MECHANICS OF NANO-STRUCTURED HIERARCHICAL AND SELF-SIMILAR TWO DIMENSIONAL CELLULAR MATERIALS

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Abstract. This paper presents the results of the elastic and geometrical properties of four types of nano-structured hierarchical and self-similar honeycombs. It is shown that at the nanometer scale, the elastic properties are size-dependent; the thinner the first order cell walls, the stiffer the hierarchical honeycombs. As an initial strain can be applied and controlled to the first order cell walls by application of an electric potential, both the elastic and geometrical properties of hierarchical honeycombs can be controlled to vary over large a range.

1 INTRODUCTION

Almost all the natural living materials have a cellular structure, examples include plants, vegetables, and the bones or lungs in the human body. To enable different types of biological functions and to ensure that living species can survive, the mechanics of cellular materials plays a fundamental role and is hence of vital importance.

The mechanics of macro-sized cellular materials has been well established. Using dimensional analysis and taking the cell wall bending as the sole deformation mechanism, Gibson et al. [1] found that the Young’s modulus of a regular hexagonal honeycomb is proportional to the cube of the honeycomb relative density. Warren and Kraynik [2] obtained the elastic properties of honeycombs by considering the cell wall bending, axial stretching and transverse shearing as the deformation mechanisms. Masters and Evans [3] took the cell wall junction hinging as an additional deformation mechanism for honeycombs. Zhu and Chen [4] explored the combined effects of relative density and material distribution on the mechanical properties of honeycombs. Silva et al [5] studied the elastic properties of irregular honeycombs by computer simulation. Zhu et al investigated the effects of cell irregularity on the elastic properties of Voronoi honeycombs [6] and related their elastic properties to their geometrical properties [7].

The mechanics established for macro-sized two dimensional cellular materials, however, may not apply to their nano-sized counterparts due to the surface stress effects [8-12] and the initial stress effects [8, 13, 14] at the nano-meter scale. The surface stress is given by $\tau = S\varepsilon + \tau_0$, where $S$ and $\varepsilon$ are the surface elastic modulus and surface strain, and $\tau_0$ is the initial surface stress. It has been experimentally found that the amplitude of the initial surface stress $\tau_0$ is controllable by adjusting an applied electric potential [15-19]. For example, the initial surface stress of Au (111) is about 1.13 N/m. However, the adsorbate-induced initial surface stress $\tau_0$ of nanoporous Au material can be controlled to reach 17-26 N/m by adjusting the chemical energy [19]. There is a linear correlation between the surface stress and surface charge in anion adsorption on Au (111) [17]. Nano-porous materials have been experimentally demonstrated to deform and to recover by controlling the amplitude of the initial surface stress via adjusting an applied electric potential [18, 19].

Natural materials, such as bones, are usually hierarchical materials with the basic building blocks at the nanometer scale [20, 21]. Lakes, Taylor et al. [22] and Fan et al. [24] studied the mechanical properties of macro-sized hierarchical two dimensional cellular materials, but did not explore the size-dependent and the tunable properties of their nano-sized counterparts. Zhu et al. [8, 25-27] have studied the size-dependent and tunable/controllable elastic and geometrical properties of two dimensional hierarchical cellular materials with hexagonal, square, equilateral-triangular, and irregular Voronoi cells. This paper will present the main mechanical and geometrical
properties of two dimensional hierarchical and self-similar cellular materials with the basic building elements at the nano-meter size scale.

2 GEOMETRICAL MODELS

In this paper, we focus on the mechanical and geometrical properties of four types of hierarchical and self-similar honeycombs, as shown in Figure 1. It is assumed that all the cell walls have the same uniform thickness at each hierarchy level and the cell wall thickness of the first order honeycombs is at the nano-meter scale.

![Diagram of hierarchical and self-similar honeycombs with four different types of cells.](image)

Figure 1. Hierarchical and self-similar honeycombs with four different types of cells.

3 THE TUNABLE MECHANICAL PROPERTIES OF NANO-SIZED CELL WALLS

For the first order honeycombs, the basic building elements are the nano-sized cell walls, which have a length $L$, width $b$ and uniform thickness $h$. The wall width $b$ is assumed to be much larger than the thickness $h$. When the first order nano-honeycomb is subjected to in-plane deformation, the cell walls undergo plane-strain bending because the width dimension of the cell walls is much larger than the cell wall thickness. For simplicity, both the surface and the bulk material of the first order cell walls are assumed to be isotropic and to have the same Poisson ratio $\nu_s$. When the initial surface stress $\tau_0$ is present, the amplitudes of the initial stresses in the
bulk material in the length and the width directions of the first order cell walls are the same and obtained as

$$\sigma_{Ec} = \sigma_{0c} = -2\tau_0 + h$$,

where \(h\) is the current thickness of the cell walls [28]. At the nano-meter scale, the yield strength of the first order cell wall material, \(\sigma_{Ec}\), can well reach \(0.1E_s\) or a larger amplitude [29]. For recoverable elastic deformation, the initial von Mises stress should not exceed the yield strength \(\sigma_y\) of the bulk material.

Thus, \(\sigma_{Ec} = |\sigma_{0c}| = |\sigma_{0w}| = 2\tau_0 / h \leq \sigma_y = 0.1E_s\). The amplitudes of the induced initial elastic residual strains in the length and width directions of the first order cell walls are the same and can be related to the initial stress in the bulk material by [28]

$$\varepsilon_{Ec} = \varepsilon_{0c} = \frac{\sigma_{Ec}}{E_s} = \frac{2\tau_0}{hE_s}(1 - v_s)$$  \(1\)

The initial elastic strain in the thickness direction of the first order cell walls is obtained as

$$\varepsilon_{h0} = \frac{4v_s\tau_0}{E_s h} = \frac{2v_s}{E_s} \frac{\sigma_{h0}}{1 - v_s} = \frac{2v_s}{1 - v_s} \varepsilon_{Ec}$$  \(2\)

When the effect of the initial stress/strain is present, the bending, transverse shear and axial stretching/compression rigidities of the nano-sized first order cell walls are given as [8, 14, 28]

$$D_0 = \frac{E_s b h_0^2}{1 - v_s^2} \left[1 + \frac{6v_s}{E_s h} \frac{2\tau_0}{v_s}(1 + v_s)\right] = \frac{E_s b h_0^2}{1 - v_s^2} \left[1 + \frac{1}{2} \frac{6v_s}{h} \frac{2\tau_0}{v_s}(1 + v_s)\right]$$  \(3\)

$$D_s = G_b b \left[\frac{6v_s}{h} + \frac{v_s}{1 - v_s} \varepsilon_{0c}^2\right]$$  \(4\)

$$D_t = E_s b h(1 + 2l_0 / h)$$  \(5\)

Where \(S\) is the surface elasticity modulus, and \(l_s = S/E_s\) is the intrinsic length of the solid material at the nanometer scale. \(D_0 = \frac{E_s b h_0^2}{12(1 - v_s^2)}\) is the bending stiffness of the first order cell walls with a unit width when the effects of both the surface elasticity and the initial stress/strain are absent. It should be noted that the bulk material, from which the first order and the hierarchical nano-sized honeycomb and open-celled foam are made, can be any type of metallic, or polymeric or biological material. Therefore, the material nano-scale intrinsic length \(l_s\) could be in the range from 0.01 to 1 nm, or even negative [8, 10]. When the effect of the initial stress is present, the current width, thickness and length of the first order cell walls can be obtained as [8, 25, 27, 28]

$$b = b_0(1 + \varepsilon_{0c}^w) = b_0(1 + \varepsilon_{0c}^c)$$  \(6\)

$$h = h_0(1 + \varepsilon_{0c}^h) = h_0(1 + \frac{2v_s}{E_s} \sigma_{h0}^c)$$  \(7\)

and

$$L = L_0(1 + \varepsilon_{0c}^l)$$  \(8\)

Where, \(L_0\), \(b_0\) and \(h_0\) are the initial cell wall length, width and thickness when the initial surface stress \(\tau_0\) is absent. As the initial surface stress \(\tau_0\) is tunable and controllable [17-19], when it is present, the cell wall dimensions and the bending, stretching and transverse shearing rigidities can be controlled to vary over a large range. As the nano-sized first order cells are usually single crystal, the range of linear elastic deformation can be from -0.1 to 0.1. Thus the cell wall length, width, thickness, the bending, transverse shearing and axial stretching or compression rigidities all could be controlled to vary over a large range.

4 THE TUNABLE MECHANICAL PROPERTIES OF THE FIRST ORDER NANO-HONEYCOMBS

Relative density is one of the most important parameters for cellular materials. It is the volume of the solid material over the volume of the whole cellular material. The elastic properties of a cellular material can be related to those of the solid material, from which the cellular material is made, by the relative density. For all the four types of first order honeycombs, their dimensionless out-of-plane Young’s moduli are the same in form, and given as

$$\frac{E_s}{E_s} = \frac{E_s}{E_s} = (1 + \frac{2h}{h} \frac{2v_s}{1 - v_s}) \frac{(1 - \frac{2v_s}{1 - v_s})}{(1 + \varepsilon_{0c}^l)}$$  \(9\)
and their dimensionless out-of-plane shear modulus can be easily derived as
\[
(G_{s1})_0 = (G_{s1})_0 \rho_0 = \frac{1}{2} \left(1 + \frac{2h}{r} \right) \frac{1}{\rho_0} \left(1 - 2v_s \frac{\varepsilon_s^e}{1 + \varepsilon_s^e} / (1 + \varepsilon_s^e) \right) \tag{10}
\]

Where, $\rho_0$ is the initial relative density of the first order honeycomb when the effects of the initial stress or strain are absent. It is noted that the dimensionless out-of-plane shear modulus given by Eq. (10) is correct for the first order triangular, square and hexagonal honeycombs, and approximately correct for first order Voronoi honeycombs. As the Poisson ratio of the surface is assumed to be the same as that of the bulk material, the out-of-plane Poisson ratio of all the four types of nano-honeycombs, $v_{13}$, is obviously the same as $v_s$.

### 4.1 Honeycombs with equilateral triangular cells

The relative density of an equilateral triangular honeycomb is
\[
\rho = 2\sqrt{3}h/L = \frac{1 + \varepsilon_t^e}{1 + \varepsilon_t^e} \rho_0 \tag{11}
\]

Where $\rho_0 = 2\sqrt{3}h_0 / L_0$ is the initial relative density when the initial surface stress or strain is absent.

There are five independent elastic constants for equilateral triangular honeycombs. As the Poisson ratio of the surface is assumed to be the same as that of the bulk material, the out-of-plane Poisson ratio of an equilateral triangular honeycomb is given by Eq. (13) is very close to 1/3.

### 4.2 Honeycombs with square cells

The relative density of a honeycomb with square cells is
\[
\rho = 2h/L = \frac{1 + \varepsilon_0^e}{1 + \varepsilon_0^e} \rho_0 \tag{14}
\]

Where $\rho_0 = 2h_0 / L_0$ is the initial relative density when the initial surface stress or strain is absent.

There are six independent elastic constants for equilateral triangular honeycombs. As the three out-of-plane elastic constants are already given above, we only need to give the other two in-plane elastic constants. These are the in-plane dimensionless Young’s modulus, given as
\[
(E_y)_0 = \frac{1}{3} \frac{E_y \rho_0}{\rho_0} \tag{12}
\]

and the in-plane Poisson’s ratio, given as
\[
(v_{12})_0 = \frac{1 + 1 + 10L^2}{5(1-v_s)} + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} h^2 \rho^2 + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} \rho^2 \tag{13}
\]

\[
(v_{12})_0 = \frac{1 + 1 + 10L^2}{5(1-v_s)} + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} h^2 \rho^2 + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} \rho^2 \tag{13}
\]

\[
(v_{12})_0 = \frac{1 + 1 + 10L^2}{5(1-v_s)} + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} h^2 \rho^2 + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} \rho^2 \tag{13}
\]

\[
(v_{12})_0 = \frac{1 + 1 + 10L^2}{5(1-v_s)} + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} h^2 \rho^2 + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} \rho^2 \tag{13}
\]

\[
(v_{12})_0 = \frac{1 + 1 + 10L^2}{5(1-v_s)} + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} h^2 \rho^2 + \frac{1 + 10L^2}{1 + 6L^2 + 30L^2} \rho^2 \tag{13}
\]
4.3 Honeycombs with hexagonal cells

The relative density of a honeycomb with hexagonal cells is

\[ \rho = 2h_0 / (\sqrt{3} L_0) = \frac{1 + \rho_0}{1 + \rho_0} \rho_0 \]

Where \( \rho_0 = 2h_0 / (\sqrt{3} L_0) \) is the initial relative density when the initial surface stress or strain is absent.

There are five independent elastic constants in total for hexagonal honeycombs \[8\]. The in-plane dimensionless Young’s modulus can be obtained as

\[ \left( \frac{E_i}{E} \right) = \frac{1}{1.5 E \rho} \left[ 1 + 6 \frac{L}{h} + 2 \frac{h}{L} \left( \frac{1}{1-v_i} \right) + 1.8 \rho \frac{h}{L} \left( 1 + 10 \frac{L}{h} + 30 \frac{h}{L} \right) \left( 1 + 2 \frac{L}{h} \left( 1 + v_i \right) \right) + \frac{9}{4} \rho^2 \frac{h}{L} \left( 1 + 2 \frac{L}{h} \left( 1 + v_i \right) \right) - \frac{1}{v_i} \right] \]

and the in-plane Poisson’s ratio is given as

\[ \left( \nu_{i,v} \right) = \frac{1}{1.5 E \rho} \left[ 1 + 6 \frac{L}{h} + 2 \frac{h}{L} \left( \frac{1}{1-v_i} \right) + 1.8 \rho \frac{h}{L} \left( 1 + 10 \frac{L}{h} + 30 \frac{h}{L} \right) \left( 1 + 2 \frac{L}{h} \left( 1 + v_i \right) \right) + \frac{9}{4} \rho^2 \frac{h}{L} \left( 1 + 2 \frac{L}{h} \left( 1 + v_i \right) \right) - \frac{1}{v_i} \right] \]

4.4 Honeycombs with Voronoi cells

The relative density of a honeycomb with Voronoi cells is \[27\]

\[ \rho = (\sum_{i=1}^{n} L_i) / L_0 = \frac{1 + \rho_0}{1 + \rho_0} \rho_0 \]

Where \( \rho_0 = (h_0 \sum_{i=1}^{n} L_i) / L_0 \) is the initial relative density when the initial surface stress or strain is absent.

As the first order nano-sized Voronoi honeycombs are in-plane isotropic, there are only five independent elastic constants. As the three out-of-plane elastic constants of the first order Voronoi honeycomb are the same as those given above, the other two size-dependent and tunable elastic constants are given in Figure 2 \[27\].

Figure 2. Effects of the cell wall thickness and initial stress/strain on the relationship between the in-plane elastic properties and the relative density of the first order nano-sized random irregular honeycombs with regularity \( \alpha = 0.7 \). (a) size-dependent Young’s modulus normalized by \( 1.5E \rho_0 / (1 - v_i^2) \); (b) tunable Young’s modulus normalized by \( 1.5E \rho_0 / (1 - v_i^2) \); (c) size-dependent Poisson’s ratio; (d) tunable Poisson’s ratio.
5  THE TUNABLE MECHANICAL PROPERTIES OF THE FIRST ORDER NANO-HONEYCOMBS

All the four types of hierarchical honeycombs are assumed to be self-similar, as can be seen in Fig. 1. At all different hierarchy levels, they are treated as materials whose size is much larger than the individual cells at the same hierarchy level. The relative density of the nth order self-similar hierarchical honeycombs with equilateral triangular cells, or square cells, or hexagonal cells, or Voronoi cells can be easily obtained as

$$\rho_n = (1 - \frac{2\varepsilon_0^c}{1 - \varepsilon_0^c})(\rho_0)^n / (1 + \varepsilon_0^c)$$  \hspace{1cm} (21)

where \(\rho_0\) can be found in the previous section. When the initial strain \(\varepsilon_0^c\) is 0, \(\rho_n\) reduces to \((\rho_0)^n\).

For all the four types of the nth order self-similar hierarchical honeycombs, the three independent out-of-plane dimensionless elastic constants can be obtained as

$$\overline{(E_i)_n} = (E_i)_n / E_i \rho_0 = (\rho_0)^{n-1} \cdot (E_i)_1$$  \hspace{1cm} (22)

$$\overline{(G_{ij})_n} = (G_{ij})_n / G_i \rho_0 = (\rho_0)^{n-1} \cdot (G_{ij})_1$$  \hspace{1cm} (23)

and \((v_{ij})_n = v_s\). Where, \(n\) is the hierarchy level of the self-similar hierarchical honeycombs. In equations (22), and (23), \((E_i)_1\), and \((G_{ij})_1\) are the dimensionless Young’s modulus in the \(z\) direction and the dimensionless shear modulus in the \(xz\) plane of the 1st order honeycomb, respectively.

When the initial strain is absent, the initial cell diameter, area, and volume of an nth order self-similar hierarchical honeycomb are assumed to be \((L_n)_s\), \((A_n)_s\), and \((V_n)_s\) respectively. When the initial strain \(\varepsilon_0^c\) is present, the dimensionless cell diameter, cross-sectional area, and volume of all the different types of nth order self-similar hierarchical honeycombs become

$$(L_n)_s / (L_0)_s = 1 + \varepsilon_0^c$$  \hspace{1cm} (24)

$$(A_n)_s / (A_0)_s = (1 + \varepsilon_0^c)^2$$  \hspace{1cm} (25)

and

$$(V_n)_s / (V_0)_s = (1 + \varepsilon_0^c)^3$$  \hspace{1cm} (26)

If \(\varepsilon_0^c\) can be controlled to change from -0.1 to 0.1, the dimensionless cell diameter, area, and volume of an nth order self-similar hierarchical honeycomb would vary over ranges from 0.9 to 1.1, 0.81 to 1.21, and 0.729 to 1.331, respectively.

5.1 Hierarchical honeycombs with equilateral triangular cells

For the nth order self-similar hierarchical honeycombs with equilateral triangular cells, the other two in-plane independent dimensionless elastic constants can be obtained as \([25]\)

$$\overline{(E_i)_y} = (E_i)_y / E_y \rho_0 = (\rho_0)^{n-1} \cdot (E_i)_1$$  \hspace{1cm} (27)

$$(v_{yz})_y \approx 1/3$$  \hspace{1cm} (28)

5.2 Hierarchical honeycombs with square cells

For the nth order self-similar hierarchical honeycombs with square cells, the other three in-plane independent dimensionless elastic constants can be obtained as \([25]\)

$$\overline{(E_i)_x} = (E_i)_x / E_x \rho_0 = (\rho_0)^{n-1} \cdot (E_i)_1$$  \hspace{1cm} (29)

$$\overline{(G_{ij})_{xy}} = (G_{ij})_{xy} / G_y \rho_0 = (\rho_0)^{n-1} \cdot (G_{ij})_1$$  \hspace{1cm} (30)

and

$$(v_{yz})_x = (\rho_0)^{n-1} \cdot (v_{yz})_1$$  \hspace{1cm} (31)

5.3 Hierarchical honeycombs with hexagonal cells

For the nth order self-similar hierarchical honeycombs with hexagonal cells, the other two in-plane independent dimensionless elastic constants can be obtained as \([26]\)

$$\overline{(E_i)_x} = (E_i)_x / E_x \rho_0 / (1 - v_x^2) = (\rho_0)^{n-1} \cdot (E_i)_1$$  \hspace{1cm} (32)
(v_{12})_{i+1} = \frac{1 + c_i \rho_i^2}{1 + c_i \rho_0^2}, \quad \text{for } i = 1, \ldots, n-1 \tag{33}

In Eqs (32-33), $c_i = [4.05 + 1.8(v_{12})]/(1-v_{12}^2)$ and $c_2 = [1.05 + 1.8(v_{12})]/(1-v_{12}^2)$.

5.4 Hierarchical honeycombs with Voronoi cells

For the $n$th order self-similar hierarchical honeycombs with hexagonal cells, the other two in-plane independent dimensionless elastic constants can be obtained as

$$
(E_i)_{v} = \frac{(E_i)_{v}(1-v_i^2)}{1.5E_i \rho_i^n} \approx [f(\alpha, \rho_i)]^{-1} \cdot (E_i)_{v}
$$

$$
(v_{12})_{v} \approx v(\rho_i), \quad n \geq 2
$$

For hierarchical and self-similar random irregular honeycombs with $n \geq 2$ and fixed values $\rho_0 = 0.2$ or $\rho_0 = 0.3$, the numerical results of the function $f(\alpha, \rho_i) = (E_i)_{v} / ((E_i)_{v-1} \rho_i^3)$ in Eq. (34) are obtained by computer simulation, and are plotted against the honeycomb regularity $\alpha$, as shown in Fig. 3.

![Figure 12](image)

Figure 12. Relationship between the value of $f(\alpha, \rho_i) = (E_i)_{v} / ((E_i)_{v-1} \rho_i^3)$ and cell regularity of micro- or nano-structured hierarchical and self-similar random irregular honeycombs with $n \geq 2$ and different relative densities $\rho_0 = 0.2$ and $\rho_0 = 0.3$.

6 Discussion

As can be seen from the results section 4, for all the four types of first order honeycombs, their dimensionless in-plane Young’s modulus and shear modulus are size-dependent (i.e. depend on $l_n / h$). As $l_n$ is a material length scale property of the solid material from which the hierarchical honeycomb is made, the thinner the cell thickness $h$, the larger the dimensionless Young’s and shear moduli. As the first order cell walls are made of single crystal, the range of the reversible linear elastic strain in the cell wall length and thickness directions could be from -0.1 to 0.1. The initial strain $\varepsilon_0^{n}$ could be controlled to vary over range of -0.06 to 0.06 (or -0.1 to 0.1), thus, the in-plane dimensionless Young’s modulus and shear modulus of the first order honeycombs can be controlled to increase 60% or to drop 50%. Equation (8) indicates that the cell diameter of the first order honeycomb cells can be controlled to increase about 10% or to drop 10%. The cell cross-section area can be controlled to increase about 21% or drop 19%. The cell volume of the first order honeycombs can be controlled to increase about 33% or to reduce about 27%.

For nano-structured hierarchical and self-similar honeycombs, equations (22-35) indicate that both their elastic and geometrical properties are functions of those of their first order honeycombs. As both the elastic and geometrical properties of the first order nano-sized honeycombs can be controlled to vary over a large range by application of an electric potential (hence an initial strain), the elastic and geometrical properties of the nano-structured hierarchical and self-similar honeycombs can also be controlled to vary over a large range.

REFERENCES


