots.

In the case of auxetic behavior from rotating rectangles, as illustrated in Fig. 2.5.9(a), Grima et al. (2004) derived the following elastic properties

\[ v_{21} = \frac{1}{v_{12}} = \frac{a^2 \sin^2\left(\frac{\theta}{2}\right) - b^2 \cos^2\left(\frac{\theta}{2}\right)}{a^2 \cos^2\left(\frac{\theta}{2}\right) - b^2 \sin^2\left(\frac{\theta}{2}\right)} \]  

(2.5.24)

\[ E_1 = 8K_h \frac{a \cos\left(\frac{\theta}{2}\right) + b \sin\left(\frac{\theta}{2}\right)}{[a \cos\left(\frac{\theta}{2}\right) + b \sin\left(\frac{\theta}{2}\right)][-a \sin\left(\frac{\theta}{2}\right) + b \cos\left(\frac{\theta}{2}\right)]^2} \]  

(2.5.25)

\[ E_2 = 8K_h \frac{a \sin\left(\frac{\theta}{2}\right) + b \cos\left(\frac{\theta}{2}\right)}{[a \cos\left(\frac{\theta}{2}\right) + b \sin\left(\frac{\theta}{2}\right)][a \cos\left(\frac{\theta}{2}\right) - b \sin\left(\frac{\theta}{2}\right)]^2} \]  

(2.5.26)

based on the nomenclature furnished in Fig. 2.5.9b.

These property expressions are based on unit thickness, \( z = 1 \), and are reduced to the particular case of rotating square when \( a = b = l \) is substituted into Eqs. (2.5.24)–(2.5.26), i.e. Equation (2.5.24) simplify to \( v = -1 \) when \( a = b \) and both Eqs. (2.5.25) and (2.5.26) become Eq. (2.5.3) by substituting \( a = b = l \) and \( z = 1 \). Figure 2.5.10 shows the variation of Poisson’s ratio and the dimensionless Young’s moduli for aspect ratio of \( a/b = 2 \) using Eqs. (2.5.24) to (2.5.26).

For the case of connected different-sixed squares and rectangles, Grima et al. (2011) show that such systems can exhibit scale-independent auxetic behavior for stretching in particular directions, with Poisson’s ratios being dependent on the shape and relative size of different rectangles in the model and the angle between them.

A real structure that exhibits similar mode of deformation was given by Taylor et al. (2013) for hole aspect ratio \( a/b \) that is sufficiently large and \( L_{\text{min}}/L_0 \) ratio that is sufficiently low, as shown in the simulated results (Fig. 2.5.11). Experimental validation on the finite element method (FEM) simulation’s horizontal and vertical displacements has also been performed by Taylor et al. (2013) using digital image correlation (DIC), as shown in Fig. 2.5.12.
Fig. 2.5.8 Off-axis plots of a Poisson’s ratio, b Young’s modulus, and c shear modulus of the stretching mechanism at varying degrees of openness, assuming $k_s = 1$ and $z = 1$ (Grima et al. 2008). With kind permission from Springer Science+Business Media.
Fig. 2.5.9  a Auxetic behavior from rotating rectangles, and b dimensions adopted by Grima et al. (2004)
2.6 Rotating Triangles Models

In addition to the rotating square model, Grima and Evans (2006) also pioneered the study on auxetic behavior using rotating triangles, as shown in Fig. 2.6.1a. Based on the schematics in Fig. 2.6.1b and adopting $K_h$ and $l$ as the rotational stiffness coefficient and length of the triangle side, respectively, Grima and Evans (2006) obtained the following elastic properties for rotating rigid triangles:

$$v_{12} = v_{21} = -1$$

(2.6.1)

and

$$E_1 = E_2 = \frac{4\sqrt{3}}{l^2} \frac{K_h}{\left[1 + \cos\left(\frac{\pi}{3} + \theta \right)\right]}^{-1}.$$  (2.6.2)

Sheets made from easily available conventional non-crystalline materials which contain star or triangular shaped perforations were simulated through FE models and were shown by Grima et al. (2010) to be capable of exhibiting auxetic behavior,
Fig. 2.5.11  a Results of the numerical investigation on the effect of the hole aspect ratio \( a/b \) for an infinite periodic square array in an elastic matrix. Four different values of porosity are considered. The RVE considered in the analysis is shown as an inset. b All data collapse on a single curve when the Poisson’s ratio is plotted as a function of \( L_{\text{min}}/L_0 \) (Taylor et al. 2013). With kind permission from John Wiley & Sons.
Fig. 2.5.12 Contour maps for the horizontal ($u_x$) and vertical ($u_y$) component of the displacement field. Numerical (left) and experimental (right) results are quantitatively compared, showing excellent agreement. In (a) and (b), the applied strain is 0.34 %, while in (c) and (d), the applied strain is 0.07 %. Note that gray areas on experimental results show regions where DIC data could not be obtained (Taylor et al. 2013). With kind permission from John Wiley & Sons.
a property which may be observed for loading in both tension and compression. An attempt was then made to explain this behavior in terms of analytical models based on “rotating rigid triangles” and they also showed that through careful choice of the shape and density of the perforations, one may control the magnitude and sign of the Poisson’s ratio. This observation provides an easy and cost-effective method for the manufacture of systems at any scale which can be tailor made to exhibit particular values of the Poisson’s ratio (auxetic or non-auxetic) so as to fit particular practical applications (Grima et al. 2010). A model based on scalene rigid triangles that rotate relative to one other was introduced and analyzed by Grima et al. (2012).

It was demonstrated that this model can give a very wide range of Poisson’s ratio values, the sign and magnitude of which depends on the shape of the triangles and the angles between them. An advantage of this model is that it is very generic and could possibly be employed for elucidating the behavior in various types of materials, such as auxetic foams and their relative surface density (Grima et al. 2012).

Chetcuti et al. (2014) proposed an extended model which not only allows for relative rotation of the units (joints), represented by non-equilateral triangular units, but also for differing amount of material at the joints as well as deformation of the joints themselves, a scenario that is more representative of real auxetic foams. This model shows that, by permitting deformation mechanisms other than rotation of the
triangles, the predicted extent of auxeticity decreases when compared to the equivalent idealized rotating rigid triangles model, thus resulting in more plausible predictions of the Poisson’s ratios. Furthermore, Chetcuti et al. (2014) showed that in the manufacturing process, a minimum compression factor, which is dependent on the amount of materials at the joints, is required to obtain an auxetic foam from a conventional foam, as one normally observed in experimental work on foams.

2.7 Tetrahedral Framework Structure

A 3D version to the rotating squares, rectangles and triangles has been performed by Alderson and Evans (2001) in order to understand the auxetic properties of $\alpha$-cristobalite via concurrent rotation and dilatation. The unit cell employed is tetragonal and contains four regular tetrahedron of uniform size, with edge length $l$, as depicted in Fig. 2.7.1a. The tetrahedra are connected at the corners such that in the extended network each corner is shared between two tetrahedral. Each tetrahedral is tilted about its tilt axis by an angle $\delta$, as indicated in Fig. 2.7.1b, c, with

![Diagram](image)

**Fig. 2.7.1** a Unit cell for the tetrahedral framework by Alderson and Evans (2001), defining the geometrical parameters and coordinate system. The unit cell contains four tetrahedral: A, B, C and D. b $x_3$-[-110] projection of the unit cell, showing tetrahedral axes and “untilted” tetrahedron (B) to define tilt angle $\delta$. c $x_3$-[-110] projection of the unit cell, showing tetrahedral axes and “untilted” tetrahedron (C) to define tilt angle $\delta$ (Alderson and Evans 2001). With kind permission from Springer Science+Business Media
\[ \delta = 0 \] corresponding to the situation where the top and bottom edges of each tetrahedron are perpendicular to the \( x_3 \) axis.

In the rotating tetrahedral model (RTM), the tetrahedra are assumed to be rigid and free to rotate cooperatively around the tilt axis defining \( \delta \), whilst maintaining network connectivity, as shown in Fig. 2.7.2. In other words, the application of an external load results in a variation in \( \delta \) (Alderson and Evans 2001). This mode of deformation is an extension of previous models, in which rigid SiO\(_4\) tetrahedral rotation was used as a model for lattice parameter changes in silica structures undergoing phase transitions or thermal expansion.

In the second mode of deformation, which is termed the dilating tetrahedral model (DTM) by Alderson and Evans (2001), the tetrahedra are assumed to be fixed in orientation but free to deform by changing size (while maintaining tetrahedral regularity) in response to an applied load, i.e. \( l \) varies (Fig. 2.7.3). 2D analogies of this can be found in Rothenburg et al. (1991) and Milton (1992).

The third mode is a combination of RTM and DTM concurrently, hence the concurrent tetrahedral model (CTM). The Poisson’s ratio \( \nu_{ij} \) for each mode was thus derived using the following constraints:
RTM : $dl = 0$ \hspace{1cm} (2.7.1)

DTM : $d\delta = 0$ \hspace{1cm} (2.7.2)

CTM : $l \frac{d\delta}{dl} = \kappa$ \hspace{1cm} (2.7.3)

where $\kappa$ is a weight parameter determining the relative strengths of the two concurrent deformation mechanisms. Alderson and Evans (2001) obtained

$v_{12} = v_{21} = -1$ \hspace{1cm} (2.7.4)

for DTM, RTM and hence also for CTM modes of deformation, while
based on the DTM mode of deformation,
\[ v_{31} = -1 \]  \hspace{1cm} (2.7.5)

based on the RTM mode of deformation, and
\[ v_{31} = -\frac{\cos \delta}{1 + \cos \delta} \]  \hspace{1cm} (2.7.6)

for the CTM.

A particular feature of CTM is that there exists a range of \( \kappa \) values for any given value of \( \delta \) for which positive values of \( v_{31} \) are realized, even though the two mechanisms in the model are each auxetic when acting independently, as shown in Fig. 2.7.4 (Alderson and Evans 2001).

### 2.8 Hard Cyclic Hexamers Model

The occurrence of negative Poisson’s ratio in 2D system was suggested in the case of hard cyclic hexamers by Wojciechowski (1987) using Monte Carlo method. Wojciechowski (1987) commented that at high densities the molecules form a “tilted phase”, whereby their centers of mass vibrate around sites of a hexagonal lattice and their axes librate around directions slightly rotated with reference to the crystal axes. See Fig. 2.8.1 for the definition of molecular axis, which joins the molecular center of mass and the point of contact between adjacent atoms.
When the ratio of the actual area to the area of the system at close packing exceeds a particular value, the system transforms to the straight phase, i.e. the lattice of the centers of mass remains hexagonal but the mean directions of molecular axes are now oriented with the crystal axes. In addition to vibrational and librational motions these molecules also experience “jump-like” reorientations of about $\pi/3$ (Branka et al. 1982). Wojciechowski (1987) gave the following compliance:

$$S_{11} = \frac{C_{11}}{C_{11} - C_{12}} = \frac{1}{16\lambda_1} + \frac{1}{8\lambda_2}$$

(2.8.1)

$$S_{12} = -\frac{C_{11}}{C_{11} - C_{12}} = \frac{1}{16\lambda_1} - \frac{1}{8\lambda_2}$$

(2.8.2)

$$S_{66} = \frac{1}{C_{66}} = \frac{1}{2\lambda_2}$$

(2.8.3)

in which the quantities $\lambda_1$ and $\lambda_2$ can be calculated upon experimental measurement of $C_{11}$ and $C_{66}$. It is known the following compliance

$$S_{12} = S_{11} - \frac{1}{2}S_{66}$$

(2.8.4)

typically possesses negative values, thereby indicating positive Poisson’s ratio. Hence Wojciechowski (1987) discovered an auxetic case in which $S_{12}$ is a positive value for the tilted phase. Wojciechowski (1989) then studied a 2D lattice model of hexagonal molecules on a triangular lattice interacting through a nearest-neighbor n-inverse-power site-site potential, which reveals negative Poisson ratio at high densities when the anisotropy non-convexity of the molecules is substantial, and proposed that such a behavior could be observed in some real systems. In a related investigation using a simple free-volume (FV) approximation, Wojciechowski and Branka (1989) examined a 2D system of hard cyclic hexamers with negative

![Molecular axis](image.png)

Fig. 2.8.1  Schematic diagram of a hard cyclic hexamer, with the molecular axis indicated
Poisson ratio in a high-density crystalline phase, in which the FV approximation and a lattice model indicate the crucial role of broken mirror symmetry for the observed auxeticity.

2.9 Missing Rib Models

A missing rib model was proposed by Smith et al. (2000) for modeling the elastic properties of auxetic foams. The missing rib model is called as such because its idealized microstructure is derived from the intact model (which is conventional) and the removal of some ribs leads to the cut version, or the missing rib model, which is auxetic. See Fig. 2.9.1 (top). With reference to the Fig. 2.9.1 (bottom left), Smith et al. (2000) obtained the following elastic moduli

\[
\nu_{21} = \frac{1}{\nu_{12}} = \tan^2 \left( \frac{\gamma}{2} \right)
\]

(2.9.1)

Fig. 2.9.1 The idealized networks of the intact version (top left) and the cut version (top right) with the unit cells shaded, as well as the unit cells chosen for the intact version (bottom left) and cut version (bottom right) along with their geometrical parameters (Smith et al. 2000). With kind permission from Elsevier
for the intact model, where $k_\zeta$ is the spring constant that restraints the change to the angle $\zeta$.

With reference to Fig. 2.9.1 (bottom right), Smith et al. (2000) obtained the following elastic moduli

\[ E_1 = \frac{4k_\zeta}{a^2} \cot \left( \frac{\zeta}{2} \right) \csc^2 \left( \frac{\zeta}{2} \right) \]  
\[ E_2 = \frac{4k_\zeta}{a^2} \tan \left( \frac{\zeta}{2} \right) \sec^2 \left( \frac{\zeta}{2} \right) \]  

for the missing rib model, where $k_\theta$ is the spring constant that restrains the change to the angle $\theta$.

A Poisson’s ratio function comparison between the hexagonal model, as described in Eq. (2.2.1) for both conventional and auxetic foams with the intact model, as well as the intact and missing rib models, as described by Eqs. (2.9.1) and (2.9.4) respectively, with experimental results is shown in Fig. 2.9.2. The values of $\theta$ in the hexagonal model are obtained when fitted to the conventional and auxetic foams, as furnished in Table 2.9.1.

The true stress versus true strain behavior of both the honeycomb and the rib model by Smith et al. (2000) are shown in Fig. 2.9.3 using the best fit predictions.

---

**Fig. 2.9.2** Poisson’s function and the true strain data of the foam specimens by Smith et al. (2000). With kind permission from Elsevier.
The conventional foam possesses a higher Young’s modulus as expected. More importantly, Smith et al. (2000) noted that the traditional 2D honeycomb model by Masters and Evans (1996) is valid for describing the strain-dependent behavior of conventional foams but not for auxetic ones; i.e. the missing rib model caters to the realistic cell geometries.

Following up on this work, Gaspar et al. (2005) compared the behavior of two conventional and two auxetic honeycomb structures, as shown in Fig. 2.9.4(a). Based on the test procedure shown in Fig. 2.9.4(b), Gaspar et al. (2005) obtained a set of experimental data for the measured angles of \( \zeta \) and \( \phi \), as shown in Fig. 2.9.4 (d). Plots of the Poisson’s ratio versus strain in the loading direction are shown in Fig. 2.9.4(c).

### Table 2.9.1 Values of the parameters used to calculate the Poisson’s function data in Fig. 2.9.2 for the hexagonal array honeycomb (hexagonal shape for conventional and re-entrant shape for auxetic foams), as well as the intact and missing rib models for the conventional and re-entrant foams respectively by Smith et al. (2000)

<table>
<thead>
<tr>
<th>Honeycomb array</th>
<th>Hexagonal shape (conventional)</th>
<th>Re-entrant shape (auxetic)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( h )</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>( l )</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \theta )</td>
<td>( 19.2^\circ )</td>
<td>( -25.99^\circ )</td>
</tr>
<tr>
<td>( k )</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>Rib model by Smith et al. (2000)</td>
<td>Intact model or rhombus unit cell (conventional)</td>
<td>Missing rib model or swastika unit cell (auxetic)</td>
</tr>
<tr>
<td>( a )</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>85.7</td>
<td>77.3^\circ</td>
</tr>
<tr>
<td>( \phi )</td>
<td>–</td>
<td>24.1^\circ</td>
</tr>
<tr>
<td>( \theta_1 )</td>
<td>( 73.4^\circ ) and 48.1^\circ</td>
<td></td>
</tr>
<tr>
<td>( \theta_2 )</td>
<td>( 73.4^\circ ) and 48.1^\circ</td>
<td></td>
</tr>
<tr>
<td>( k_0 ) or ( k_\zeta )</td>
<td>( k_\zeta = 0.01429 )</td>
<td>( k_0 = 0.08333 )</td>
</tr>
</tbody>
</table>

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**Fig. 2.9.3** True stress versus true strain of experimental data and theoretical predictions by the honeycomb and the rib models by Smith et al. (2000). With kind permission from Elsevier

The conventional foam possesses a higher Young’s modulus as expected. More importantly, Smith et al. (2000) noted that the traditional 2D honeycomb model by Masters and Evans (1996) is valid for describing the strain-dependent behavior of conventional foams but not for auxetic ones; i.e. the missing rib model caters to the realistic cell geometries.
An alternate missing rib model was introduced by Lim et al. (2014) upon observing photomicroscopy of both the conventional and auxetic materials using light microscopy, as shown in Fig. 2.9.5. It could be clearly seen that the conventional foam resembles hexagonal microstructures, while the auxetic foam did not give a clear view. In order to provide a clearer view, thin slices of both foam materials were made and viewed under coarse microscopy. Figure 2.9.6a clearly shows again that the assumption of hexagonal microstructure is quite valid. However, no clear indication can be seen for the case of auxetic foams. Thereafter, a finer imaging using light microscopy was made, with startling results.

As shown in Fig. 2.9.6b, the assumption of re-entrant structure that is commonly adopted for modeling auxetic materials is invalid. Rather, the microscopy image shows that there is high level of irregularity in the microstructure in both the shape
and size. Consideration of Figs. 2.9.5 and 2.9.6 shows that the individual cells in conventional foams are convex from the outside or concave from the inside, while both concave and convex surfaces are found on both sides of individual cell’s wall.
in the case of auxetic foams. Furthermore the individual cells are of similar sizes for conventional foams but very different in the case of auxetic foams.

Based on these two observations, a possible model is proposed for auxetic foams by means of missing rib from hexagonal cellular structure, as shown in Fig. 2.9.7. Unlike the cells in Fig. 2.9.6a, which are all almost about the same size, the cells in Fig. 2.9.6b are of different sizes. As such, the model displayed in Fig. 2.9.7 allows the RVE to be represented both by larger and smaller cells, as inspired by Fig. 2.9.6b and the works by Pozniak et al. (2013).

The experimentally studied foams are isotropic at macro level, which is a consequence of their disordered structure. The model considered is highly ordered as its structure is periodic. It is well known that 6-fold axis implies isotropic elastic

![Fig. 2.9.6 Microphotography from thin slices of PU foams: a conventional specimen, and b auxetic specimen. With kind permission from John Wiley & Sons](image)

![Fig. 2.9.7 Hexagonal-based missing rib model for describing auxetic foams: a before rib deletion (ribs to be removed are denoted as thin lines), and b after rib deletion by Lim et al. (2014). With kind permission from John Wiley & Sons](image)
properties in planes perpendicular to the axis but the studied structure does not exhibit 6-fold symmetry by a lower, 3-fold symmetry axis. The fact that this is a sufficient symmetry to obtain planar isotropy has been pointed out by Wojciechowski (2003). Typical foams are strongly disordered but nevertheless isotropic. Although the proposed model is perfectly ordered, its rotation-based deformation allows isotropic auxetic characteristics to be manifested.

In this model, the relative difference between the small and large cell sizes is comparable to those shown in Fig. 2.9.6(b), in which the smaller cells generally exhibit regular polygonal shapes while the larger cells exhibit more distorted shapes. In addition, this model allows auxetic behavior to be exhibited by means of rotation. It is possible to compare this missing rib model with the missing rib model proposed by Smith et al. (2000) for describing auxetic behavior in reticulated foams, which is based on a network of ribs with biaxial symmetry that exhibits rhombus cells, such that the removal of a proportion of the cell ribs leads to swastika network that manifests auxetic property via rotation mechanism. The proposed model by Lim et al. (2014) is based on hexagonal cells such that the removal of a proportion of the cell ribs leads to both large distorted cells and small regular-shaped cells to exhibit auxetic behavior by means of rotation, and at the same time partially reflect the foam microstructural geometry.

With reference to Fig. 2.9.8a for an RVE, the small cells are surrounded by foam walls on all six sides, and are therefore of comparatively high stiffness. The center of the RVE is a highly “open” partial cell, which is surrounded by only three walls, thereby allowing greater deformation. The remaining hexagons are filled with partial cells that are surrounded by four or five walls, and are therefore of moderate stiffness. The surrounding regions of high, moderate and low stiffness are shown in Fig. 2.9.8b. For this missing rib model, the rigidity of the high stiffness region, denoted by “H”, avails its function as a rotating unit. The rotation of the

![Diagram](image)

Fig. 2.9.8 The proposed model showing: a an RVE with regions of high stiffness (H), moderate stiffness (M) and low stiffness (L), and b a central RVE surrounded by six other RVEs, with the rotating cells shaded in black (Lim et al. 2014). With kind permission from John Wiley & Sons
comparatively rigid units leads to the collapse or expansion of the low stiffness region, denoted by “L”. Figure 2.9.9a, b shows how the direction of rotation of the H regions opens or closes the L regions, leading to 2-dimensional iso-expansion and iso-contraction respectively.

### 2.10 Chiral and Anti-chiral Lattice Models

Another model that gives rise to auxetic behavior is the chiral lattice model. In this model, each rigid ring is connected by six ligaments that are attached in a tangential fashion, as illustrated in Fig. 2.10.1. It can be easily seen from this model that tensile loading in one direction causes the elongation in the direction of loading by means of clockwise rotation of the rigid rings. The ring rotation consequently enlarges the entire network, thereby leading to an in-plane auxetic property.

A theoretical and experimental investigation was conducted of a two-dimensionally chiral honeycomb by Prall and Lakes (1997), in which the honeycomb exhibits a Poisson’s ratio of $\nu = -1$ for in-plane deformation. This Poisson’s ratio is maintained over a significant range of strain, in contrast to the variation with strain seen in known
negative Poisson’s ratio materials. The ligament is modeled as beam of thickness $t$ and length $L$, while the ring has a radius $r$ (Fig. 2.10.2). For a base material of Young’s modulus $E_s$, Prall and Lakes (1997) gave the in-plane Young’s modulus as

$$E = \sqrt{3} E_s \left( \frac{L}{r} \right)^2 \left( \frac{t}{L} \right)^3$$

(2.10.1)

in which a similar dependence on $(t/L)^3$ is found for the honeycomb model by Gibson and Ashby (1988).
A chiral lattice investigated with an equivalent, micropolar-continuum model was attempted to remove the indeterminacy $v = -1$ encountered by Prall and Lakes (1997) and Spadoni et al. (2009). Based on the geometry nomenclature laid out in Fig. 2.10.3, Spadoni and Ruzzene (2012) developed constitutive models for two cases. In the first case the nodes are assumed rigid while in the second case the nodes are allowed to deform. The constitutive relation for the rigid node case was developed analytically while the constitutive relation for the deformable node case was developed numerically via a finite element model.

For the case of rigid nodes, Spadoni and Ruzzene (2012) obtained the constitutive relation

\[
\begin{align*}
\{\sigma_{11} & \sigma_{22} & \sigma_{12} & \sigma_{21} & m_{13} & m_{23}\} = \\
\begin{bmatrix}
D_{11} & D_{12} & 0 & 0 & 0 & 0 \\
D_{21} & D_{22} & 0 & 0 & 0 & 0 \\
0 & 0 & D_{33} & D_{34} & 0 & 0 \\
0 & 0 & D_{43} & D_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & D_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & D_{66}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{12} \\
\varepsilon_{21} \\
\kappa_{13} \\
\kappa_{23}
\end{bmatrix}
\end{align*}
\]

(2.10.2)

where

\[
D_{11} = D_{22} = \frac{\sqrt{3}E_s t (t^4 - L^4) \cos^2 \beta + L^4 + 3L^2 \tan^2 \beta}{4L^3} \frac{\cos^2 \beta + L^2}{(t^2 - L^2)}
\]

(2.10.3)

\[
D_{12} = D_{21} = -\frac{\sqrt{3}E_s t L^4 \tan^2 \beta + t^4 - L^2 \tan^2 \beta (1 + \tan^2 \beta)}{4L^3} \frac{L^2 \tan^2 \beta + t^2}{L^2}
\]

(2.10.4)

\[
D_{33} = D_{44} = \frac{\sqrt{3}E_s t 2L^4 \tan^2 \beta + L^2 R^2 + t^2(2L^2 + R^2)}{4L^3} \frac{R^2}{L^2}
\]

(2.10.5)
\[
D_{34} = D_{43} = -\frac{\sqrt{3}E_t t 2L^4 \tan^2 \beta - L^2 R^2 + t^2 (2L^2 - R^2)}{4L^3} \quad (2.10.6)
\]

\[
D_{55} = D_{66} = \frac{\sqrt{3}E_t t}{4L^3} \left( L^4 \tan^2 \beta + \frac{4}{3} L^2 t^2 \right). \quad (2.10.7)
\]

Using the treatments of Nakamura and Lakes (1995) and Yang and Huang (2001), the engineering constants in terms of stiffness coefficients \( E = (D_{11}^2 - D_{12}^2)/D_{11} \) and \( v = D_{12}/D_{11} \) were expressed by Spadoni and Ruzzene (2012) as

\[
E = \frac{2\sqrt{3} \left[ 1 + \left( \frac{t}{L} \right)^2 \right] \left( \frac{t}{L} \right)^3}{\left( \frac{t}{L} \right)^4 \cos^2 \beta + \sin^2 \beta + 3 \left( \frac{t}{L} \right)^2} E_s \quad (2.10.8)
\]

\[
v = \frac{4 \left( \frac{t}{L} \right)^2}{\left( \frac{t}{L} \right)^4 \cos^2 \beta + \sin^2 \beta + 3 \left( \frac{t}{L} \right)^2} - 1 \quad (2.10.9)
\]

\[
G = \frac{\sqrt{3}}{4} \frac{t}{L} \left[ 1 + \left( \frac{t}{L} \right)^2 \right] E_s. \quad (2.10.10)
\]

Due to the complexity in obtaining analytical expressions for the case of deformable rings, Spadoni and Ruzzene (2012) adopted FE model with the imposed displacements and rotations to the corresponding strain states as shown in Fig. 2.10.4. Results of the Young’s modulus, shear modulus and Poisson’s ratio for both the case of rigid node by analytical approach and the case of deformable node by the finite element approach are shown in Fig. 2.10.5, whereby the Young’s and shear moduli were plotted in normalized forms, i.e. \( \bar{E}_m/(t/L)^3 \) and \( \bar{G}_m/(t/L)^3 \) respectively, in which

\[
\left\{ \frac{\bar{E}_m}{\bar{G}_m} \right\} = \frac{1}{E_s} \left[ \begin{array}{c} E \\ G \end{array} \right]. \quad (2.10.11)
\]

In relation to this chiral lattice, the auxeticity of chiral and anti-chiral lattices, such as those shown in Fig. 2.10.6, have also been studied by Alderson et al. (2010b). Other investigations on chiral and anti-chiral models have been performed by Alderson et al. (2010a), Miller et al. (2010), Lorato et al. (2010), Michelis and Spitas (2010), Abramovitch et al. (2010), Kopyt et al. (2010).

The anti-tetrachiral structure model by Chen et al. (2013) was investigated analytically and by finite element approach. Based on the structure shown in Fig. 2.10.7, Chen et al. (2013) established the following elastic moduli:

\[
v_{xy} = -\frac{L_x}{L_y} \quad (2.10.12)
\]
Fig. 2.10.4  a FE model of the unit cell employed to study configurations with deformable rings with boundary degrees of freedom prescribed for each considered strain state, and b imposed displacements corresponding to six independent strain states (Spadoni and Ruzzene 2012). With kind permission from Elsevier.
Fig. 2.10.5 Micropolar engineering constants for the chiral lattice with two values of ligament aspect ratio $t/L = 1/100, 1/20$ with rigid rings (plus and multiplication symbols) and deformable rings (square and triangle symbols) rings. Normalized a Young’s modulus, b shear modulus, and c Poisson’s ratio (Spadoni and Ruzzene 2012). With kind permission from Elsevier

\[
E_x = \frac{E_c \beta^3 \alpha_x}{12(1 - \beta/2)^2 \alpha_y} \left( \frac{1}{\alpha_x - 2\sqrt{2\beta - \beta^2}} + \frac{1}{\alpha_y - 2\sqrt{2\beta - \beta^2}} \right) \tag{2.10.13}
\]

\[
E_y = \frac{E_c \beta^3 \alpha_y}{12(1 - \beta/2)^2 \alpha_x} \left( \frac{1}{\alpha_x - 2\sqrt{2\beta - \beta^2}} + \frac{1}{\alpha_y - 2\sqrt{2\beta - \beta^2}} \right) \tag{2.10.14}
\]

\[
E_c = \frac{\beta [\alpha_x + \alpha_y + \pi (2 - \beta)] - 2[\phi - (1 - \beta) \sin \phi]}{\alpha_x \alpha_y} E_c \tag{2.10.15}
\]
Fig. 2.10.6 Rapid prototype chiral honeycombs investigated: a trichiral; b anti-trichiral; c tetrachiral; and d anti-tetrachiral, in the study by Alderson et al. (2010b). With kind permission from Elsevier

where

$$\phi = \cos^{-1}(1 - \beta)$$

and the dimensionless parameters are defined as

$$\begin{align*}
\begin{pmatrix} \alpha_x \\ \alpha_y \\ \beta \\ \gamma \end{pmatrix} &= \frac{1}{r} \begin{pmatrix} L_x \\ L_y \\ t \\ b \end{pmatrix}
\end{align*}$$

in which $E_c$ is the Young’s modulus of the core material and $b$ is the cell depth.
For equal ligament length \((x = y = a)\), Eqs. (2.10.12)–(2.10.15) reduce to
\[
v_{xy} = -1,
\]
\[
E_x = E_y = \frac{E_c \beta^3}{6(1 - \beta/2)^2} \left( \frac{1}{\alpha - 2\sqrt{2\beta - \beta^2}} \right) \tag{2.10.18}
\]
and
\[
E_z = \frac{\beta[2\alpha + \pi(2 - \beta)] - 2[\phi - (1 - \beta)\sin \phi]}{\alpha^2} E_c. \tag{2.10.19}
\]

Figure 2.10.8a shows the FE model for comparison with the analytical model, while the experimental procedure is graphically summarized in Fig. 2.10.8b, in which more details are described by Chen et al. (2013). Figure 2.10.9 furnishes the analytical and FE results of the Poisson’s ratio by Chen et al. (2013). This, and other results contained therein, presents a parametric analysis showed that one can expect large variations of the in-plane negative Poisson’s ratios through changing the length of the ligaments along the \(x\) and \(y\) directions, and hence provides overall guidelines to develop and manufacture a new type of core for sandwich structures for a variety of engineering applications.

By using finite element simulation, Pozniak and Wojciechowski (2014) determined the Poisson’s ratio of anti-chiral structures built on rectangular lattices with disorder introduced by stochastic distributions of circular node sizes. Their investigated models were parameterized by the lattice anisotropy, the rib thickness, and the radii distribution of circular nodes. In this investigation, Pozniak and Wojciechowski (2014) developed three approaches. In the first approach, exact in the limit of infinitely large system and infinitely dense mesh, uses only planar elements (CPS3). Two other approaches are approximate and exploit one-dimensional
elements utilizing the Timoshenko beam theory. Pozniak and Wojciechowski (2014) showed that in the case of sufficiently large anisotropy of the studied structures PR can be highly negative, reaching any negative value, including those lower than −1, and that thin ribs and thin-walled circular nodes favor low values of Poisson’s ratio, i.e. in the case of thick ribs and thick-walled circular nodes the Poisson’s ratio is higher. In both cases the dispersion of the values of circular nodes radii has a minor effect on the lowest values of PR. A comparison of the results obtained with three different approaches shows that the Timoshenko beam based approximations are valid only in the thin rib limit, i.e. the difference between them grows with increasing thickness (Pozniak and Wojciechowski 2014).

Fig. 2.10.8 a Finite element model of repeating unit cell layout, and b honeycomb structures experimental setup: (A) flatwise compression tests; (B) three-point bending tests; (C) and (D) tensile tests by Chen et al. (2013). With kind permission from Elsevier
The effects of hierarchy on the in-plane elastic properties of honeycombs have been examined by Taylor et al. (2011), in which the effects of adding hierarchy into a range of honeycombs, with hexagonal, triangular or square geometry super and sub-structure cells, were explored by finite element simulation. It was found that a negative Poisson’s ratio sub-structure engenders substantial increases to the density modulus versus conventional honeycombs—partial result of this work is summarized in Fig. 2.10.10.

2.11 Interlocking Hexagons Model

Using the interlocking hexagons model shown in Fig. 2.11.1a, Ravirala et al. (2007) developed a micromechanical model that exhibits auxetic behavior. In addition to the geometries, the adoption of spring constants, as shown in Fig. 2.11.1b, aids the development of the Young’s moduli expressions. While a hexagonal array of honeycomb with hexagonal and re-entrant structures give conventional and auxetic behavior respectively, a hexagonal array of interlocking hexagonal and re-entrant structures give auxetic and conventional behavior, respectively. See Fig. 2.11.1c for the interlocking re-entrant structure.
Fig. 2.10.10  a The internal angle of the substructure versus the elastic moduli $E_1$ and $E_2$ (referring to the $X_1$ and $X_2$ axes) for 50 % mass distribution (open symbols) and 75 % mass distribution within the sub-structure (closed symbols). For all cases $\theta$ in the super-structure was 30°. b The anisotropy present in re-entrant hierarchical structures shown by a polar plot of the Young’s modulus versus loading angle for two hierarchical honeycombs with a NPR sub-structures ($\theta = -10^\circ$), with mass distributions of 50 and 25 % respectively. A conventional hexagonal honeycomb is shown for comparison (Taylor et al. 2011). With kind permission from Elsevier
Based on the geometrical parameters given in Fig. 2.11.1, the elastic moduli established by Ravirala et al. (2007) are

\[
v_{xy} = \frac{1}{v_{yx}} = - \frac{(l_1 + l_2 \cos \alpha + a) \cos \alpha}{l_2 \sin^2 \alpha + a \cos \alpha} \tag{2.11.1}
\]

\[
E_x = k_h \left( \frac{2 \cos^2 \alpha + 1}{\sin \alpha} \right) \left( \frac{l_1 + l_2 \cos \alpha + a}{l_2 \sin^2 \alpha + a \cos \alpha} \right) \tag{2.11.2}
\]

\[
E_y = k_h \left( \frac{2 \cos^2 \alpha + 1}{\sin \alpha \cos^2 \alpha} \right) \left( \frac{l_2 \sin^2 \alpha + a \cos \alpha}{l_1 + l_2 \cos \alpha + a} \right) \tag{2.11.3}
\]
Fig. 2.11.2 Poisson’s ratio as functions of: a angle $\alpha$ ($l_1 = l_2 = 1$; $a = 0.01$), b gap parameter $a$ ($\alpha = 30^\circ$; $l_1 = 2$; $l_2 = 0.5$), c edge length $l_1$ ($\alpha = 60^\circ$; $l_2 = 1$; $a = 0.01$), and d edge length $l_2$ ($\alpha = 60^\circ$; $l_1 = 1$; $a = 0.01$) plotted by Ravirala et al. (2007). With kind permission from Springer Science+Business Media.

Fig. 2.11.3 Young’s moduli as functions of: a angle $\alpha$ ($l_1 = l_2 = 1$; $a = 0.01$), b gap parameter $a$ ($\alpha = 30^\circ$; $l_1 = 2$; $l_2 = 0.5$), c edge length $l_1$ ($\alpha = 60^\circ$; $l_2 = 1$; $a = 0.01$), and d edge length $l_2$ ($\alpha = 60^\circ$; $l_1 = 1$; $a = 0.01$) plotted by Ravirala et al. (2007). With kind permission from Springer Science+Business Media.
where the spring stiffness constant, $k_h$, is shown in Fig. 2.11.1b. It can be easily seen that

$$v_{xy}E_y = v_{yx}E_x = -k_h \left( \frac{2 \cos^2 \alpha + 1}{\sin \alpha \cos \alpha} \right)$$

(2.11.4)

and that substitution of $l_1 = l_2$ and $\alpha = 60^\circ$ into Eq. (2.11.1) and (2.11.4) reduces them to $v_{xy} = v_{yx} = -1$ and $v_{xy}E_y = v_{yx}E_x = -2k_h \sqrt{3}$.

Figures 2.11.2 and 2.11.3 show the plots of Poisson’s ratio and Young’s moduli, respectively, for various combinations of edge lengths $l_1$, $l_2$, gap parameter $a$, and the angle $\alpha$, using Eqs. (2.11.1)–(2.11.3). Comparison with
experimental results by Ravirala et al. (2005) gives the fitted results $l_1/l_2 = 2.86$ and $\alpha = 69.2^\circ$. The predicted transverse total true strain ($\varepsilon_y$) versus axial total true strain ($\varepsilon_x$) for $l_1/l_2 = 2.86$ and $\alpha = 69.2^\circ$ assuming an initially fully dense structure (i.e. $a = 0$ for the undeformed structure) is shown in Fig. 2.11.4. Also shown, for comparison, is the experimental transverse versus axial (extrusion) total true strain.

Fig. 2.12.2 a The structural formulae of the repeat units for the molecular ‘double calix’ structures, and b the simulated single crystalline Poisson’s ratios ($v_{ij}$) and Young’s moduli ($E_i$) of the two molecular systems (a) and those predicted for the idealized folded macrostructure shown in Fig. 2.12.1 (Grima et al. 2005). With kind permission from The Royal Society of Chemistry.
data by Ravirala et al. (2005) assuming the extrusion direction corresponds to the model \( x \)-direction. Combining the hexagonal shape of nodules in this section with the re-entrant fibrils discussed in Sects. 2.3 and 2.4, Lim and Acharya U (2009) proposed a hexagonal array of fourfold interconnected hexagonal nodules for modeling auxetic microporous polymers in 2D and 3D.

### 2.12 Egg Rack Structure

Based on an “egg rack” structure, shown in Fig. 2.12.1, Grima et al. (2005) proved the auxeticity of networked calix[4]arene polymers using molecular simulation (Fig. 2.12.2).

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