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Periodic boundary conditions for unit cells of periodic cellular solids in the determination of effective properties using beam elements

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ABSTRACT

Finite element analysis using solid elements to determine effective elastic properties of periodic cellular solids from their unit cells has been extensively studied. Using solid elements in this type of analysis is computationally expensive. Since many periodic cellular solids resemble frame structures, it is reasonable to represent their struts by beam elements instead of solid elements. Models of unit cells of periodic cellular solids that use beam elements are easier to create and require less computational resources. To obtain effective elastic properties from a unit cell of a periodic cellular solid, periodic boundary conditions must be applied to the unit cell. When solid elements are used, the application of periodic boundary conditions is quite straightforward. This is not true for beam elements. For a periodic cellular solid, there will always be more than one possible unit-cell configuration. Some unit-cell configurations may have some struts that are cut transversely, longitudinally or both. Correct periodic boundary conditions when beam elements are used can be quite obscure. This study aims to discuss this obscurity. The correct ways to prescribe periodic boundary conditions of unit cells are mentioned. The distinctions between periodic boundary conditions for solid elements and beam elements are shown. Moreover, the appropriate choices of unit-cell configurations are suggested for the effectiveness of the analysis.

1. INTRODUCTION

Cellular solids are useful materials and they are used in various applications. They can provide special properties such as light weight, low density, low thermal conductivity, and high energy absorption. According to the orderliness of their pores, cellular solids can be classified into two groups, namely random cellular solids and periodic cellular solids. Periodic cellular solids are composed of repeating structures called unit cells. Their properties can be designed by changing their unit-cell topologies

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and, likewise, their properties can be analyzed from their unit cells. The properties of periodic cellular solids can be designed to obtain materials with extreme mechanical properties such as Poisson's ratio close to -1, 0, and 0.5 (Milton 1992, Sigmund 1995). Unit-cell scaffolds in tissue engineering are examples of periodic cellular solids. Since tissue-engineering scaffolds are commonly used in human bodies for medical treatments, they require specific physical, mechanical, and biological properties. Mechanical properties of unit-cell scaffolds are important especially when they are used to replace load bearing tissues. Unit cells of tissue-engineering scaffolds are very small, usually in the micrometer scale, and tissue-engineering scaffolds generally contain large amounts of unit cells. For a periodic cellular solid, changing the number of unit cells causes changes in apparent properties. However, the properties will converge to constants called effective properties when the number of unit cells is sufficiently large. In other words, if the size of the unit cell is sufficiently small when compared to the size of the whole solid, the apparent properties converge to the effective properties. By using a homogenization theory, the effective properties of a periodic cellular solid can be analyzed from its unit cell under prescribed periodic boundary conditions.

Some periodic cellular solids resemble frame structures. Their structures are composed of connecting slender struts (Wallach and Gibson 2001, Yan *et al.* 2006, Yeong *et al.* 2010). Presently, finite element analysis using solid elements is extensively used in the determination of effective elastic properties of periodic cellular solids (Jean and Engelmayr 2010, Lin *et al.* 2004, Xia *et al.* 2007) even though using solid elements in this type of analysis is quite computationally expensive. In order to simplify the process of finite element modeling and reduce computational resources, it is reasonable to represent slender struts by beam elements instead of solid elements. When a unit cell is selected for the analysis, various configurations are possible depending on individual judgment. The struts of the cellular solid can be cut transversely or longitudinally to obtain the unit cell. If solid elements are used, correct modeling and correct periodic boundary conditions can be quite evident although their implementation can be rather involved. Oppositely, if beam elements are used, correct modeling and correct periodic boundary conditions can be quite obscure but their implementation can be quite simple. Especially when there are longitudinally cut struts in the unit cell, finite element modeling by beam elements requires careful consideration of beam elements' sectional properties. Finite element modeling of unit cells by beam elements, including correct periodic boundary conditions, are discussed in this paper. The distinctions between the periodic boundary conditions for solid elements and beam elements are shown. The study considers only 2D periodic cellular solids.

2. STRAIN-ENERGY BASED HOMOGENIZATION

The homogenization method of periodic cellular solids based on strain energy has been studied by many researchers (Dai and Zhang 2009, Wang *et al.* 2008, Xu and Zhang 2011, Zhang *et al.* 2007). The method allows the effective properties of a periodic cellular solid to be determined from its unit cell. Only a brief discussion on the method is shown here. Consider a periodic cellular solid that is composed of a significantly large number of unit cells. Define the effective material constant C^*_{ijkl} of the solid as

$$\langle\sigma_{ij}\rangle = C^*_{ijkl}\langle\epsilon_{kl}\rangle, \tag{1}$$

where $\langle\sigma_{ij}\rangle$ and $\langle\epsilon_{kl}\rangle$ are the average stress and strain, averaged over the whole volume of the domain. A set of kinematic boundary conditions is applied to the domain such that it results in the displacement field u_i written as

$$u_i = \epsilon^o_{ij}x_j + u^p_i. \tag{2}$$

Here, ϵ^o_{ij} is a constant tensor and u^p_i is the periodic component of u_i, whose volume average is zero. It can be shown that the displacement field in Eq. (2) yields $\langle\epsilon_{kl}\rangle = \epsilon^o_{ij}$. The displacement field in Eq. (2) also allows the strain energy of the unit cell U_c to be written in terms of the average strain ϵ^o_{ij}, i.e.,

$$U_C = \frac{1}{2}C^*_{ijkl}\epsilon^o_{kl}\epsilon^o_{ij}V_C\ , \tag{3}$$

where V_C is the volume of the unit cell.

By prescribing different modes of ϵ^o_{ij} to the unit cell and numerically computing the corresponding strain energy values, Eq. (3) allows C^*_{ijkl} to be computed (Dai and Zhang 2009, Wang *et al.* 2008, Zhang *et al.* 2007). Two-dimensional periodic cellular solids are usually orthotropic materials, which can be defined by four independent material constants. As a result, four different unit strain states are required in the determination of the effective material constants, i.e.,

$$\begin{Bmatrix}\epsilon^0_{11}\\ \epsilon^0_{22}\\ 2\epsilon^0_{12}\end{Bmatrix} = \begin{Bmatrix}1\\0\\0\end{Bmatrix}, \quad \begin{Bmatrix}0\\1\\0\end{Bmatrix}, \quad \begin{Bmatrix}0\\0\\1\end{Bmatrix}, \quad \begin{Bmatrix}1\\1\\0\end{Bmatrix}. \tag{4}$$

3. FINITE ELEMENT DOMAINS OF UNIT CELLS

In analysis of a periodic cellular solid, a unit cell has to be selected from the periodic cellular solid. Depending on individual judgment, various unit-cell configurations are possible. The boundary of the selected configuration may cut through the struts transversely or longitudinally. Fig 1 shows an example periodic cellular solid, which is composed of square unit cells. The figure also shows two different unit-cell configurations. All struts of the unit cell in configuration *i* are cut transversely and all struts of the unit cell in configuration *ii* are cut longitudinally. When solid elements are used, the two configurations simply have different domains but the two domains do not require any special treatment. However, when beam elements are used, the axial and bending rigidities of struts in configuration *ii* must be only half of those in configuration *i*.

If the unit cells of configuration *ii* are reassembled back together, each beam element and its adjacent element must together provide the original axial and bending rigidities. The half axial and bending rigidities can be obtained by simply reducing the values of the sectional area and moment of inertia by half.

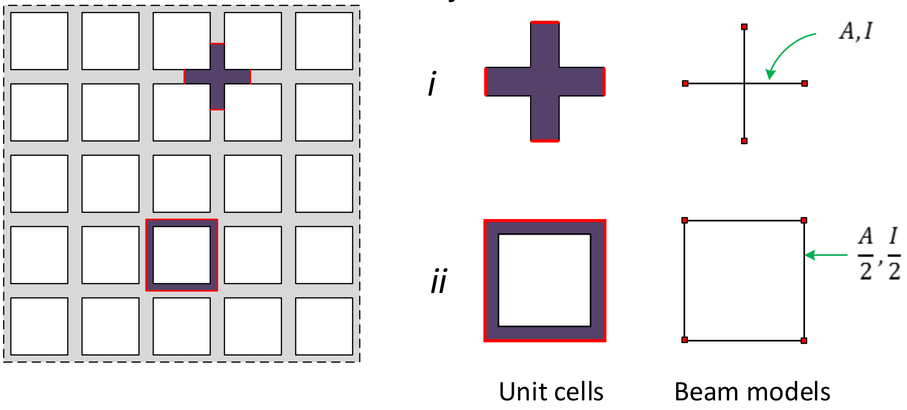


Fig. 1 Periodic cellular solid and two different unit cells

4. PERIODIC BOUNDARY CONDITIONS

In the determination of the effective properties of a periodic cellular solid from its unit cell, periodic boundary conditions have to be used (Drago and Pindera 2007, Nguyen *et al.* 2012, Pecullan *et al.* 1999). Periodic boundary conditions must satisfy the periodicity of the displacement field given by Eq. (2). Prescribing periodic boundary conditions requires two types of boundary prescription. The first type is the ordinary prescription of exact values of some degrees of freedom. The second type is the prescription of relative values between some degrees of freedom. The first type of boundary condition is required to prevent rigid body displacements. The second type of boundary condition comes from the periodic displacement field u_i^p in Eq. (2). Fig. 2 shows the periodic boundary conditions of the example unit cells from the previous section. The figure shows the locations on the boundary where u_i^p must be the same due to the periodicity. If any two nodal points on the boundary have the same u_i^p, the relative displacements between the two points can be obtained from Eq. (2) for each prescribed strain mode. Then, the obtained relative displacement conditions have to be prescribed on the two nodal points. For models that use beam elements, when u_i^p of two nodal points are the same, their rotational degrees of freedom θ must also be the same.

Since the second type of boundary condition is required in prescribing correct periodic boundary conditions, it is preferable to have unit cells that do not have large cut boundary surfaces when solid elements are used. Otherwise, there will be a large number of relative displacement conditions to be prescribed. It is therefore obvious that, in Fig. 1, configuration *i* is better than configuration *ii* in this respect. This kind of difference between configurations is not significant when beam elements are used. Consider the unit cell of configuration *ii* that employs beam elements. The relative displacement conditions along the two vertical cut boundary surfaces of the unit cell are satisfied automatically if the relative displacement conditions between the corner nodes are correctly satisfied. This is because the same displacement interpolation function is used in all beam elements. In any case, models that use beam elements always require much less effort to prescribe relative displacement conditions than those that use solid elements.

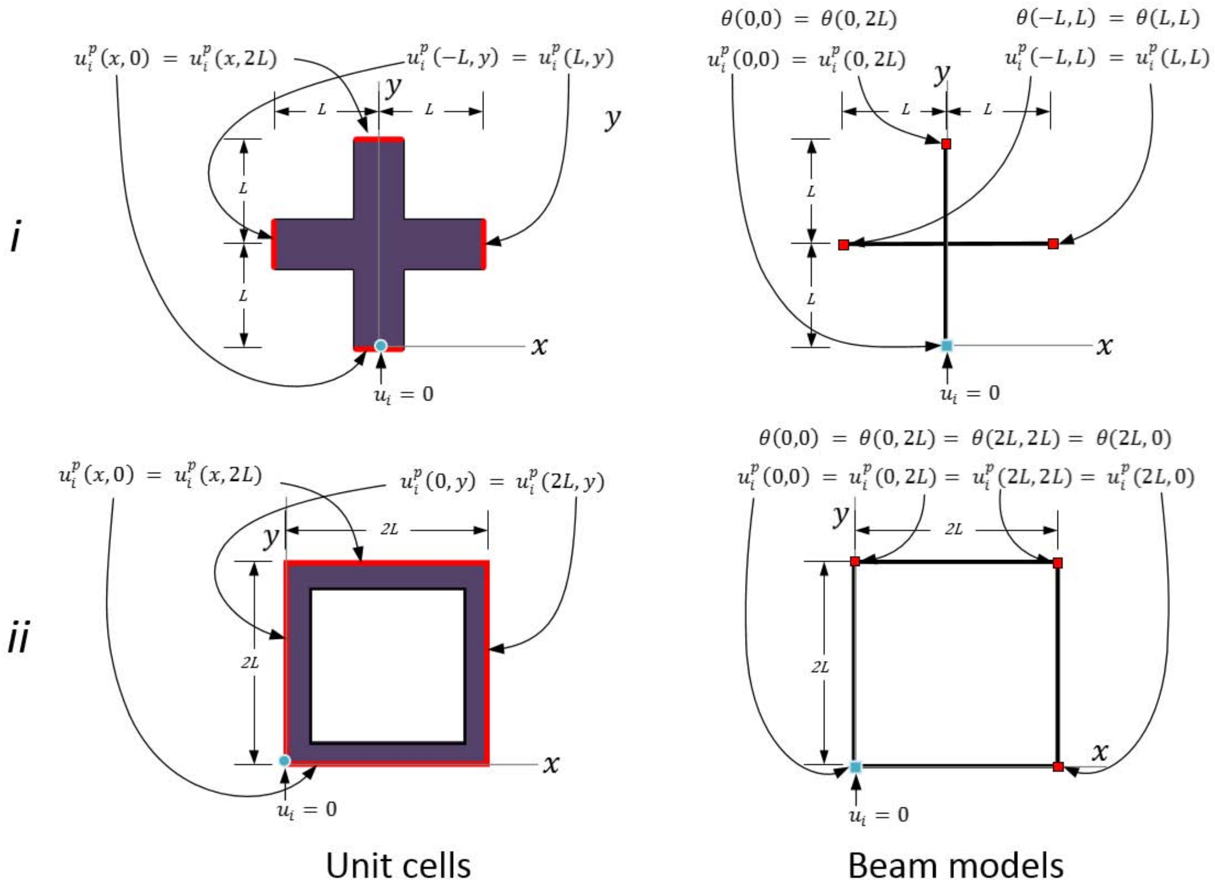


Fig. 2 Periodic boundary conditions of unit cells

5. EXAMPLES

As examples, the effective Young's moduli and Poisson's ratio of the periodic cellular solid shown in Fig. 3 are determined. The cellular solid is composed of hexagonal unit cells. The distance between the opposing struts of a hexagonal unit cell is 1 mm. Each strut has a square cross section of 0.1×0.1 mm. There are many possible unit-cell configurations, some of which are shown in Fig. 3. Between the three unit-cell configurations in Fig. 3, the H3 configuration has the smallest cut boundary surfaces. Consequently, the H3 configuration has the smallest number of relative displacement conditions. This configuration is therefore selected as the example model in this study. The H3 unit cell is modeled by 4-noded quadrilateral plane stress elements and Euler beam elements. The constitutive material is assumed to be linear elastic isotropic with Young's modulus equal to 1 GPa and Poisson's ratio equal to zero.

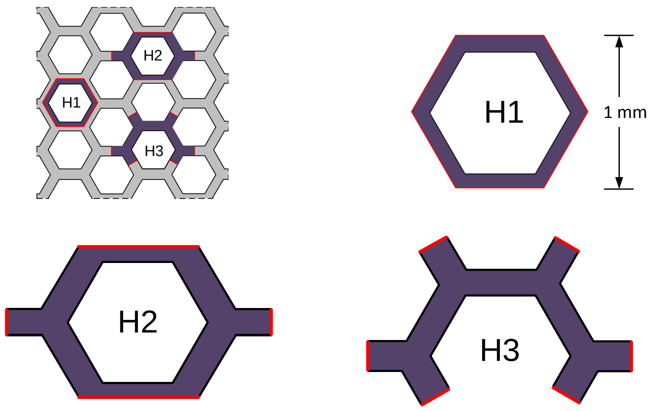


Fig. 3 Periodic cellular solid with hexagonal unit cells

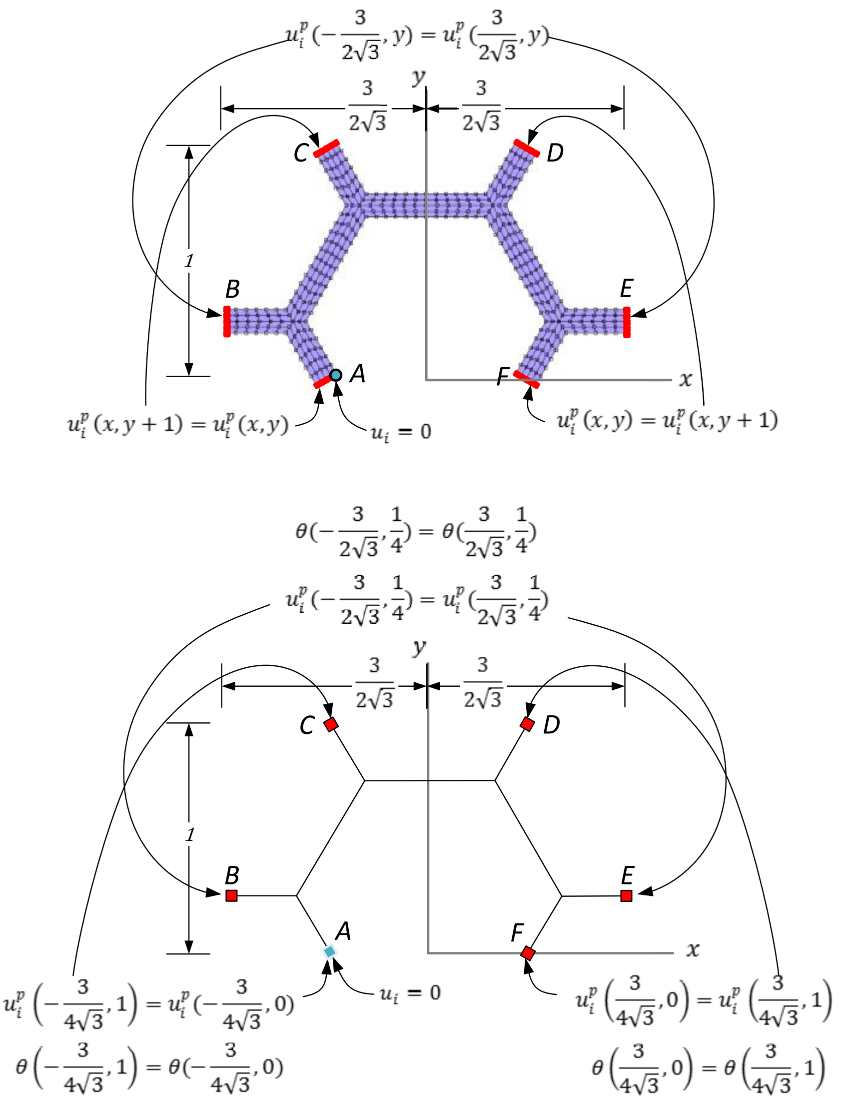


Fig. 4 Periodic boundary conditions of the H3 unit cell

5.1 Periodic boundary conditions

Fig. 4 shows the periodic boundary conditions of the H3 unit cell both for the models using solid elements and beam elements. All translational displacements of a selected node in each model are fixed to prevent rigid body displacements. For this unit-cell configuration, there are three pairs of boundaries where relative displacement conditions must be considered as shown in Fig. 4.

As examples, the periodic displacement boundary conditions for the unit shear strain state ($\epsilon_{11}^o = \epsilon_{22}^o = 0,\ 2\epsilon_{12}^o = 1$) for the unit cell modeled by beam elements are shown in detail here. Eq. (2) is written for u_1 of points *A* and *C* in the figure as

$$u_1\left(-\frac{3}{4\sqrt{3}},0\right) = \epsilon_{11}^o x_1 + \epsilon_{12}^o x_2 + u_1^p\left(-\frac{3}{4\sqrt{3}},0\right)$$
$$= (0)\left(-\frac{3}{4\sqrt{3}}\right) + \left(\frac{1}{2}\right)(0) + u_1^p\left(-\frac{3}{4\sqrt{3}},0\right) = u_1^p\left(-\frac{3}{4\sqrt{3}},0\right), \quad (5)$$

$$u_1\left(-\frac{3}{4\sqrt{3}},1\right) = \epsilon_{11}^{o}x_1 + \epsilon_{12}^{o}x_2 + u_1^p\left(-\frac{3}{4\sqrt{3}},1\right)$$
$$= (0)\left(-\frac{3}{4\sqrt{3}}\right) + \left(\frac{1}{2}\right)(1) + u_1^p\left(-\frac{3}{4\sqrt{3}},1\right) = \frac{1}{2} + u_1^p\left(-\frac{3}{4\sqrt{3}},1\right). \quad (6)$$

Since $u_i = 0$ at $\left(-\frac{3}{4\sqrt{3}},0\right)$, Eq. (5) yields

$$u_1^p\left(-\frac{3}{4\sqrt{3}},0\right) = u_1\left(-\frac{3}{4\sqrt{3}},0\right) = 0. \quad (7)$$

Since $u_1^p\left(-\frac{3}{4\sqrt{3}},1\right) = u_1^p\left(-\frac{3}{4\sqrt{3}},0\right) = 0$, Eq. (6) yields

$$u_1\left(-\frac{3}{4\sqrt{3}},1\right) = \frac{1}{2}. \quad (8)$$

Eq. (2) is written for u_1 of points *F* and *D* as

$$u_1\left(\frac{3}{4\sqrt{3}},0\right) = (0)\left(\frac{3}{4\sqrt{3}}\right) + \left(\frac{1}{2}\right)(0) + u_1^p\left(\frac{3}{4\sqrt{3}},0\right) = u_1^p\left(\frac{3}{4\sqrt{3}},0\right), \quad (9)$$

$$u_1\left(\frac{3}{4\sqrt{3}},1\right) = (0)\left(\frac{3}{4\sqrt{3}}\right) + \left(\frac{1}{2}\right)(1) + u_1^p\left(\frac{3}{4\sqrt{3}},1\right) = \frac{1}{2} + u_1^p\left(\frac{3}{4\sqrt{3}},1\right). \quad (10)$$

Since $u_1^p\left(\frac{3}{4\sqrt{3}},0\right) = u_1^p\left(\frac{3}{4\sqrt{3}},1\right)$, Eqs. (9) and (10) give

$$u_1\left(\frac{3}{4\sqrt{3}},1\right) = u_1\left(\frac{3}{4\sqrt{3}},0\right) + \frac{1}{2}. \quad (11)$$

Eq. (2) is written for u_1 of points *B* and *E* as

$$u_1\left(-\frac{3}{2\sqrt{3}},\frac{1}{4}\right) = (0)\left(-\frac{3}{2\sqrt{3}}\right) + \left(\frac{1}{2}\right)\left(\frac{1}{4}\right) + u_1^p\left(-\frac{3}{2\sqrt{3}},\frac{1}{4}\right) = \frac{1}{8} + u_1^p\left(-\frac{3}{2\sqrt{3}},\frac{1}{4}\right). \quad (12)$$

$$u_1\left(\frac{3}{2\sqrt{3}},\frac{1}{4}\right) = (0)\left(\frac{3}{2\sqrt{3}}\right) + \left(\frac{1}{2}\right)\left(\frac{1}{4}\right) + u_1^p\left(\frac{3}{2\sqrt{3}},\frac{1}{4}\right) = \frac{1}{8} + u_1^p\left(\frac{3}{2\sqrt{3}},\frac{1}{4}\right). \quad (13)$$

Since $u_1^p\left(-\frac{3}{2\sqrt{3}},\frac{1}{4}\right) = u_1^p\left(\frac{3}{2\sqrt{3}},\frac{1}{4}\right)$, Eqs. (12) and (13) yield

$$u_1\left(\frac{3}{2\sqrt{3}},\frac{1}{4}\right) = u_1\left(-\frac{3}{2\sqrt{3}},\frac{1}{4}\right). \quad (14)$$

Similarly, the following conditions can be obtained for u_2, i.e.,

$$u_2\left(-\frac{3}{4\sqrt{3}},1\right) = u_2\left(-\frac{3}{4\sqrt{3}},0\right), \tag{15}$$

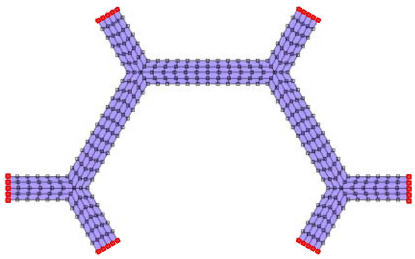
$$u_2\left(\frac{3}{4\sqrt{3}},1\right) = u_2\left(\frac{3}{4\sqrt{3}},0\right), \tag{16}$$

$$u_2\left(\frac{3}{2\sqrt{3}},\frac{1}{4}\right) = u_2\left(-\frac{3}{2\sqrt{3}},\frac{1}{4}\right) + \frac{3}{2\sqrt{3}}. \tag{17}$$

The periodic boundary conditions for the other strain states can be calculated in the same manner.

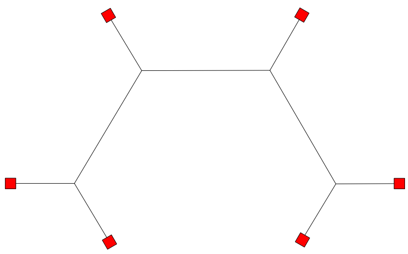
5.2 Results

The effective moduli E_x^*, E_y^*, and G^*, normalized by the Young's modulus of the constitutive material E_m, and the effective Poisson's ratios ν^* of the example periodic cellular solid are shown in Fig. 5. The normalized effective Young's moduli from the models using solid and beam elements are 0.0115 and 0.0110, respectively. The difference between the two results is 4.47%. The normalized shear moduli are 0.0031 for the model using solid elements and 0.0029 for the model using beam elements. The difference is 5.13%. The effective Poisson's ratios from the models using solid and beam elements are 0.8882 and 0.8899, respectively, in which the difference is 0.19%.



Solid elements

$$\frac{E_x^*}{E_m} = \frac{E_y^*}{E_m} = 0.0115$$
$$\frac{G^*}{E_m} = 0.0031$$
$$\nu^* = 0.8882$$



Euler beam elements

$$\frac{E_x^*}{E_m} = \frac{E_y^*}{E_m} = 0.0110$$
$$\frac{G^*}{E_m} = 0.0029$$
$$\nu^* = 0.8899$$

Fig. 5 The obtained effective properties

6. CONCLUSIONS

For frame-like periodic cellular solids, Euler beam elements can be used instead of solid elements in the determination of effective properties. The advantages of the Euler beam element in this type of analysis are that finite element models using Euler beam elements are easier to create, and require less computational resources. In addition, it is easier to prescribe periodic boundary conditions when beam elements are used. Since beam elements idealize the domain as connecting lines, models of unit cells that use beam elements must be carefully created. If a strut is split in half longitudinally to create a unit cell, an Euler beam element with half axial and half bending rigidities must be used to represent each half of the split strut. Using beam elements simplifies the prescription of relative displacement conditions on cut boundary surfaces of unit cells. Using solid elements may result in a large number of relative displacement conditions to be prescribed. When solid elements are used, it is important that unit-cell configurations are selected in such a way that cut boundary surfaces are as small as possible. This is to reduce the number of relative displacement conditions. Finally, in this study, the differences between the effective properties obtained from models using solid and Euler beam elements are found to be small.

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REFERENCES

Dai, G. and Zhang, W. (2009), "Cell Size Effect Analysis of the Effective Young's Modulus of Sandwich Core", *Computational Materials Science,* **46**(3), 744-748.

Drago, A. and Pindera, M.J. (2007), "Micro-Macromechanical Analysis of Heterogeneous Materials: Macroscopically Homogeneous Vs Periodic Microstructures", *Compos. Sci. Technol.,* **67**(6), 1243-1263.

Jean, A. and Engelmayr, G.C. (2010), "Finite Element Analysis of an Accordion-Like Honeycomb Scaffold for Cardiac Tissue Engineering", *J. Biomech.,* **43**(15), 3035-3043.

Lin, C.Y., Kikuchi, N. and Hollister, S.J. (2004), "A Novel Method for Biomaterial Scaffold Internal Architecture Design to Match Bone Elastic Properties with Desired Porosity", *J. Biomech.,* **37**(5), 623-636.

Milton, G.W. (1992), "Composite Materials with Poisson's Ratios Close to - 1", *Journal of the Mechanics and Physics of Solids,* **40**(5), 1105-1137.

Nguyen, V.D., Béchet, E., Geuzaine, C. and Noels, L. (2012), "Imposing Periodic Boundary Condition on Arbitrary Meshes by Polynomial Interpolation", *Computational Materials Science,* **55**(390-406.

Pecullan, S., Gibiansky, L.V. and Torquato, S. (1999), "Scale Effects on the Elastic Behavior of Periodic and Hierarchical Two-Dimensional Composites", *Journal of the Mechanics and Physics of Solids,* **47**(7), 1509-1542.

Sigmund, O. (1995), "Tailoring Materials with Prescribed Elastic Properties", *Mech. Mater.,* **20**(4), 351-368.

Wallach, J.C. and Gibson, L.J. (2001), "Mechanical Behavior of a Three-Dimensional Truss Material", *IJSS,* **38**(40–41), 7181-7196.

Wang, H.B., Zhang, W.H., Xu, Y.J. and Zeng, Q.F. (2008), "Numerical Computing and Experimental Validation of Effective Elastic Properties of 2d Multilayered C/Sic Composites", *Mater. Sci. Technol.,* **24**(11), 1385-1398.

Xia, Z., Ju, F. and Sasaki, K. (2007), "A General Finite Element Analysis Method for Balloon Expandable Stents Based on Repeated Unit Cell (Ruc) Model", *Finite Elements in Analysis and Design,* **43**(8), 649-658.

Xu, Y. and Zhang, W. (2011), "Numerical Modelling of Oxidized Microstructure and Degraded Properties of 2d C/Sic Composites in Air Oxidizing Environments Below 800°C", *Mater. Sci. Eng., A,* **528**(27), 7974-7982.

Yan, J., Cheng, G., Liu, S. and Liu, L. (2006), "Comparison of Prediction on Effective Elastic Property and Shape Optimization of Truss Material with Periodic Microstructure", *IJMS,* **48**(4), 400-413.

Yeong, W.Y., Sudarmadji, N., Yu, H.Y., Chua, C.K., Leong, K.F., Venkatraman, S.S., Boey, Y.C.F. and Tan, L.P. (2010), "Porous Polycaprolactone Scaffold for Cardiac Tissue Engineering Fabricated by Selective Laser Sintering", *Acta Biomater.,* **6**(6), 2028-2034.

Zhang, W., Dai, G., Wang, F., Sun, S. and Bassir, H. (2007), "Using Strain Energy-Based Prediction of Effective Elastic Properties in Topology Optimization of Material Microstructures", *Acta Mechanica Sinica/Lixue Xuebao,* **23**(1), 77-89.

Zhang, W., Wang, F., Dai, G. and Sun, S. (2007), "Topology Optimal Design of Material Microstructures Using Strain Energy-Based Method", *ChJA,* **20**(4), 320-326.