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A K A P I T

2-/3-D DIGITAL MATERIAL REPRESENTATION AND EVALUATION OF METAL FOAMS

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Abstract

Recently metal foams are becoming popular in engineering application due to their high energy absorption ability and low density, which are being utilised in automotive engineering and aerospace engineering as well as biomedical engineering. As a typical porous or cellular material, from the material design's point of view, metal foams have typical heterogeneous structures crossing length scales, which can be defined by only two phases: matrix material and voids. The voids are termed as cells or pores. Their structures can be characterised by several main geometric parameters related to the cells, such as size, shape, spatial distribution and arrangement and so on. The digital material representation (DMR) of metal foams has been employed to represent metal foams accounting for their complex structures. However random distributions of the size and shape of cells in most foam materials make the digital material representation and modelling of such materials very complicated. Furthermore, effects of size and shape of cells on mechanical behaviours of metal foams have been found and investigated numerically and experimentally in authors' previous studies in which the authors have developed a digital framework for the representation, modelling and evaluation of multi-phase materials including metal foams.

In this study, the developed digital framework for the representation, modelling and evaluation of microstructured or multi-phase materials has been further developed with a multi-scale sense including both two-/three-dimensional (2-/3-D) finite element modelling to represent metal foams with a certain distribution on cell size and shape, which can be used for digital or virtual testing to determine mechanical properties and behaviours of such foams. A linkage between 2-D and 3-D finite element models has been built up through a comparativeness analysis between them. For validation and verification purpose, the results obtained from these models have been compared with those from experimental work and good agreement has been found which demonstrated the effectiveness of the digital framework developed for metal foams.

Key words: metal foams, mechanical behaviour, digital material representation, finite element modelling, virtual testing and compression

1. INTRODUCTION

Metal foams, as a new generation material, have superb material properties, i.e., high stiffness in conjunction with very low specific weight, or high compression strength combined with good energy absorption characteristics (Gibosn, 2000; Ashby, 2000). They are ideal material candidates in a wide range of engineering applications, including automotive engineering and aerospace engineering, in which the engineers are seeking light metals to re-

place the traditionally 'heavy' materials, i.e., steels. Therefore such porous materials have attracted a lot of research interests on material fabrication, evaluation and optimisation design purposes. Except for experimental studies, with the aid of modern computer power, numerical modelling and simulations have been widely developed and utilsed to study metal foams in literature (Shen & Brinson, 2006, 2007; Shen et al., 2006; An et al., 2010; Yang et al., 2014).

Metal foams are typically heterogeneous materials, which can be regarded inhomogeneous at different length scales. They have only two distinct phases: solid phase (cell walls) and hollow phase (cells or pores). The foams can be characterised by several main geometric parameters of the hollow phase–cells, existing in the materials, such as their size, shape, spatial distribution, compactness (space occupied by phases regarding the total space), and arrangement (regular and irregular or random), and so on (Jurczyk et al., 2007; Madej et al., 2009, Chen and Krill, 2002; Groeber, 2007). Their material properties and mechanical behaviours greatly depend on their geometric structures, especially for cells. Recently the experimental and numerical studies on metal foams have revealed the geometry and spatial distribution of cells in titanium foams including their size and shape have significant influences on their material properties and mechanical behaviours (An et al., 2010; Yang et al., 2014). To incorporate the spatial arrangement of phase components in numerical modelling and simulations, it is essential to quantitatively characterise the randomly-distributed representative structures in such materials. From digital representation reconstruction and fabrication's point of view, several different methods have been developed and employed to generate such material structures (Brahme et al., 2006; Pyrz & Bochenek, 2004; Riesch-Oppermann et al., 2002; Asgari et al., 2009; Michailidis et al., 2010, 2011), i.e., Voronoi tessellation method, cellular automata grain growth algorithm, sphere growth algorithm, and image analysis methods, etc. If the cells in closed-cell metal foams are treated as circular shape in 2-D and spherical shape in 3-D, the circle (2-D)/sphere (3-D) growth algorithm is found an appropriate tool and it enables researchers to create large structures with high dispersion of cell size and random spatial distribution of cells.

In this study, following the authors' recent work on development of a digital framework for the representation, finite element modelling and evaluation of microstructured or multi-phase materials, a 2-/3-D digital framework for closed-cell foam materials with random cell distributions is further developed with the implementation of a multi-scale sense. This framework includes digital material representation and fabrication, finite element model generation and digital testing on the characterisation and evaluation of material properties and mechanical behaviours of such materials. Both 2-/3-D finite element models of closed-cell metal foams have been developed and

the linkage between 2-D model and 3-D model is investigated and created at the first time to authors' knowledge. For verification and validation, the numerical results extracted from the current digital framework are compared to those obtained from experimental work. Based on these ideas, the main body of the paper is structured with six main sections. In Section 2 the experimental work on fabricating titanium foams with a 70% porosity is performed to determine their internal structure, i.e. cell size, cell shape and distribution, etc. and Section 3 describes the digital representation and fabrication of these closed-cell foams are then conducted using the sphere growth algorithm from an inverse problem's point of view, considering both 2-/3-D geometries of characteristic material structures. In Section 3, the generation of the 2-/3-D finite element models and their meshes are also performed based on the geometries obtained using a free mesh generator – Gmsh (Geuzaine & Remacle, 2009) and analysed using the commercial finite element analysis package – Abaqus. The linkage between the 2-D and 3-D models is also identified, in which the utilisation of 2-D model can greatly improve the efficiency of numerical simulations of metal foams. Section 4 gives the whole idea and procedure of the virtual testing for the evaluation of material properties and mechanical behaviours of titanium foams via focusing on uniaxial compression test only. Section 5 investigates the material properties and mechanical behaviours of this typical metal foam material through checking the stress-strain curves obtained in virtual testing, which are validated using the experimental data. Section 6 summarises the conclusions based on the discussions and research findings and outlooks the future work.

2. EXPERIMENTAL FABRICATION AND EVALUATION OF METAL FOAMS

Steel, aluminium, magnesium and titanium are the most popular materials used as energy absorber in automotive applications. Among these metals, titanium and its alloys are well known as chemically inactive and stable at high temperature and easy to fabricate in the laboratory and thus that was chosen for the matrix material in the current study. In fact its cell structures are typical and similar to those of steel, aluminium and magnesium foams and the samples made the experimental study in a general sense. Powder metallurgy technique, one of the most popular fabrication techniques of powder materials was used to fabricate the titanium foams. This fabri-

cation method includes four main steps: selection of starting materials, compaction of powders, removal of space-holders and sintering. Figure 1 shows schematically the illustration of the processing of porous metals through powder metallurgy using space holders.
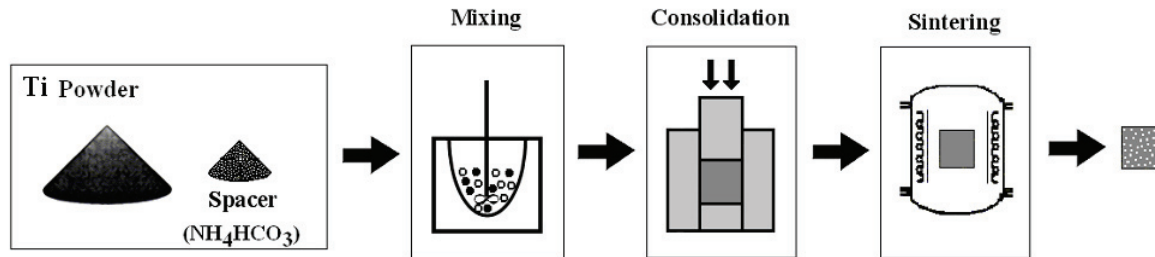

Fig. 1. *Illustration of powder metallurgy route for fabrication of metal foams using spacer holders.*

In the current research, commercially available titanium powders from Atlantic Equipment Engineers, USA, were purchased and used as metal powders. The purity and average particle size of the powders are 99.7% and 45 µm, respectively. The other starting material used was ammonium bicarbonate, NH_4HCO_3, as the space-holder material. The particles of ammonium bicarbonate with a purity of 99.1% are white in colour and have angular shape. A set of eight size fractions covering a range from less 50 to 1000 µm, i.e., >50, 50-100, 100-150, 150-200, 200-300, 300-500, 500-800 and 800-1000 µm were separated by sieving. These size fractions of space-holder particles were used in producing cells in the porous samples with the same porosity of 70%, but different cell sizes.

$$NH_4HCO_3 \rightarrow NH_3\uparrow + CO_2\uparrow + H_2O\uparrow \qquad (1)$$
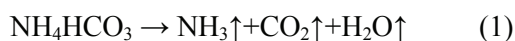
In the experimental step for removing of space-holders, a low-temperature heat treatment process was employed for 24 hours to decompose the space-holder material according to Eq. (1) and form the cells of the sizes designed. The fabricated samples are small cylinders and of 14 mm high and 10 mm in diameter as shown in figure 2. Meanwhile in order to determine the material properties of pure titanium several samples made of pure titanium were fabricated which are of the same shape and size as those of porous samples.

Microstructure analysis of the foam materials was conducted using scanning electron microscope (SEM) considering the variations of cell sizes from 50 to 1000 µm. Figures 3 (a) and (b) show the SEM images of a titanium foam manufactured by powder metallurgy and the cell sizes were found 50 – 100 µm in (a) and 300 - 500 µm in (b), respectively.

The distribution of these cells in foam is random. The cell shapes in these foams are also random; basically, these samples can be catalogued into three groups: sphere-like, cube-like and diamond-like shapes, etc. It can also be seen that the thickness of the cell walls varies over a large range. As measured from figure 3 (a), the smallest thickness of cell wall in this foam is only 15 µm while the largest thickness is 120 µm; i.e. 8 times larger than the smallest one. In current research only sphere-like shape of cells was considered for the implementation of the circle/sphere growth algorithm into digital material presentation.


Fig. 2. *Ti foam samples for uniaxial compression.*

The typical shapes of cells found in the SEM images are summarized in figure 4, which indicates the circular and elliptical shapes of cells can used to characterise the material and that was why we focused on circularly shaped cells in current research only based on the circle (2-D) / sphere (3-D) growth algorithm.

To characterise the material properties and mechanical behaviours of these materials fabricated, a standard uniaxial compression test was employed and a typical engineering stress-strain curved for foam samples with an average cell size of 200 ~ 300 µm is shown in figure 5. From such a curve, the material data can be obtained, including Young's modulus, yield strength, and a relation between stress and strain, as well as experimental data for the

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verification and validation of finite element modelling.
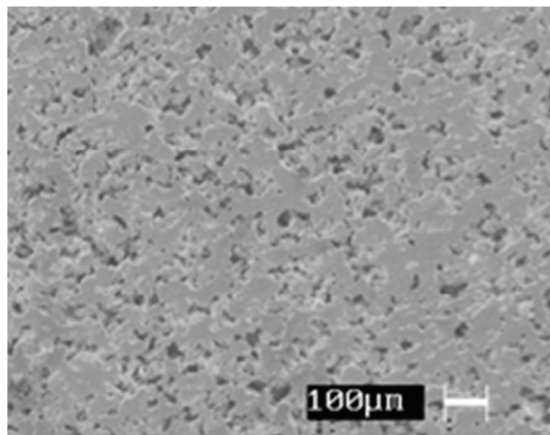
(a) 50-100 μm
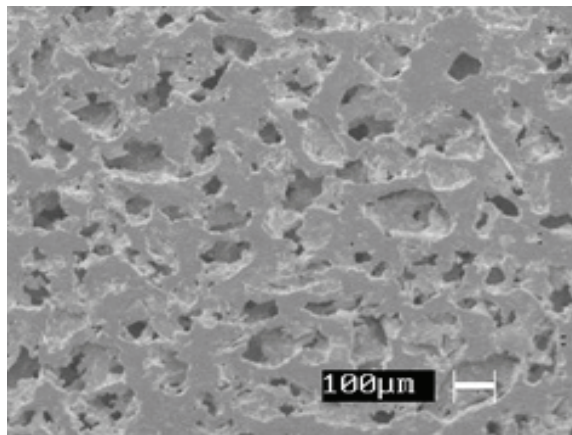
(b) 300-500 μm

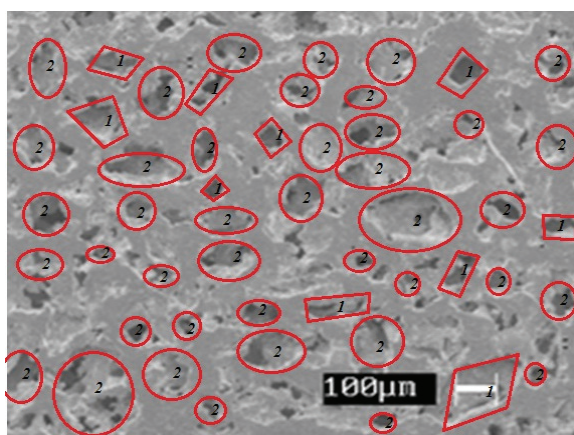**Fig. 3.** *SEM images of titanium foams with a porosity of 70%.*

Fig. 4. *Cell shapes of a sample with average cell size of 200~300 μm: (1) quadrilateral; (2) circular or elliptical.*
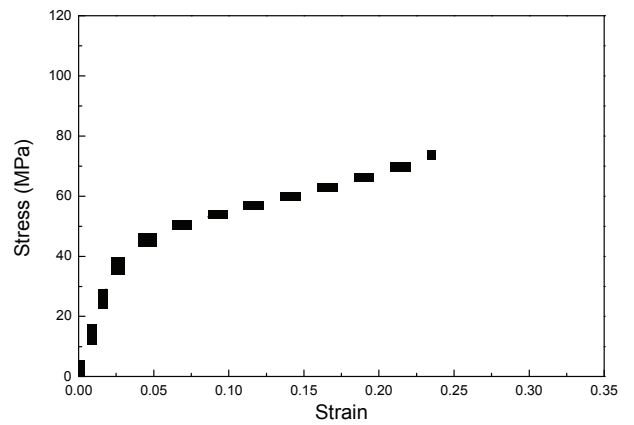
Fig. 5. *Typical stress-strain curve of titanium foams.*

The stress-strain curves of pure titanium were also obtained from the standard uniaxial compression test by using pure titanium samples, which were also fabricated with the above-mentioned pure titanium powders through powder metallurgy. Based on these curves, Young's modulus of pure titanium was determined as 100 GPa. The Poisson's ratio of titanium was chosen as 0.36. The raw data have been further processed and used as input data to define plastic material model in finite element modelling as listed in table 1.

Table 1. *Plastic strain and yield stress of pure titanium*

Plastic Strain	Yield Stress (Mpa)
0	186.0644
0.001767	224.1
0.002625	238.8
0.005354	267.84
0.007229	282.15
0.009198	287.508
0.012159	295.5
0.014109	303.747
0.017057	314.58
0.019018	322.74
0.021954	336.375
0.02344	341.6985
0.026537	340.6455

3. DIGITAL MATERIAL REPRESENTATION AND FINITE ELEMENT MODELLING OF METAL FOAMS

In this study, the circle/sphere growth algorithm was employed to generate 2-/3-D closed-cell metal foam materials without considering the intersecting

among cells and considering the characteristic size of the cells and a certain value of porosity, i.e., 70%, a number of circles/spheres starting from a selected one are generated and each newly-generated circle/sphere added is tangent to an existing one. The codes with the implementation of the sphere growth algorithm were programmed using Matlab codes. As mentioned-above, for metal foams, there are only two phases existing in the materials: a) hollow phase – cells, which can be treated with a circular shape for 2-D and a spherical shape for 3-D, respectively; and b) solid phase – cell walls made of base or matrix materials, i.e., steel, aluminium, magnesium, and titanium, etc.

In the digital material presentation, the internal structure of the metal foams was not reconstructed based on the real materials but treated as an inverse problem, which is defined via the geometric parameters, porosity, characteristic cell size and random distribution of the cells, etc. As we know the porosity of a metal foam material as well as the other characteristics of its microstructure, i.e., cell size and distribution, we also can treat the fabrication as an inverse problem. In such a case, the centres of cells of different sizes are allocated randomly but the cells are created via following the appropriate relative positions between the neighboured cells' centres considering the existence of cell walls between cells. In the developed Matlab codes, the main control and input parameters include the dimensional type of the problem (2-D or 3-D), the sizes of the 2- and 3-D models which can be shaped as circle, square, and rectangle in 2-D cases, and cylinder, cube, and brick for 3-D cases, the total type numbers of cell size, the total numbers of cells at each size, and the radius of cells at each cell, etc. for such an inverse problem. By this way, the dimensions and the positions of the elementary cell could be easily defined using an algorithm for the generation of a set of random numbers. An algorithm based on a random uniform distribution into the parameter range variability was considered adequately and the uniformly random distribution is characterised by a mean value and a variance equal respectively to $(a + b) / 2$ and $(b - a)^2 / 12$, in which, a and b are the minimum and maximum values of the radii of the cells considered.

The 2- and 3-D geometrical models created using the proposed Matlab codes are then output in a file with a required format and saved as geo files, which can be further processed by the free finite element meshing generator–Gmsh, developed by Geuzaine and Remacle. It has four modules: geome-

try, mesh, solver and post-processing and we just use the mesh module in current study. The finite element meshes can be discretised by linear elements or quadratic elements in both 2-D and 3-D cases up to the need. Figures 6 (a) and (b) show typical digital representations of the 2-D square and 3-D cubic models, respectively.

The generated mesh is then output in a file with a required format of the input file with a filename extension of inp via importing FE models to Abaqus, which is a commonly-used powerful finite element analysis (FEA) package. Once the mesh is input into Abaqus, the boundary conditions can be further conveniently applied or adjusted using Abaqus/CAE if any needed to finalise in the developed finite element model.
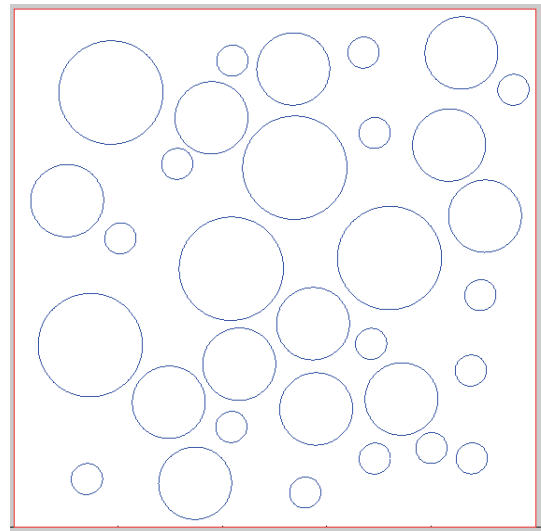
(a) 2-D square model
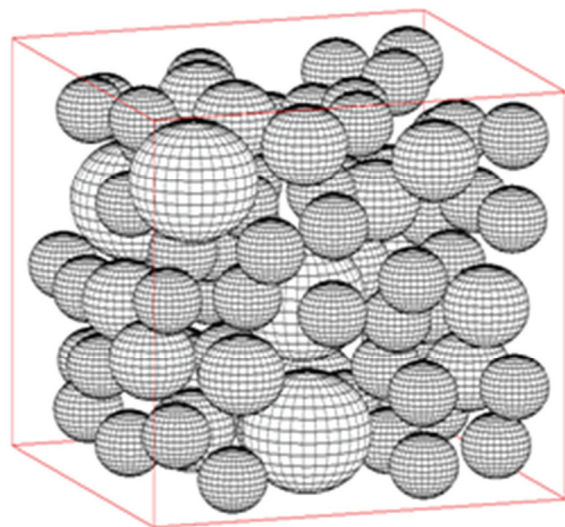
(b) 3-D cube model

Fig. 6. *2- and 3-D digital representation and fabrication of foam materials.*
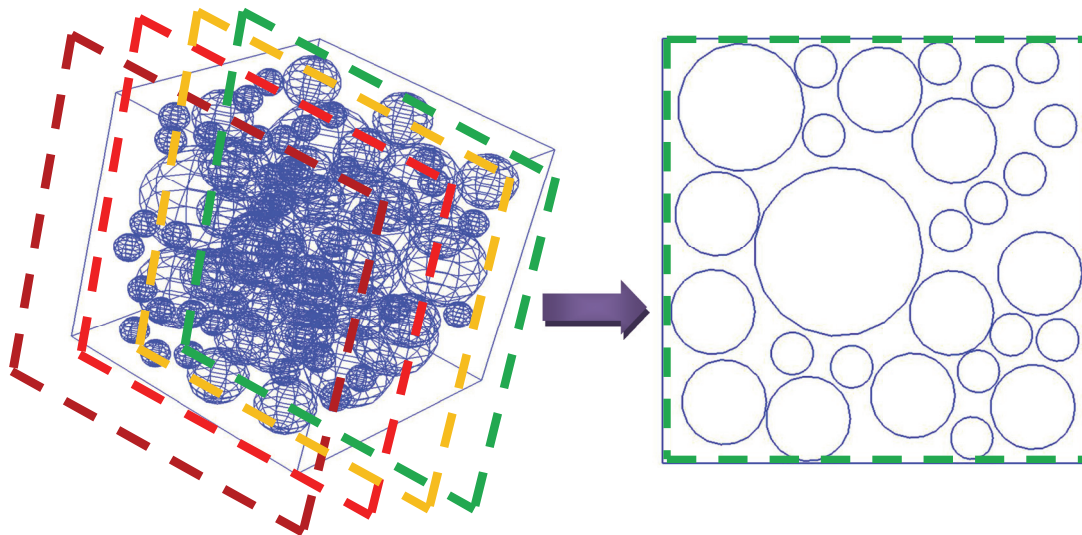
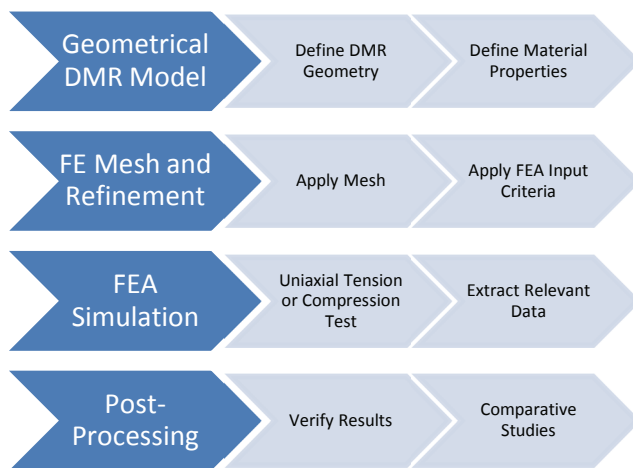**Fig. 7.** *Effective models from 3-D to 2-D subject to compression tests.*

Fig. 8. *Digital material representation (DMR) and material evaluation process.*

Although the 2-/3-D finite element models of metal foams can be easily generated, the simulations of 3-D models take a lot of CPU time, which are not cost-effective. 2-D models are relatively economical compared to 3-D simulations. In the current research, a link between 2-D and 3-D digital material representations is of interest. The idea here is to generate effective 2-D models based on 3-D models which effectively link these models. Since the simulations of 2-D models take much less CPU time than 3-D model, it would greatly improve the efficiency of finite element modelling and simulation of metal foams. As shown in figure 7, the methodology developed here is that a 3-D finite element model was firstly generated and then based on this 3-D model, several cutting operations to get a series of cross sections were performed along one direction. Using these cross sections obtained, a series of 2-D mod-

els, termed as slices, were created, which may have different porosities one another. For each 2-D model, the simulation of uniaxial compression was then conducted to extract the numerical results wanted, i.e., stress-strain curves. Final results from all the 2-D models were taken at average to compare the results obtained from 3-D model. Through this procedure, a much quicker but still effective 2-D finite element analysis procedure was constructed to replace the highly-expensive 3-D modelling and simulation.

The material model of the metal foams can be defined much easier now, which is used to define to the elastoplasticity of solid phase–cells wall only, by two parts: a) elastic model defined by giving the values of the Young's modulus and the Poisson's ratio of pure titanium; and b) plastic model defined by a true stress-true strain curve which was obtained from experimental work on pure titanium. Note that since we developed the digital representation of metal foams, the complex plasticity models for metal foams were not required to be implemented in current FE models and those models need to be defined using a lot of input parameters determined by several different experimental tests, including hydrostatic tension/compression, uniaxial compression, uniaxial tension, pure shear and indentation, etc. The details on these can be found in authors' recent work (Yang, et al., 2014). The whole procedure to fabricate the structure of microstructured material and generate its finite element model digitally by integrating the outcomes of the developed Matlab code with the free 2-/3-D finite element mesh generator – Gmsh and the FEA package – Abaqus is summarised in figure 8.

4. VIRTUAL TESTING OF METAL FOAMS

The porous structures of foam materials make them have quite different material properties and mechanical behaviours compared to solid materials. In general, foams can be characterised structurally by its cell or cell topology such as open or closed cell, relative density, cell size and cell shape, etc. One of the benefits from using foam materials is the controllable material properties from material design's point of view. For example, as a common sense, it is well known that the stiffness of foam materials decreases with the square of relative density. On the one hand, engineers always pursuing lighter metallic materials with higher porosity but on the other hand the reduced stiffness, strength and ductility may accompany. Therefore, it is very important to accurately predict material properties and elastoplastic behaviours of metal foams for application. In reality, metal foams can be regarded as a mixture of solid cell walls and cells or pores which show remarkable mechanical behaviours involving in extremely large strain and deformation. Normally in experimental studies, their mechanical behaviours can be characterised by using several tests, including hydro-static tension/compression, uniaxial compression, uniaxial tension, pure shear and indentation, etc., and among them, uniaxial compression is the most commonly used experimental technique for evaluating material properties of foam materials. In this case study, only the uniaxial compression on digital samples of Ti-based metal foams with a porosity of 70% was studied according to the experimental work done.

In the virtual testing of uniaxial compression, two sets of finite element models with a constant porosity of 70% were designed as shown in figure 9: a) one cubic 3-D model of 1 mm × 1 mm × 1 mm (Sample-3D: figure 8a); and b) eight square 2-D models of 1 mm × 1 mm (Sample-I to Sample-VIII: figures 8b to 8i) with periodic boundary conditions (P.B.C.s) in the multiscale sense. The 3-D model was generated firstly and then the eight 2-D models as slices were created via cutting-off operations along one direction and the interval between slices was set as 0.1 mm. As mentioned above, the generated 2-D models have different porosities, which were found 48%, 59%, 65%, 66%, 71%, 76%, 77% and 78%, respectively. It is reasonable to have lower or higher porosity in 2-D models compared to 70% in the 3-D model.
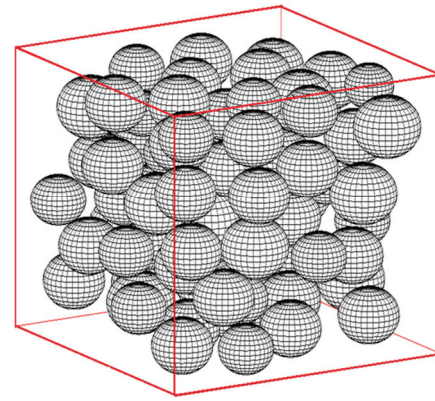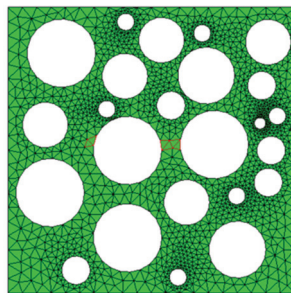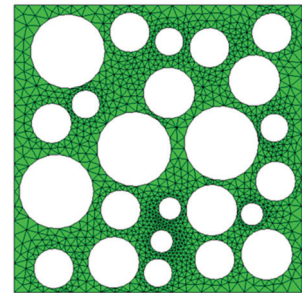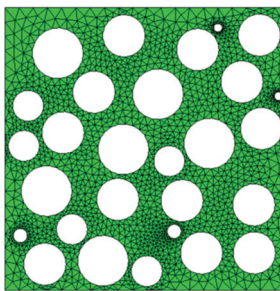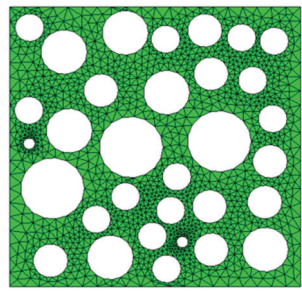

a. Sample-3D
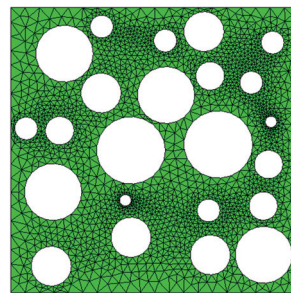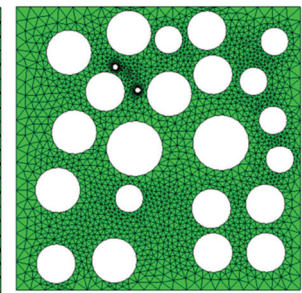
b. Sample-I   *c. Sample-II*

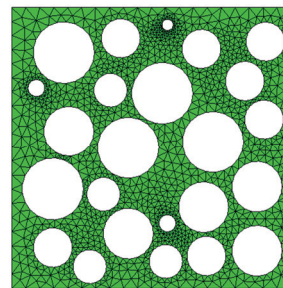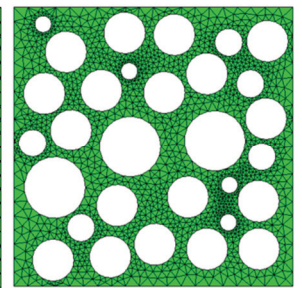*d. Sample-III*   *e. Sample-IV*

f. Sample-V   *g. Sample-VI*

h. Sample-VII   *i. Sample-VIII*

Fig. 9. *2-/3-D digital samples for virtual compression testing.*

The finite element used in the 3-D models was the 3-D solid element – C3D4, a 4-node linear tetrahedron element, having four nodes with three degrees of freedom each and reduced integration, available in Abaqus. Meanwhile, a plane element CPS4R was used in the 2-D models via treating the stress state as plane strain. In the virtual testing of uniaxial compression of these two sets of finite element models, two rigid plates on the top and bottom surfaces of the cubic models were created to apply the compressive loading by moving the top one downwards at a strain rate of 0.02 s⁻¹ while keeping the bottom one fixed during the dynamic analysis using Abaqus/Explicit. As for the 2-D models, periodic boundary conditions were also employed to represent those current models with a repeated structure.

of the envelope. To compare to the numerical results from the 3-D model and experiment data, an additional curve in purple colour with symbol was also generated and the values are the averaged values of all the eight samples, which is closer to the curve from Sample III.

In figure 11, the comparison between the 2- and 3-D results and experimental data is conducted. Good agreement between these results has been found to some extent. Considering the 2-D results, a good fitting with experimental curve has been found in elastic and plastic zones close to the turning point for 2-D model but when the strain increases (large than 12.5%) the averaged 2-D numerical results show flat differently. 3-D results give a good trend at all zones and shape compared to that of experimental one but does like 2-D results to fit very well in the elastic
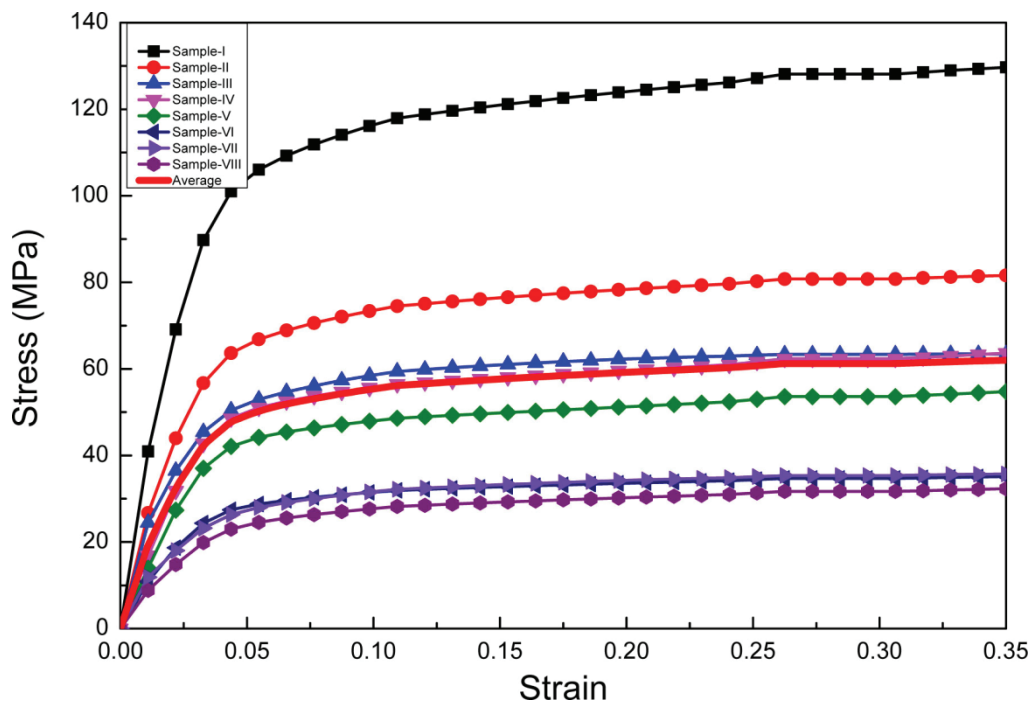

Fig. 10. Strain-stress curves of titanium foams with different cell sizes under uniaxial compression.

5. EVALUATION OF MATERIAL PROPERTIES AND MECHANICAL BEHAVIOURS OF METAL FOAMS

Eight stress-strain curves were obtained via numerical simulations from the proposed 2-D FE models as shown in figure 10 and due to the different porosities for samples, it clearly indicates the porosity's influence on the material behaviour and that is the higher porosity, the lower material strength or the softer material. However all curves have the similar trends to clearly show the elastic and plastic zones in them. The two curves extracted for Sample I and Sample VIII are making the upper and lower bounds

zone. Both of the 2-/3-D models cannot exactly capture the mechanical behaviours at high strain zone when the strain is larger than 12.5% for 2-D and 22.5% for 3-D. The reason for these discrepancies may be sourced from the internal structures of the real samples in the experimental study since those samples fabricated using powder metallurgy may have a situation of co-existing closed and open cells internally.

The deformation patterns of these eight 2-D models were shown in figure 12 to check whether or not periodic boundary conditions have been applied correctly. The deformations are all at the maximum stain of 35% and in all the cases the circular pores
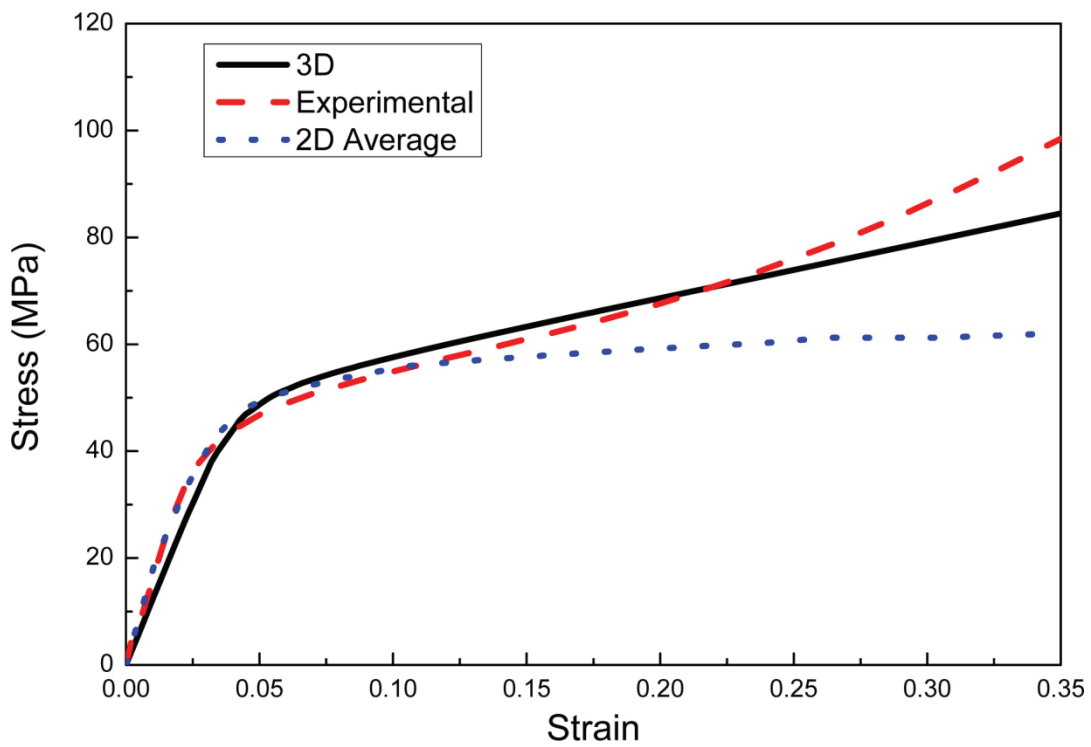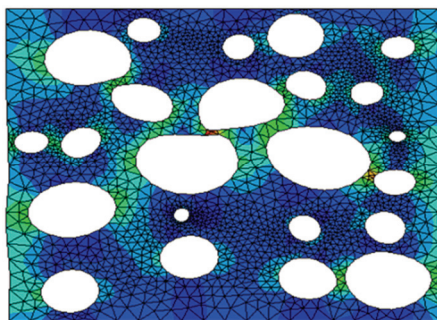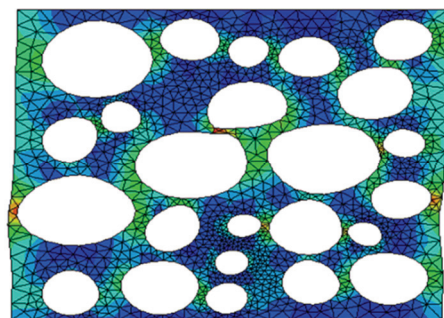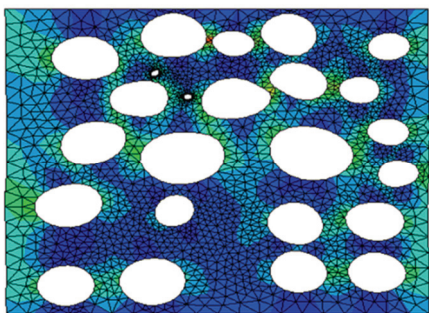
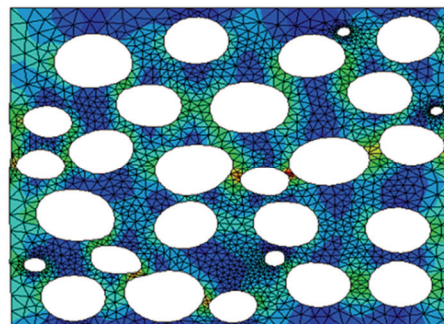***Fig. 11.*** *Strain-stress curves of titanium foams with different pore sizes under uniaxial compression.*
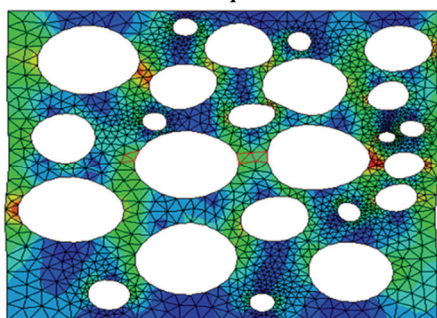

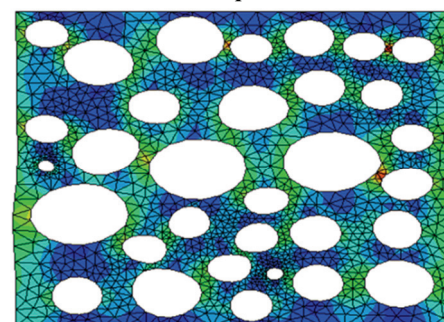*a. Sample-I*

d. Sample-IV

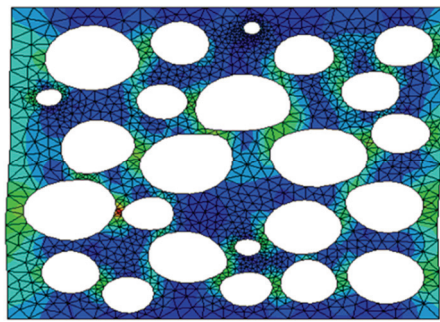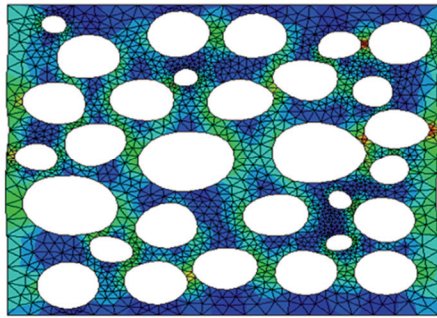*b. Sample-II*

e. Sample-V

c. Sample-III

f. Sample-VI

g. Sample-VII

h. Sample-VIII

Fig. 12. *Deformation patterns of 2-D finite element models subject to compression at maximum strain of 35%.*

have been deformed to be elliptic but under such a deformation, there is still no closure of hole or self-contact found but lager pores deform more than those smaller ones. In each image, the deformations of side edges of the models clearly show these two parallel boundaries have the same deformation when under compression.

The best benefit to create the 2-D models based on a 3-D model is to greatly reduce the simulation costs and in the current study, it took 174,513 seconds finishing a 3-D simulation but eight 2-D simulations only took 29,800 seconds in total to finish using a desktop workstation (Intel i7, 8 GB memory and 128 GB hard drive).

6. CONCLUSIONS

In this study, a 2-/3-D digital framework integrated with digital material representation and virtual testing on metal foams has been further developed at a multi-scale sense and based on the 3-D digital material representation of metal foams, their 2-D digital material presentation has been created with different porosities each slice.

The linkage between 2-D and 3-D models has been also found compared to experimental data and it can be summarised as follows:

− As for geometric characteristic, the porosities in 2-D models are different from one another and 3-D model as well: 70% for the 3-D model;

48%, 59%, 65%, 66%, 71%, 76%, 77% and 78% for the 2-D model, respectively.

− As for mechanical behaviours obtained from 2-D and 3-D models, the averaged 2-D results can well reflect the elastoplastic behaviours when the strain is small (less than 12.5%), especially for elastic zone. Meanwhile, 3-D models can capture the elastoplastic behaviours when the strain is less than 22.5% as well as a better trend compared to experimental data. Both 2- and 3-D results can fit with the experimental results to some extent considering different elastic and plastic zones in the stress-strain curves.

− As for computing costs, the 2-D simulation provides a fast and efficient mean compared to the expensive 3-D simulation.

Based on the current results obtained, the future work is to further extend the digital material representation and fabrication, modelling and evaluation of other typically microstructured materials with more complex structures, such as nanocomposites as well as the user-kind interface with other commercial FEA packages, i.e., ANSYS, and extensive application to multi-scale modelling of microstructured materials.

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2-/3-D CYFROWA REPREZENTACJA MATERIAŁU I JEJ EWALUACJA DLA PIANEK METALICZNYCH

Streszczenie

Ze względu na ich dużą zdolność do absorpcji energii i niską gęstość pianki metaliczne znajdują ostatnio szerokie zastosowanie w przemysłach samochodowym i lotniczym, a także w bioinżynierii. Jako typowy materiał porowaty lub komórkowy pianki metaliczne mają strukturę niejednorodną, która może być zdefiniowana przez dwie fazy: materiał osnowy i pustki nazywane komórkami lub porami. Struktury komórek są charakteryzowane przez ich główne parametry geometryczne, takie jak rozmiar, kształt, rozkład w przestrzeni i aranżacja. Cyfrowa reprezentacja materiału została wykorzystana do reprezentowania pianek metalicznych z uwzględnieniem ich złożonej struktury. Z drugiej strony nierównomierność rozkładu rozmiaru i kształtu komórek w większości pianek powoduje, że taka cyfrowa reprezentacja i modelowanie stają się bardzo trudne.

Wpływ rozmiaru i kształtu komórek na własności mechaniczne pianek metalicznych był badany numerycznie i doświadczalnie we wcześniejszych pracach autorów. W tych pracach opracowana została numeryczna platforma dla reprezentacji, modelowania i oceny wielofazowych materiałów, w tym pianek metalicznych.

W niniejszej pracy przedstawiono dalszy rozwój tej platformy. Stworzono wieloskalowe modele 2D i 3D połączone z metodą elementów skończonych (MES) do opisu pianek metalicznych z zadanym rozkładem rozmiaru i kształtu komórek. Ten program może być dalej stosowany do wyznaczania własności mechanicznych oraz do opisu zachowania się pianek metalicznych pod obciążeniem. Połączenie między modelami 2D i 3D MES zostało zbudowane na podstawie analizy podobieństwa między tymi rozwiązaniami. Dla walidacji i weryfikacji modelu porównano otrzymane wyniki z badaniami doświadczalnymi i otrzymano dobrą zgodność, co potwierdziło efektywność cyfrowej platformy dla pianek metalicznych.

COMPUTER METHODS IN MATERIALS SCIENCE