Homogenized Properties of Porous Microstructure: Effect of Void Shape and Arrangement

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Abstract. This paper aims to investigate the effect of void shape and arrangement on the effective elastic properties of porous microstructure. The characteristics of the voids are in different shapes, sizes and arrangement. The porous microstructure models were developed using CATIA. Then, VoxelCon was employed to analyse the multiscale finite element model and determine the homogenized properties. Based on the results, void shape, size, and arrangement of porous microstructure were found sensitive to the elastic (homogenized) properties. Ellipsoidal shape having the highest Young’s modulus, whereas the spherical shape has the highest Poisson’s ratio and shear modulus. Cubical shape was the lowest for all the elastic properties. Moreover, the formation arrangement in void cubical shape produced the highest Young’s modulus and shear modulus.

1. Introduction

Porous material is a material containing pores or it can be called as voids. The pores have porosity that might contained air, and other particles that can stick on the wall as a pores. The characteristics of a porous material may vary depending on its size, arrangement and shape of the pores, as well as the porosity. Porous materials has been used in many applications. For instance, wood contain pores and it may not always can be seen by naked eye, but it has strong material properties that can serve as the structural foundation of a home. Porous materials with open pores are mainly used for industrial applications such as filters and carriers for catalysts and bioreactors [1]. Closed porous materials are used for thermal insulators and low specific gravity structural components and biomedical field.

Chan and Francis [2] had developed a multi scale method that allows one to predict the mechanical performance, where it includes the elastic modulus and yield strength of the 3D scaffold of a given pore geometry on the basis of properties of constituents at smaller length scales and higher structural hierarchies. From their researched, a first-principles computational method had been used to compare and analyse the mechanical properties of nano-scaled particles. On the other hand, Wang and Hu [3] had studied on the mechanical properties and pores structure deformation behaviour for porous titanium. Porous titanium has been exhibited into desirable properties as biomedical materials. Porosity of porous titanium is varying from 36% to 66% and pores size has average of 230μm, then, were fabricated by powder sintering. Its microstructure features were using scanning electron microscopy as its characteristics. Porous titanium has mechanical properties that found to be close to

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those of human bone. Its stiffness value is ranging from 1.86GPa to 14.7GPa and compressive strength values are 85.16MPa to 461.94MPa.

According to Roberts and Garboczi [4], the elastic properties of 2D phase (solid phase) porous materials depend on the geometrical nature of the pore space and solid phase and also the porosity ratio. The relevant aspects of porous materials include pore shape, size and type of the interconnections between solid areas. Besides that, they used finite element method to derive simple formulae that relate with Young’s modulus and Poisson’s ratio to porosity and microstructure for three different models of microstructure. They have created or test the three different models by overlapping solid spheres, overlapping spherical pores and overlapping ellipsoidal pores. Hence, the main objective of this study was to develop the finite element model of porous microstructure with variation of voids characteristics in order to analyse the effect of voids shape and formation on the effective elastic properties of porous microstructure.

2. Computational Analysis

2.1 Homogenization Method
Homogenization Method is macroscopic structure supposed to be made of a material that has the microscopic heterogeneity. If we can define a microscopic unit cell structure \( Y \) that can represent the global heterogeneity, the macroscopic properties can be defined as the volumetric average of the microscopic properties in the unit cell. The heterogeneous material can be replaced by the equivalent homogenized model. Then, it assumed that the unit cell is repeated periodically. By using the two scale singular perturbation theory, all the equation was followed based on previous studies [5-7].

\[
    u_i(x,y) = u_i^0(x) + \varepsilon u_i^1(x,y)
\]  

(1)

In this equation, \( u_i^0 \) microscopic or homogenized displacement and \( u_i^1 \) is a perturbed term due to the microscopic heterogeneity. Suppose that the traction \( t_i \) applied on the boundary \( \Gamma \) and the body force is neglected. An elasticity tensor is denoted as \( E_{ijkh} \). By taking the lim of \( \varepsilon \to 0 \) for homogenization, the decoupled microscopic and macroscopic equations are finally obtained. In this derivation, \( u_i^1 \) in Equation (1) is assumed to be written as below :

\[
    u_i^1(x,y) = -\chi_i^{kh}(y) \frac{\partial u_i^0(x)}{\partial x_h}
\]  

(2)

Where \( \chi_i^{kh} \) is a characteristic displacement that is a periodic function with respect to the microscale. The microscopic equation to solve for the unit cell \( Y \) under the periodic boundary condition is as follows:

\[
    \int_Y (E_{ijkh} - E_{ijmn} \frac{\partial x_k^{kh}}{\partial y_n}) \frac{\partial^2 u_i^1}{\partial y_j} dY = 0 \quad \text{for} \quad \forall u_i^1
\]  

(3)

Due to the existence of the solution in Equation (3), the macroscopic equation can be derived as below:

\[
    \int_\Omega E_{ijkh}^H \frac{\partial u_i^0}{\partial x_h} \frac{\partial u_j^1}{\partial x_j} d\Omega = \int_\Gamma t_i v_i^0 d\Gamma \quad \text{for} \quad \forall v_i^0
\]  

(4)

where \( E_{ijkh}^H \) is the homogenized elasticity tensor that is also symmetric defined by

\[
    E_{ijkh}^H = \frac{1}{|Y|} \int_Y (E_{ijkh} - E_{ijmn} \frac{\partial x_k^{kh}}{\partial y_n}) dY
\]  

(5)

where \(|Y|\) is the volume of the unit cell.
2.2 Geometrical Model
The development of porous model for void regular and void formation arrangement in this study is using CATIA Software. The model that decided to be investigated for one of the porous characteristic are cubical, spherical and ellipsoidal, where there are 18 models. Each of the arrangement has 9 models. There are 3 sizes; small, medium and large. The dimensions for the shapes were obtained by calculating the same volume for each shape. The number of voids is set to be 4 x 4 x 4 in 3D, where there are 64 numbers of voids. Total volume is 1000 mm³, where 10 mm x 10 mm x 10 mm of an outer box dimensions. Porosity or volume fraction can be calculated by number of voids divided by total volume. Porosity that decided to be determined is 15%, 20% and 25% for cubical and spherical void while ellipsoidal void is 8.03%, 10.03% and 12.78%.

![Figure 1](image1.png)

**Figure 1:** Void regular arrangement porous model; (a) Cubical, (b) Spherical, (c) Ellipsoidal.

![Figure 2](image2.png)

**Figure 2:** Void formation arrangement porous model; (a) Cubical, (b) Spherical, (c) Ellipsoidal.

2.3 Meshing
Voxel (cubical) was used as element type for all models in this study. Since validation of the present analysis using experiment work is very difficult due to the small scale size imposed in the modelling, the element size becomes very crucial in order to ensure the accuracy of numerical result. Hence, convergence test was performed in order to obtain the optimum element size. Table 1 shows the results of convergence test for all models with different void shape. The test was conducted for 0.1³, 0.2³, 0.3³, 0.4³ and 0.5³ mm³ of element size. Based on the result, element size of 0.2 was selected for all analysis in the present study.
### Table 1: Convergence test of unit cell models with variation of void shape.

| No. | Element Type | Cubical |
|-----|--------------|---------|
| 1   | Convergence Test | ![Graph](image1.png) |
|     | No. of element | 6272, 12881, 30105, 103048, 859392 |
| 2   | Element Type | Spherical |
|     | Convergence Test | ![Graph](image2.png) |
|     | No. of element | 7936, 15409, 35409, 123272, 985344 |
| 3   | Element Type | Ellipsoidal |
|     | Convergence Test | ![Graph](image3.png) |
|     | No. of element | 7680, 14533, 33429, 116264, 930048 |
2.4 Mechanical Properties of Constituent
The constituent material used is porous alumina. It has been widely used in industrial such as nanostructure template in various nano-applications. The porous structure consists of numerous hexagonal cells perpendicular to the aluminium substrate and each cell has several tens or hundreds of nano-scale pores at its centre. Because the nano-morphology of anodic porous alumina is limited by the electrolyte during anodizing, the discovery of additional electrolytes would expand the applicability of porous alumina. Porous alumina has Young’s modulus ($E$) of 404 GPa and Poisson’s ratio ($ν$) of 0.239.

3. Results & Discussion
Based on all the obtain result, the project is more clarified in term of analysis of model and theoretical of project. Convergence test was conducted in order to get the finest result for the analysis. The size of voxel element mesh that chosen to analyse all the model is 0.1mm. It is generally known that, small size of element tends to take longer time to compute the result analysis.

The result for void shape that on Young’s modulus ($E$); $E_{11}$, $E_{22}$, $E_{33}$ is shown in figure 3. Ellipsoidal shape has the highest value than spherical shape, while cubical shape is the lowest value. Next, the result on Poisson’s ratio ($ν$); $ν_{12}$, $ν_{23}$, $ν_{31}$ is depicted in figure 4. The $ν_{12}$ result shows that spherical shape has the highest value than ellipsoidal shape, while for cubical shape is the lowest. Result for $ν_{23}$, and $ν_{31}$ is the same where ellipsoidal is the highest that spherical, while cubical shape is still the lowest. Then, figure 5 shows the effect of void shape on shear modulus ($G$). $G_{12}$, $G_{23}$, $G_{31}$ was found has the same pattern as Young’s modulus ($E$); $E_{11}$, $E_{22}$, $E_{33}$.

The result for void formation effect on Young’s modulus and shear modulus is shown in figure 6. The result shows that the elastic properties was not sensitive to the void arrangement. The line graph for both arrangement (regular and formation) almost in the same line. Based on the past research, some research papers found that the elastic properties of the porous materials are not sensitive to the shape of the voids but depends on the void’s number and size. But, some papers are said the opposite. Therefore, this project is conducting for investigate and compare the problem whether the shape of the voids really affect the elastic properties and mechanical properties of the porous microstructure. The result for void shape and void formation are affect the effective elastic properties of porous microstructure.
Figure 3: Effect of shape on; (a) $E_{11}$, (b) $E_{22}$, (c) $E_{33}$.

Figure 4: Effect of shape on; (a) $\nu_{12}$, (b) $\nu_{23}$, (c) $\nu_{31}$.

Figure 5: Effect of shape on; (a) $G_{12}$, (b) $G_{23}$, (c) $G_{31}$.
Figure 6: Effect of arrangement on; (a) $E_{11}$, (b) $E_{22}$, (c) $E_{33}$.

4. Conclusion
As the conclusion, the objective of the project had been achieved. The project successfully developed the finite element model of porous microstructure with variation of voids characteristics. The project also managed to analyse the effect of voids shape on the effective elastic properties of porous microstructure. Besides that, the project had also investigated the effect of voids formation on the effective elastic properties of porous microstructure. Based on the results and analysis, ellipsoidal shape having the highest Young’s modulus. Next, spherical shape has the highest Poisson’s ratio and shear modulus. Whereas, cubical shape is the lowest for all the elastic properties. Besides that, the effect of void arrangement on cubical shape, void formation has the highest Young’s modulus and shear modulus. While for spherical shape void arrangement, void formation has the highest value for both Young’s modulus and shear modulus. Moreover, ellipsoidal shape has the highest Young’s modulus and shear modulus on void regular arrangement. Hence, all of the factors does affect the elastic properties of porous microstructure.

The result obtained based on the study of previous research papers and significant information also knowledge on the effect of void in porous microstructure. It is important to study and know whether the void affect or not on the structural element of the porous microstructure. This is especially for those in manufacturing or building industry.

5. References
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