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The Negative Compressibility in 3D Cellular Elongated Octahedron Model

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Abstract. A new three-dimensional cellular system based on the elongated octahedron model [1] is analyzed and discussed mathematically for its compressibility properties. It is shown that there exists negative linear and area compressibility for some certain conformations in this model. In addition, when compared with the octahedral structure, it can be found that this structure has better negative compression effect in the horizontal direction.

1. Introduction

Generally, materials will contract in every direction when they are subjected to a hydrostatic pressure. However, a slight number of materials [1-10] become elongate at lowest one direction, which defined as negative compressibility [2]. The behavior of relative reduction in length of a line is named as negative linear compressibility (NLC), and equally in two or three directions is known as negative area compressibility (NAC) and negative volume compressibility (NVC).

Over the past few decades, several natural materials with NLC have been discovered, such as methanol monohydrate [3], ZAG-4 [4], and α-BiB_3O_6 [5]. Baughman et al. [2] proposed a wine-rack mechanism to explain the NLC effect and it has been shown that this mechanism can be used to explain the experimentally measured or predicted NLC in many systems including methanol monohydrate [3] and α-BiB_3O_6 [5]. Except for the wine-rack structure, there are many other 2D structure such as hexagonal honeycombs structures [6], truss-type systems [7] and rotating rigid units [8-9].

Different from 2D structures, there are very few 3D structures with negative compressibility in present study, mainly including the hexagonal dodecahedron [10], the octahedron model [1] and the dodecahedron model [1]. In view of the lack of research on 3D structures, we propose a new 3D model similar with the octahedron model [1] as shown in the fig. 1, which adds four rods in the both horizontal directions. It is proved to have NLC and NAC and the characteristics in both horizontal directions are the same. When compared with octahedral structure, it can be found that this structure has better negative compression effect in the horizontal direction, which provides a reference for future material design.

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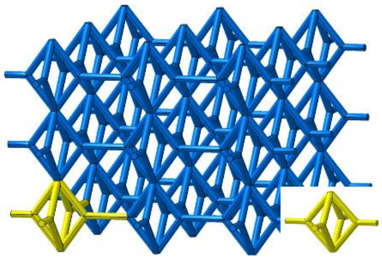

Figure. 1 the Structural sketch of the elongated octahedron model: unit cell array and unit cell

2. Analytical Model

As shown in Fig.1, it is a structure based on the elongated octahedron model proposed in our previous paper [1] with two horizontal directions adding four rods. The dimensions θ, l, h are defined as in Fig. 2, so the projections of the unit cell in the OX_i (i=1, 2, 3) directions can be given by

$$X_1 = 2l_1 \cos\theta_1 + l_3 \tag{2.1}$$

$$X_2 = 2l_2 \cos\theta_2 + l_4 \tag{2.2}$$

$$X_3 = 2l_1 \sin\theta_1 = 2l_2 \sin\theta_2 \tag{2.3}$$

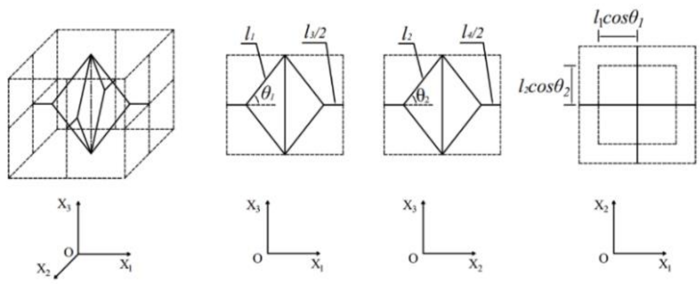

Figure. 2 The unit cell models and its two-dimensional projections in the three axes.

Then the expressions of the linear compressibility in the OX_i directions can be given by

$$\beta_L(OX_1) = \frac{l_1^2}{2k_h}\frac{\sin^2\theta_1 \tan\theta_1}{\tan^2\theta_1 + \tan^2\theta_2}\left(\frac{X_2X_3}{X_1}\tan\theta_1 + X_3\tan\theta_2 - X_3\right) \tag{2.4}$$

$$\beta_L(OX_2) = \frac{l_1^2}{k_h}\frac{\sin^2\theta_1 \tan\theta_2}{\tan^2\theta_1 + \tan^2\theta_2}\left(\frac{X_1X_3}{X_2}\tan\theta_2 + X_3\tan\theta_1 - X_1\right) \tag{2.5}$$

$$\beta_L(OX_3) = \frac{l_1^2}{k_h}\frac{\sin^2\theta_1}{\tan^2\theta_1 + \tan^2\theta_2}\left(\frac{X_1X_2}{X_3} - X_1\tan\theta_2 - X_2\tan\theta_1\right) \tag{2.6}$$

Moreover, the area compressibility and volume compressibility of this model can be obtained by substituting Eqs. (2.4-2.6) into Eq. (2.7) and Eq. (2.8)

$$\beta_A(OX_i - OX_j) = \beta_L(OX_i) + \beta_L(OX_j) \tag{2.7}$$

$$\beta_V = \beta_L(OX_1) + \beta_L(OX_2) + \beta_L(OX_3) \tag{2.8}$$

Note that in the case when $l_1=l_2=l$, $\theta_1=\theta_2=\theta$ (i.e. $OX_1 = OX_2$) and $k=l_3/l_1\cos\theta_1=l_4/l_2\cos\theta_2$, the expressions for the linear compressibility simplify to

$$\beta_L(OX_1) = \beta_L(OX_2) = \frac{l^3 \sin\theta \cos^2\theta}{k_h}(2\tan^2\theta - 1 - k) \tag{2.9}$$

$$\beta_L(OX_2) = \frac{l^3 \cos^3\theta \cot\theta}{2k_h}(1+k)[(1+k) - 2\tan^2\theta] \tag{2.10}$$

3. Discussion

Through the analysis of the formulas (2.4)-(2.10) and the fig.3 obtained from them, we can find that the structural formula has NLC and NAC, which mainly depends on the geometric parameters of the structure, such as the length of the rid and the angle between the two rids.

At first, we can note that NLC can be exhibited in this model when the following conditions are satisfied:

For NLC in the OX_1 and OX_2 direction

$$2\tan^2\theta < 1+k \tag{3.1}$$

For NLC in the OX_3 direction

$$2\tan^2\theta > 1+k \tag{3.2}$$

This means that in this relatively symmetrical model, the negative linear compressibility (NLC) in the OX_1 and OX_2 directions that exists simultaneously will be completely contrary to the condition of NLC in the OX_3 direction, and vice versa. From these formulas, we can also analyze the condition of zero compressibility of this system in the three directions, which corresponds to the turning point, i.e. $\theta = arctan\sqrt{0.5(1+k)}$. It shows that with the increase of k (that is, with the increase of l_3), the angle value of zero compressibility of this system increases gradually.

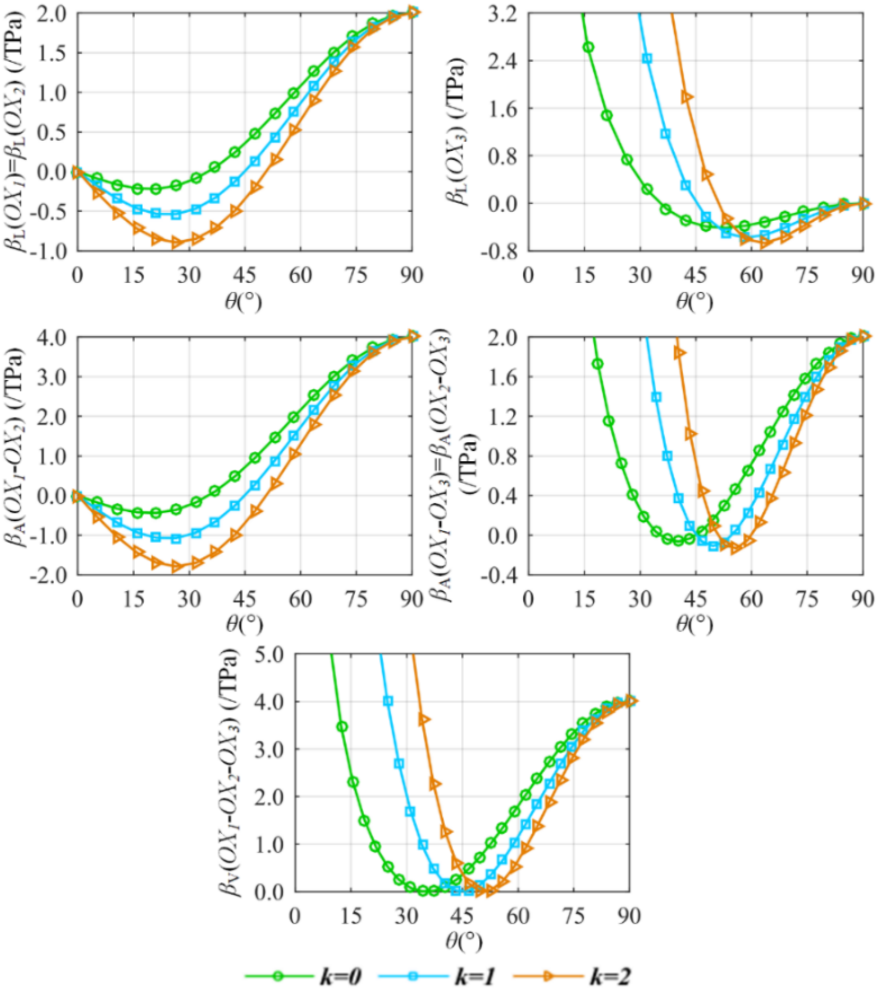

Figure. 3 The linear, area and volume compressibility across various angles of θ with k_h=1 kJ•rad^{-2} and l=1 mm

In addition, as shown in Fig. 3 (a) (b) and (c), we can find that with the increase of k, the range of NLC in OX_1 and OX_2 directions is also increasing, and so does the maximum value of NLC. On the contrary, in the OX_3 direction, the range of NLC decreases with the increase of k, but the value of maximum negative compressibility increases slightly rather than decreases. When k is zero, the corresponding octahedron structure, which we have studied in detail before. Therefore, we can draw a conclusion through this phenomenon that increasing the lengths of rods l_3 and l_4 can increase the linear negative compressibility effect in these two directions (including the range of NLC and the maximum value of NLC). Moreover, for the OX_3 direction, although the range of negative compression reduces, the maximum linear negative compression coefficient in this direction increases. This also shows that for a three-dimensional porous structure, if the length of rod in one direction is increasing without deformation, the negative compressibility effect in this direction can be increased, and the range of negative compression in the other direction will be suppressed.

Next, let's look at the expression of surface compressibility. Similar with linear compressibility, the in-axis negative area compressibility (NAC) also exists simultaneously in the OX_1 and OX_2 direction, with which the range of negative area compressibility in the OX_3 direction is completely different. That is to say, NAC can never occur in these two directions at the same time. In addition, for the condition that the area compressibility is zero, we can get two points, i.e. $\theta = arctan\sqrt{0.5(1+k)}$ and$\theta = arctan\sqrt{1+k}$.

At last, we will observe the characteristics of volume compressibility. Note that this model can never exhibit negative volume compressibility (NVC) because if one solves the equation β_V=0, we would find that this expression has a double root, i.e. $\theta = arctan\sqrt{0.5(1+k)}$, which corresponds to the turning point when $\beta_L(OX_1)$= $\beta_L(OX_2)$= $\beta_L(OX_3)$=0. All this is graphically illustrated in fig. 3(g).

4. Conclusion

Through the detailed analysis of the stretched octahedron structure, we can draw the following conclusions:

1. This elongated octahedron structure does have NLC and NAC. Because of its symmetry, the properties in OX_1 and OX_2 directions are identical.
2. By comparing the structure with the normal octahedron structure, we can conclude that increasing the length of rod without deformation in a certain direction can increase the negative compressibility effect in this direction, while weakening the range of negative compression in the repulsive direction. This conclusion provides a reference for the design of negative compressive structures in the future.

Acknowledgments
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