Design and performance evaluation of additively manufactured composite lattice structures of commercially pure Ti (CP–Ti)

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\textbf{A B S T R A C T}

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Ti alloys with lattice structures are garnering more and more attention in the field of bone repair or regeneration due to their superior structural, mechanical, and biological properties. In this study, six types of composite lattice structures with different strut radius that consist of simple cubic (structure A), body-centered cubic (structure B), and edge-centered cubic (structure C) unit cells are designed. The designed structures are firstly simulated and analysed by the finite element (FE) method. Commercially pure Ti (CP-Ti) lattice structures with optimized unit cells and strut radius are then fabricated by selective laser melting (SLM), and the dimensions, microtopography, and mechanical properties are characterised. The results show that among the six types of composite lattice structures, combined BA, CA, and CB structures exhibit smaller maximum von-Mises stress, indicating that these structures have higher strength. Based on the fitting curves of stress/specific surface area versus strut radius, the optimized strut radius of BA, CA, and CB structures is 0.28, 0.23, and 0.30 mm respectively. Their corresponding compressive yield strength and compressive modulus are 42.28, 30.11, and 176.96 MPa, and 4.13, 2.16, and 7.84 GPa, respectively. The CP-Ti with CB unit structure presents a similar strength and compressive modulus to the cortical bone, which makes it a potential candidate for subchondral bone restorations.

1. Introduction

Osteochondral defects can lead to mechanical instability of the joint and loss of joint function and can proceed to the generation of osteoarthritis (OA), which is one of the most prevalent joint diseases and a major cause of disability in the adult population [1]. In recent years, tissue engineering has emerged as a potential solution for the repair of damaged subchondral bone [2]. At present, metals, ceramics, and polymers have been used as subchondral scaffolds. Among them, metals especially Titanium (Ti) and its alloys scaffolds are widely used due to their high strength and fatigue resistance [3-5].

Porous Ti scaffolds are usually fabricated by conventional techniques, such as slurry foaming and space-holder method [7,8]. But these techniques have some limitations, for example, the shape, the size, and the distribution of pore are difficult to control accurately that leads to the expected performance cannot be achieved. Additive manufacturing (AM) is a new technology developed in recent years, which is defined as a process of joining materials to make objects from 3D model data, usually layer upon layer. With the development of additive manufacturing (AM) technology, scaffolds with unlimited arbitrary topological layouts, complex internal microstructures and particular properties (e.g. magnetic, excellent cell adhesion ability and mechanical properties) can be manufactured [9-11]. Among the additive manufacturing (AM) technology, such as selective laser sintering (SLS), electron beam melting (EBM), and selective laser melting (SLM), SLM is considered the most promising technology by which products are built by melting selected areas of powder layers under a protective atmosphere using a computer-controlled laser beam [12,13]. Compared with...
conventional fabrication methods, SLM technology is more flexible in forming complex shapes, especially for scaffolds based on lattice structures [14,15].

So far, Ti scaffolds with different lattice structures, e.g. cubic or cubic-based lattices [16,17], diamond lattices [18,19], and gyroid lattices [20,21], have been fabricated by SLM. Such as Du et al. [22] designed uniform structures of 70% porosity with the unit cells of the cube, diamond, and Rhombic dodecahedron. The results showed that the compressive modulus was in the range of 25–120.4 GPa while the yield stress was more than 400 MPa. Although the compressive stress is higher than natural bone significantly that is enough for standing loads, the remarkably higher elastic modulus than that of bones will cause “stress shielding”, which leads to bone resorption around the implants and ultimately the failure of implantation. In addition, Gyroid structures with the porosity of 70.99% ± 9.3% of Ti–6Al–4V alloy were fabricated by Zaharin et al. [23], and the results showed that the yield strength and compressive modulus were 22.44 ± 0.46 MPa and 10.6 ± 0.28 GPa, respectively. But these studies mainly focus on single lattice structures that cannot match the natural bones well at the strength and elastic modulus. Thus, from a design point of a view, it is imperative to design porous Ti scaffolds with different pore porosities and pore sizes, in order to match the mechanical and biological properties of natural bone [24–27].

Till now, there are some kinds of graded scaffolds have been fabricated by SLM to improve the mechanical and biological properties of the alloys [28–31]. Such as, Choy et al. designed and manufactured cubic lattice and honeycomb lattice structures with graded structure diameter and density, and the results demonstrated that the graded lattices performed better mechanical properties compared to uniform lattices. Zhang et al. manufactured a graded lattice structure based on diamond unit cells and it showed good mechanical properties and permeability. In order to enhance the mechanical and biological properties further, six types of composite lattice structures with different strut radius were designed in the present study. Then mechanical properties were investigated numerically using the FE method. Based on the simulated results, CP-Ti with optimized structures and strut radius were fabricated by SLM, and the morphology and compressive properties were characterised. It aims at designing the composite lattice structures and optimising the mechanical properties of CP-Ti, so as to provide basic guidance for its potential application in subchondral bone repair and restorations.

2. Materials and methods

2.1. Design of composite lattice structures

Fig. 1. The basic unit cells of A, B, C with the strut radius of 0.3 mm.

Fig. 2. The combined composite lattice structures and their front views.

Three unit cells with a length of 2 mm, namely simple cubic (A), body-centered cubic (B), and edge-centered cubic (C), were designed by
the Solidworks software, as shown in Fig. 1. It is relatively easy to design these three unit cells due to their simple structures. Additionally, they could be manufactured well due to their relatively simple design and the significantly reduced warping effect caused by internal inclined struts during the SLM process. What’s more, the inclined struts cross could reduce the flow velocity, which is beneficial for cell adhesion and proliferation. Six types of composite lattice structures were designed by the Solidworks software, i.e. AB, BA, AC, CA, BC, and CB structures. Due to the mechanical properties of lattice struts along different spatial directions are not the same and the direction of stress applied in the FEA simulations is from the top, the AB and BA structures are considered to be two different structures. The dimensions of samples were $10 \times 10 \times 12$ mm (length $\times$ width $\times$ height) and the composite lattice structures were hybridized in the direction of the Z-axis by layering two different types of unit cell from top to bottom, e.g. AB lattice: A for the first, third and fifth layers and B with the same size for the second, fourth and sixth layers. The same design method was applied with BA, AC, CA, BC, and CB. For each composite lattice structure, different strut radius of 0.2, 0.25, 0.3, 0.35, and 0.4 mm were set, therefore a total of 30 different composite lattice structures were designed. Fig. 2 shows the six composite lattice structures with a strut radius of 0.3 mm and their front views.
FE analysis of uniaxial compressive behaviors was conducted using ANSYS Workbench software to investigate the mechanical properties and visualize the stress distribution of the composite lattice structures. The parameters of material in the FE analysis process were as follows: the density of 4.46 g/cm$^3$, the elastic modulus of 110 GPa, the Poisson ratio of 0.3, and the compressive yield strength of 830 MPa based on previous study [32]. The 3D linear triangular prism elements (C3D6) were used to mesh the composite lattice structures. In terms of the boundary conditions, the bottom surface was fixed and the compressive stress of 73 MPa was applied on the top surface [33].

2.2. Materials and manufacturing

The hydride-dehydride Ti (HDH-Ti) powder (Beijing Xing Rong Yuan Co., Ltd, China) was used as raw materials. The powder was treated in a ball mill to improve the flowability. The ratio of ball and powder, milling speed, and milling time were 5:1, 200 r/min, and 4h, respectively. The detailed powder characteristic and process parameters were described elsewhere [34–39].

The CP-Ti with optimized composite lattice structures were manufactured by SLM 125HL machine (SLM Solutions GmbH, Lübeck, Germany) under an argon gas atmosphere with O$_2$ content < 0.05 wt% to reduce oxidation. The process begins with the preparation of CAD files which are subsequently sliced into two-dimensional layers by Materialise Magics [40, 41]. The detailed process parameters are as follows based on our previous study [34]: the layer thickness is 30 μm; the scanning speed is 900 mm/s; the laser power is 200 W; the hatching space is 0.14 mm; and the hatching type is a continuous laser mode, which is alternated 33° between each layer. The printing direction is along the direction of the Z-axis.

2.3. Measurement and characterisation

The manufactured specimens were sand-blasted and ultrasonically cleaned in absolute ethyl alcohol and finally dried under vacuum. The relative density was calculated based on the ASTM B962-14 standard [42], and then the porosity was obtained based on Eq. (1). Each specimen was measured five times repeatedly to obtain average results.

$$P = 1 - \frac{m_1 \times \rho_{\text{water}}}{(m_3 - m_2) \times \rho_{\text{Ti}}}$$

where $P$ is the porosity of specimen, $\%$; $m_1$ is the mass of the specimen in air, g; $\rho_{\text{water}}$ is the density of water, 1 g/cm$^3$; $\rho_{\text{Ti}}$ is the density of solid Ti, 4.507 g/cm$^3$; $m_2$ is the mass of the oil-impregnated test specimen in water with the mass of the specimen support tared, g; $m_3$ is the mass of the oil-impregnated test specimen in air, g.

The scanning electron microscopy (SEM, JSM-6480LV) was used to characterize the morphology. The pore diameter distribution was determined from 50 2D slices images obtained from Solidwords software, and $D_{50}$ is used as average pore size. Based on ISO 13314:2011(E)
3. Results and discussion

3.1. FE analysis

Von-Mises stress distribution and total deformation of designed composite lattice structures were firstly analysed by FE to evaluate the strength. Taking the structure with the strut radius of 0.3 mm for example, it can be seen from von-Mises stress distribution (Fig. 3) that the stress is mainly concentrated on the upper surface or the vertical struts. For the AB, AC, and BC structures, the stress is mainly concentrated on the upper surface and the vertical struts of the first, third, and fifth layers (from top to the bottom), while it is mainly concentrated on the vertical struts of the second, fourth, and sixth layers for BA, CA and CB structures. This is mainly related to the internal structure. As shown in Fig. 1, the number of struts in three structures is \( C > B > A \), which leads to structure C has a higher ability to bear loads than structure B and A.

| BA   | CA   | CB   |
|------|------|------|
| Strut radius (mm) 0.28 | 0.23 | 0.3  |
| Porosity (%) 71.24 | 77.12 | 51.48 |
| Maximum von-Mises stress (MPa) 688.44 | 972.67 | 360.69 |
| Maximum total deformation (mm) 0.0244 | 0.0768 | 0.0138 |

Fig. 6. Von-Mises stress distribution of optimized composite lattice structures: BA with the strut radius of 0.28 mm, CA with the strut radius of 0.23 mm and CB with the strut radius of 0.3 mm.

Fig. 7. The SEM images of optimized composite lattice structures BA, CA and CB.
As a result, the stress is concentrated on the layer composed of A or B unit cell. In addition, it can be seen from Fig. 3 that AB and AC structures exhibit higher maximum von-Mises stress (1454.50 and 1453.90 MPa, respectively) than the other four structures (384.46 MPa). In contrast, the deformation of the other four structures is relatively uniform. These results are consistent with the results of von-Mises stress distribution.

Table 1 summaries the maximum von-Mises stress and the maximum total deformation of 30 different composite lattice structures designed in this study. It can be seen that the maximum von-Mises stress and the maximum total deformation decrease along with strut radius increasing in the same type structures. In addition, compared with the AB structure, BA structure with the same strut radius and porosity exhibits smaller maximum von-Mises stress and total deformation, indicating that BA structures have higher mechanical properties. As for AC/CA and BC/CB composite lattice structures, similar results are found, namely CA and CB structures exhibit higher mechanical properties than AC and BC structures, respectively. Hence, the BA, CA, and CB structures will be focused on the following studies.

It is well known that the pore features, such as porosity and pore size, can significantly influence the biological properties of implants [44]. In this study, the pore features are directly related to the strut radius. For example, with a larger strut radius, the pore size and the porosity decrease which leads to an increase in the volume and the surface area. However, there is a reduction in specific surface area (Table 2), which is not beneficial for adhesion, proliferation, and differentiation, and the transportation of nutrients [44,45]. Meanwhile, with the larger strut radius, the maximum von-Mises stress becomes smaller, which is beneficial for the mechanical properties. That is to say, a smaller stress/specific surface area would be more desirable for both mechanical and biological properties. Fig. 5 shows the variation of strut radius of BA, CA, and CB structures with stress/specific surface area, and their corresponding fitting curves. It can be seen that the stress/specific surface area of CA and CB decreases with the strut radius firstly and then increases. So, the best strut ratios for CA and CB structures are 0.23 and 0.3 mm respectively. As for the BA structure, the stress/specific surface area decreases with the strut radius firstly and then increases, and finally decreases again. However, when the strut radius is higher than 0.4 mm, the porosity becomes too small to be used. Therefore, the best strut radius for the BA structure is 0.28 mm. The pore sizes of three designed BA, CA, and CB structures are listed in Table 3. It can be seen that the small pore size of designed structures is in the range of 400–700 μm, which may be benefit to adhesion, proliferation, and differentiation of cells based on previous studies [46,47]. In addition, the size of the large pores increasing from 700 μm to 2300 μm can be used as a path for the transportation of nutrients and metabolites, and vascularisation.

The mechanical properties of the optimized BA, CA, and CB composite lattice structures were simulated by the FE method. The total deformation and von-Mises stress distribution are shown in Fig. 6, and the FE results together with geometrical parameters are summarised in Table 4. It can be seen from Fig. 6 that the stress distributions within all structures are homogeneous. The maximum stresses for three structures are in the range of 360.69–972.67 MPa (Table 4), which is lower or close to the maximum stress of sample failure in practice [36]. In addition, as can be seen from Table 4, the porosity of all structures is above 50%, which meets the requirements of scaffolds as subchondral bone restorations [46].

3.2. Dimensions and microtopography characterisation

Fig. 7 shows the SEM images and CAD models of the local cross-section of the optimized composite lattice structures. It can be seen that the surface of the lattice structures is rough, which is due to partially melted powders boned on the surfaces of struts and the stair-stepping effect. Comparing the CAD models with the printed samples, it can be found that the geometries of fabricated lattice structures are in line with the CAD models. In addition, there is no macro defects are observed. These results indicate that the printing quality is high.

The detailed morphological parameters of the designed and as-built samples, including the strut radius and porosity were summarised in
The compressive modulus of CP-Ti with composite lattice structures in this study (30.1 ± 0.35 GPa) is significantly higher than that of CP-Ti with diamond and dodecahedron structures with a similar porosity and close to that of Ti-6Al-4V with diamond structure. Among them, the CP-Ti with CB structure exhibits similar yield strength to the cortical bones (103–222 MPa) while the compressive modulus is also in the range of cortical bones (7.7–21.8 GPa). As a result, CP-Ti with CB structure has the best potential for subchondral bone restorations.

### 3.3. Compressive mechanical properties

Fig. 8 shows the compressive stress-strain curves of CP-Ti with optimized BA, CA, and CB structures. All curves exhibit a linear elastic region. Following the linear elastic stage, the curves of CP-Ti with optimized BA and CA composite lattice structures in Fig. 8(a) show that the stress increases nonlinearly with the strain and the slopes of stress-strain curves decrease gradually until the slopes reach zero. After that, the stress-strain curves enter a softening region where the stress declines. Finally, fracture occurs in the SLM process. In addition, the distinct thermal gradient which is caused by the molten and unmolten powders leads to further adhesion of powders to the surfaces of the struts.

Table 6 compares the mechanical properties of the CP-Ti with composite lattice structures in this study, trabecular bone, cortical bone, and CP-Ti and Ti-6Al-4V with other structures in literature.

#### Table 6
Comparison of mechanical properties of the CP-Ti with composite lattice structures in this study, trabecular bone, cortical bone, and CP-Ti and Ti-6Al-4V with other structures in literature.

| Scaffold | Material | Porosity (%) | Yield strength (MPa) | Compressive modulus (GPa) | Reference |
|---------|----------|--------------|----------------------|--------------------------|-----------|
| BA      | CP-Ti    | 69.72 ± 0.2  | 42.28 ± 1.5          | 4.13 ± 0.11              | this study |
| CA      | CP-Ti    | 75.32 ± 0.35 | 30.11 ± 0.8          | 2.61 ± 0.09              | this study |
| CB      | CP-Ti    | 50.15 ± 0.2  | 176.96 ± 4.2         | 7.84 ± 0.18              | this study |
| Diamond | CP-Ti    | 81.12        | 17.75 ± 0.9          | 0.566 ± 0.021            | [50]      |
| Dodecahedron | CP-Ti | 66-81     | 8.6-36.5            | 0.58-2.61               | [51]      |
| Diamond | Ti-6Al-4V | 48.4        | 156.1 ± 20.3        | 9.01 ± 0.35              | [32]      |
| Step-wise FGPB | Ti-6Al-4V | 56.4 | 170.6 ± 15.6 | 10.44 ± 0.2           | [32]      |
| Diamond | CP-Ti    | 61.6 ± 0.4  | 36.2 ± 1.3          | 0.557 ± 0.006            | [52]      |
| Trabecular bone | bone | 80-116.9   | 0.022-0.712        |                         | [46]      |
| Cortical bone | bone | 5-10      | 10-222             | 7.7-21.8                | [46]      |

The data that support the findings of this study are available from the corresponding or first authors on reasonable request.

### CRediT authorship contribution statement

Wei Xu: Conceptualization, Data curation, Formal analysis, Writing - original draft, Writing - review & editing. Aihua Yu: Data curation, Formal analysis, Investigation. Xin Lu: Conceptualization, Data curation, Formal analysis, Writing - original draft, Writing - review & editing, Supervision, Project administration. Maryam Tamaddon: Investigation, Writing - review & editing. Mengdi Wang: Investigation, Writing - review & editing. Jiachen Zhang: Investigation, Writing - review & editing. Jianliang Zhang: Investigation, Writing - review & editing. Xuanhui Qu: Investigation, Writing - review & editing. Chaozong Liu: Investigation, Writing - review & editing. Bo Su: Investigation, Writing - review & editing.

### Declaration of competing interest

The authors declare that they have no known competing for financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Table 5. It can be seen that all of the as-built strut radius for the BA, CA, and CB composite lattice structures slightly increase (~1.3%~2.3%) and the porosity of as-built structures slightly reduces (~2.1%~2.58%) compared to the designed samples. This is mainly due to the partial melting of some powders surrounding the struts bond to the surfaces of the struts during the SLM process. In addition, the distinct thermal gradient which is caused by the molten and unmolten powders leads to the partial melting of some powders surrounding the struts bond to the surfaces of the struts [49].

#### Table 7
Comparison of mechanical properties of CP-Ti with composite lattice structures in this study, trabecular bone, cortical bone, and CP-Ti and Ti-6Al-4V with other structures in literature.

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| Diamond | CP-Ti    | 61.6 ± 0.4  | 36.2 ± 1.3          | 0.557 ± 0.006            | [52]      |
| Trabecular bone | bone | 80-116.9   | 0.022-0.712        |                         | [46]      |
| Cortical bone | bone | 5-10      | 10-222             | 7.7-21.8                | [46]      |

[Reference]
