Simulation and physical validation of triply periodic minimal surfaces-based scaffolds for biomedical applications

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Abstract

Metallic scaffolds are used as implants to help heal bones. Sheet-based Triply Periodic Minimal Surfaces (TPMS) are of interest due to their high surface-to-volume ratio (S/V), customisable stiffness, and can be realised using Additive Manufacturing (AM). Other studies investigate porosity and pore size of scaffolds but they frequently overlook S/V, which is critical for cellular response. Additionally, the limitation of AM (esp. Selective Laser Melting (SLM)) causes discrepancies between intended and actual physical and mechanical properties of those structures, and this also needs to be addressed. This work investigates three types of TPMS scaffolds made in pure Titanium, with an emphasis on design vs manufactured differences and the significance of S/V. As-designed scaffolds reported 70-75% porosity and 25-35 cm^{-1} S/V, and stiffness was measured using finite element analysis (FEA) at 6.7-9.3 GPa. The manufactured scaffolds had 59-70% porosity and 33-42 cm^{-1} S/V. Laboratory compression testing revealed an effective Young's modulus of 5-9 GPa, comparable to bone. Image-based simulation method was also employed on the built samples which reported the stiffness range of 8.3-16.6 GPa, overestimating it by 57%. It is hypothesised that these discrepancies stem from the secondary roughness deposited on the scaffold walls during SLM, causing reduction in porosity yet not contributing to structure's strength. The cyber-physical validation methods presented are a good way to quantify these discrepancies, allowing feedback to the design stages for more predictable as-manufactured structures.

1. Scaffold Design and Physical Properties

Three types of sheet-based TPMS structures (gyroid, Schwartz diamond and primitive) were generated using MATLAB v.R2021A and Magics v.22.03. Two variants were designed for each type of scaffold with an intended porosity range of 70-75% and S/V 25-35 cm^{-1}. The intended physical properties of the scaffolds are listed in Table 1.

Table 1: Intended physical properties of as-designed scaffolds.

Structure	Scaffold ID	Unit cell size (µm)	Porosity (%)	S/V (cm^{-1})	Sheet thickness (µm)	Pore Size (µm)
Gyroid	G2.50	2500	73.9	25.2	254 ± 6	872 ± 88
	G2.22	2222	73.8	28.2	229 ± 5	779 ± 77
Primitive	P1.64	1667	70.9	28.2	254 ± 22	831 ± 311
	P1.43	1428	70.6	32.8	225 ± 18	720 ± 280
Diamond	D2.50	2500	74.9	30.9	205 ± 4	761 ± 99
	D2.22	2222	74.8	34.7	188 ± 2	681 ± 81

2. Mesh Convergence and Scaffold Cell Tessellation Studies

A mesh convergence study was run in nTop v.4.6.2 on the as-designed models of G2.22, P1.43 and D2.22 scaffolds. The edge length of tetrahedral mesh elements varied [0.04-0.22 mm] for [1x1x1 to 7x7x7] lattice models creating 900-170k elements per unit cell. The resultant moduli were plotted against the number of finite elements per unit cells in Fig. 1 (b,d,e). The moduli converge was found at ~ 20k-60k elements per unit cell, in agreement with [1].

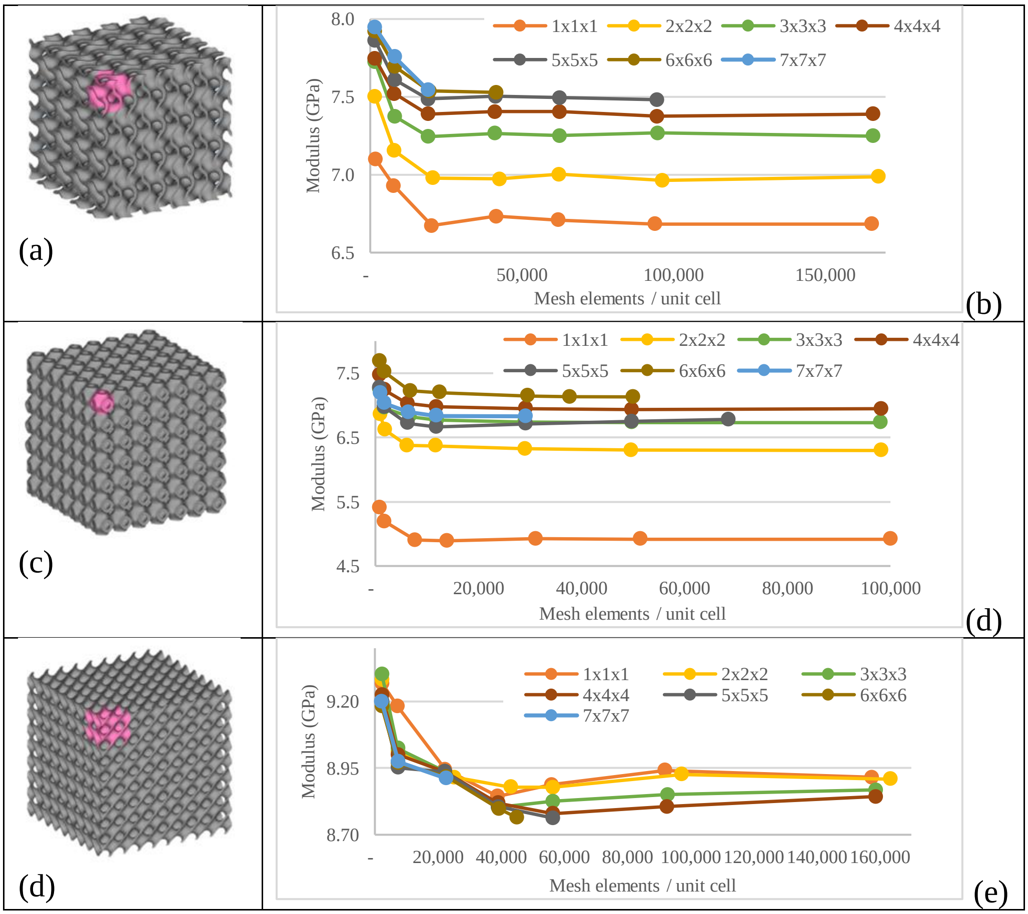

Figure 1: (a), (c), (d) 1 cm^3 scaffold variants G2.22, P1.43 and D2.22 (unit cells highlighted). Finite element mesh convergence for lattice structures(b) G2.22 (d) P1.43 (e) D2.22 comprising 1 × 1 × 1 to 7 × 7 × 7 unit cells.

The cell tessellation study was conducted on the same three design variants comparing FEA and meshless methods. The converged values of moduli from both methods were plotted against cell order (Fig 2). These graphs show that the moduli from FEA plateaued at 4x4x4 cell configuration for gyroid and primitive structures, in agreement with [1]. The results from a meshless method (i.e., Altair's SimSolid v.2023.1) show a similar trend as FEA for primitive structures, and slightly higher than FEA for gyroid and diamond, up until lattice order 5. It is noteworthy that the modulus from the meshless method for gyroid and diamond increased very significantly for lattice order n>6.

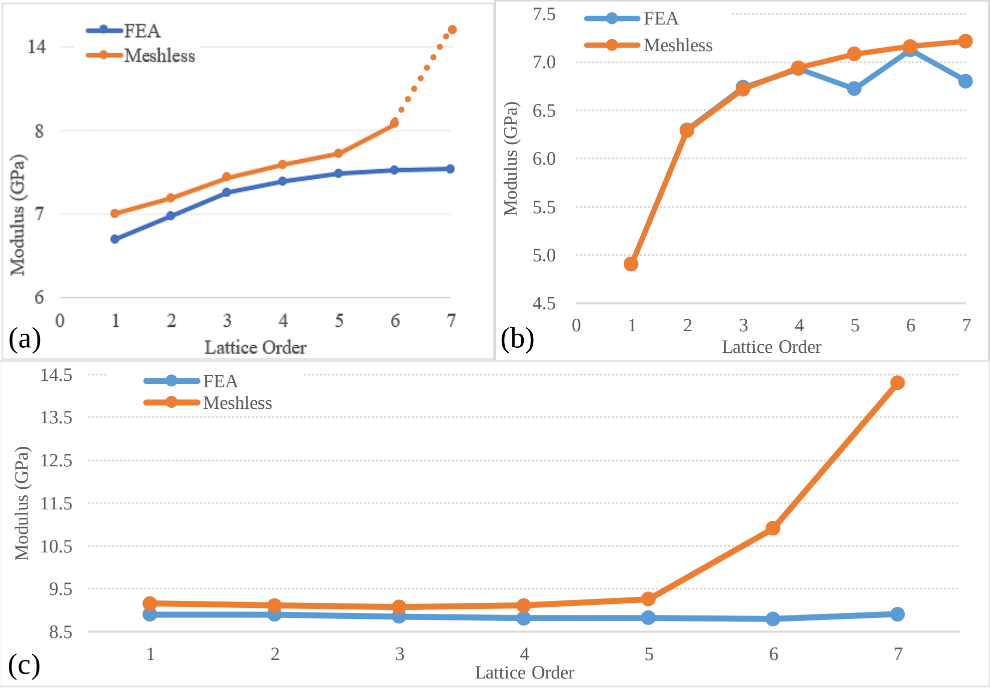

Figure 2: Lattice cell tessellation study of as-design scaffold models by FEA and meshless methods. Effective elastic modulus plotted against increasing number of lattice unit cells. (a) G2.22 (b) P1.43 (c) D2.22.

We hypothesize that SimSolid is limited to the size of the STL model/no. of mesh elements that it can handle, hence the differing results when n>6. In light of this, the following results in this study are obtained with 4x4x4 cells for as-designed (FEA method) and as-manufactured models (meshless method), with a mesh element size of 0.07mm used throughout.

3. Morphological and Mechanical Characterization

The SLM 1cm^3 printed cubes were scanned by µ-CT with 10.03 µm resolution. The porosities of the actual samples were measured by Archimedes's (using acetone) and via µ-CT data analysis, which show a reduction in the actual porosity. Scaffolds designs with smaller unit cell size (G2.22, P1.43 and D2.22) deviated more from target porosity than the larger unit cell designs. The

S/V values increased avg. 27% in all samples, compared to the intended values. These deviations are due to the presence of partly sintered particles (i.e., secondary roughness) attached to the walls. Other studies have found similar deviations in actual porosity and S/V of SLM printed scaffolds [2], [3]. Quasistatic compression results (BS ISO 13314) from printed samples were compared with FEA results on as-designed models; both results were similar for primitive and diamond structures. However, FEA overestimated the moduli for gyroid, as also found in [3].

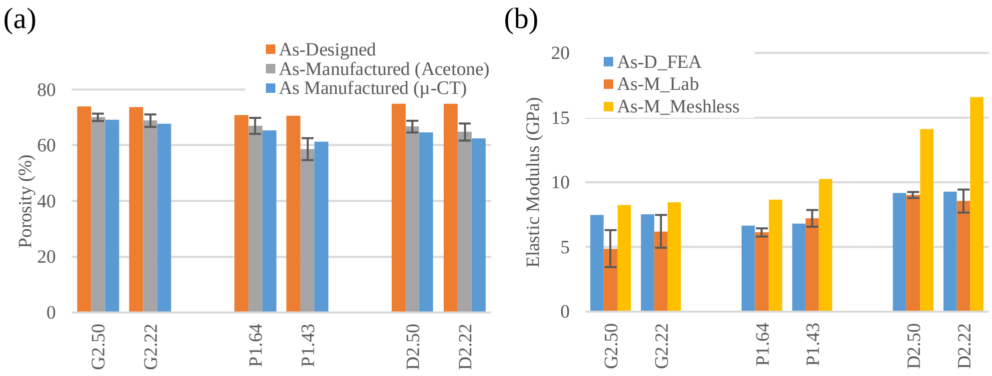

Figure 3: (a) Porosity as designed (CAD) vs as-manufactured (measured by Archimedes's and by μ-CT), (b) Elastic Moduli (as-designed by FEA, and as-Manufactured by lab testing and meshless methods).

As-manufactured scaffolds were reconstructed (in ORS-Dragonfly) and moduli obtained via static simulations (in SimSolid) (Fig. 3b). There is a difference between the lab test and the meshless method results, with diamond affected the most. The presence of secondary roughness has caused that μ-CT scan reconstruction yields lower porosity than the printed samples (Fig. 3a). A lower porosity with fewer structural details would lead to stiffer mechanical response. Another contributing factor might be the limitation of the meshless software to handle size and complexity of the geometries, as aforementioned (section 2).

4. References

[1] I. Maskery, A. O. Aremu, L. Parry, R. D. Wildman, C. J. Tuck, and I. A. Ashcroft, "Effective design and simulation of surface-based lattice structures featuring volume fraction and cell type grading," *Mater. Des.*, vol. 155, pp. 220–232, 2018.

[2] A. Timercan, V. Sheremetyev, and V. Brailovski, "Mechanical properties and fluid permeability of gyroid and diamond lattice structures for intervertebral devices: functional requirements and comparative analysis," *Sci. Technol. Adv. Mater.*, vol. 22, no. 1, pp. 285–300, 2021.

[3] S. Ma *et al.*, "Manufacturability, Mechanical Properties, Mass-Transport Properties and Biocompatibility of Triply Periodic Minimal Surface (TPMS) Porous Scaffolds Fabricated by Selective Laser Melting," *Mater. Des.*, vol. 195, 2020.