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Development of Modelling Methods for Materials to be Used as Bone Substitutes

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Abstract. The demand in the medical industry for load bearing materials is ever increasing. The techniques currently used for the manufacture of such materials are not optimized in terms of porosity and mechanical strength. This study adopts a microstructural shape design approach to the production of open porous materials, which utilizes spatial periodicity as a simple way to generate the models. A set of triply periodic surfaces expressed via trigonometric functions in the implicit form are presented. A geometric description of the topology of the microstructure is necessary when macroscopic properties such as mechanical strength, stiffness and isotropy are required to be optimised for a given value of volume fraction. A distinction between the families of structures produced is made on the basis of topology. The models generated have been used successfully to manufacture both a range of structures with different volume fractions of pores and samples of functional gradient material using rapid prototyping.

Introduction

The need for new materials which have a high porosity and low weight but also a relatively high strength and tailored stiffness, has pushed research towards a more in depth analysis of the microstructure of porous materials. The numerous applications that, today, require a good balance of mechanical properties and porosity encompass the aerospace, automotive, biomedical materials, chemical and renewable energy industries. The wide range of properties available in the form of porous materials justifies the market demand and the interest in further developing their properties. In the medical sector, porous materials are highly desired as a substitute for osseous tissue, as some of their properties resemble those of bone, being lightweight, strong and having a totally interconnected porosity [1-4]. The demand from the medical industry for a material of this kind is continuously growing, and the manufacturing processes for foaming metals, polymers and ceramics which are continuously evolving. There is also increasing interest in the production of functional gradient materials which more closely resemble the naturally occurring structures found in bone [5-7]. A limitation of the materials currently used for biomedical applications is their lack of interconnected porosity and their limited load bearing capacity. The aim of this study is to adopt a microstructural shape design approach to the manufacture of open porous materials, which utilizes spatial periodicity as a simple way to generate the models. The intention is to minimize stress concentrations in open porous materials via structural design of interconnected three-dimensional lattices hence optimising properties such as strength. The optimised models and geometries which are finally developed can be subsequently produced in material form by the use of rapid prototyping techniques.

Model development

Consider a finite volume of porous matter. Interconnected voids inside the continuous matter can be defined via a surface. In mathematical terms, let S be a surface defined by:

$$S : F(X) = 0 \quad X \in R^3 \qquad \text{Eq. 1}$$

where X is a point of coordinates x, y and z.

The surface S represents the border between the matter and the voids. A trigonometric polynomial has been used for the definition of the function *F(X)*, which can be written as a sum of *d* terms as shown in Eq. 2:

$$1 + \sum_{c=1}^{d} a_c \sin^i x \cdot \sin^j y \cdot \sin^k z \cdot \cos^l x \cdot \cos^m y \cdot \cos^n z \quad i, j, k, l, m, n = 0, 1 \qquad \text{Eq. 2}$$

This gives rise to triply periodic level surfaces: the primitive (P) surface, the diamond (D) surface and the gyroid (G) surface, having interconnectivity orders respectively equal to 6, 4 and 3.

$$\begin{aligned}
&P: \quad a_1(\cos x + \cos y + \cos z) + a_2(\cos x \cos y + \cos y \cos z + \cos z \cos x) + 1 = 0 \\
&D: \quad a_3(\sin x \sin y \sin z + \sin x \cos y \cos z + \cos x \sin y \cos z + \cos x \cos y \sin z) + \\
&+ a_4[\cos(4x) + \cos(4y) + \cos(4z)] + 1 = 0 \qquad \text{Eq. 3} \\
&G: \quad a_5(\cos x \sin y + \cos y \sin z + \cos z \sin y) + \\
&+ a_6[\cos(2x)\cos(2y) + \cos(2y)\cos(2z) + \cos(2z)\cos(2x)] + 1 = 0
\end{aligned}$$

From a topological point of view, the interconnectivity order states how many struts depart from each node of the lattice.

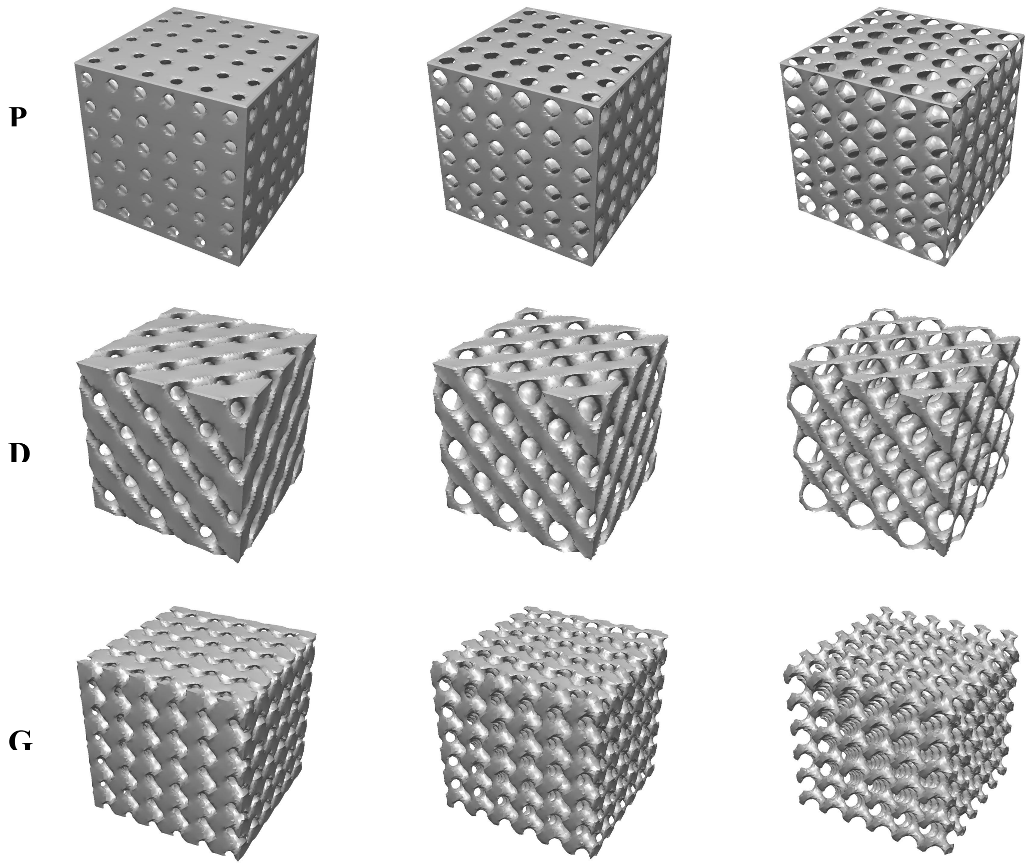


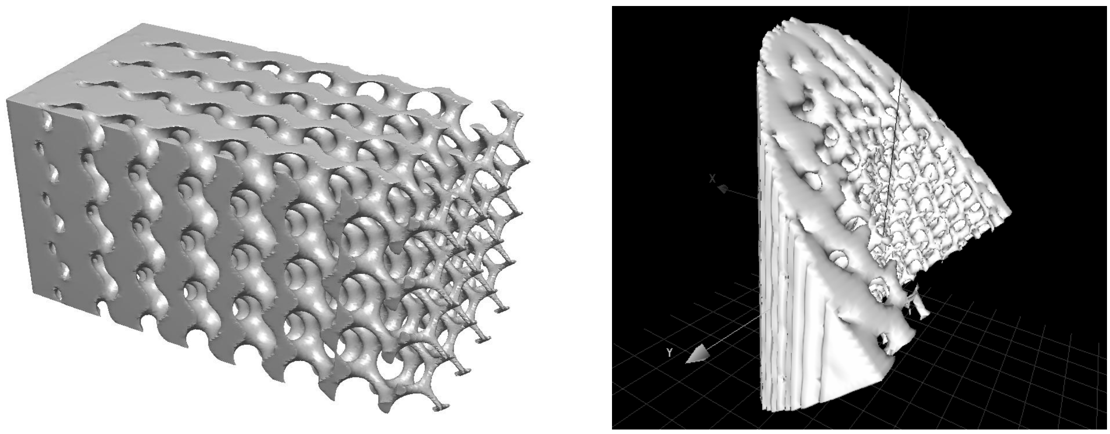
Fig.1: The P, D and G surfaces with different values of volume fraction (from left to right: 0.7, 0.5 and 0.3).

A particular advantage of using mathematical expressions to define the surface is that a desired number of parameters can be assigned to the model so that a subsequent shape optimization study can be carried out with relative ease. Subsequently, the generation of models with a range of pore volume fractions and interconnectivities is possible.

The surface has been modelled with the aid of a routine written in the computer language C which uses the GNU Triangulated Surface Library [8]. The shapes obtained are illustrated in Fig. 1 which shows P, D and G surfaces with different values of volume fraction.

Different values for volume fraction have been assigned to the scaffold geometries, demonstrating how cortical and cancellous bone (respectively ~0.7 and ~0.2 volume fraction) can be represented using the same mathematical expression, where just a few coefficients vary. The calculation time for this type and size of surface is between 0.4 and 2 s, and primarily depends on the number of cells per unit volume and the desired resolution of the output. The machine used for these operations is run by a Pentium 4 processor, 2.4 GHz with 1 GB RAM.

By adding a linear term to Eq. 1 it is possible to generate functionally graded materials with a porous inner core and a dense outer layer, imitating the transition seen in bone from the outer dense cortical to the inner porous cancellous structure. Fig. 2 shows examples of functionally graded structures produced in this way.



(a) (b)

Fig. 2: (a) Variable porosity structure resembling functional gradient material. (b) Representation of a bone wedge generated via mathematical function.

The use of the viewer K3DSurf [9] provided the opportunity to produce complex structures in a finite volume via implicit functions and inequalities. A more complex function with a radial variation of the porosity can be used to generate the bone wedge shown in Fig. 2(b). This new approach to 3-D modelling is particularly useful when dealing with the microstructure of materials, because of its ability to represent small features such as struts and pores with little computer memory allocation. Additionally, the highest degree of continuity is implicitly guaranteed over the entirety of the defined surface.

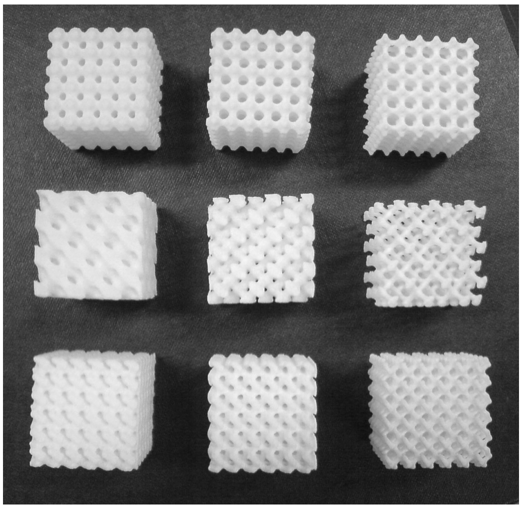
Manufacturing

The modelling outputs in Fig. 1 and Fig. 2(a) were used to generate the geometries using rapid prototyping techniques. The specimens shown in Fig. 4(a) have been manufactured using a 3DSystem SLS Vanguard Rapid Prototyping machine. In addition, a model of the functional gradient scaffold using a G surface has also been produced via SLS on a DTM Sinterstation 2500, Fig. 4(b). All the scaffolds are made from polyamide PA12, although in the longer term it is intended to pursue the direct formation of these structures in ceramic [10].

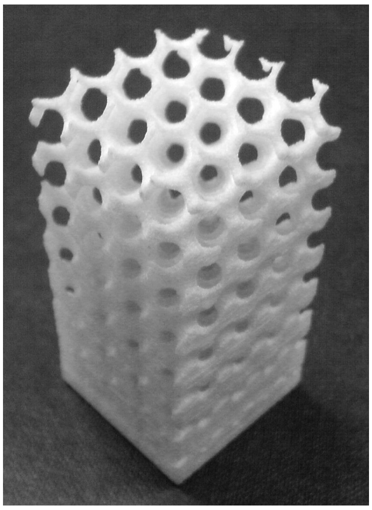
P

D

G



(a)



(b)

Fig. 4: The samples in (a) are 30x30x30 mm, the one in (b) is 30x30x60 mm.

Conclusions

A range of materials with different volume fractions have been successfully modelled and subsequently manufactured using rapid prototyping. The techniques have been further developed to produce models and prototype functional gradient samples with a similar bimodal structure to that found in natural bone. In order to optimize the mechanical properties of such structures, the load bearing capacity of such materials needs to be further investigated. However this success in developing simple, yet effective, modelling methods for the generation of materials with a diversity of microstructural features indicates the potential use of the technique to manufacture tailor made structures that could be used in dental and orthopaedic applications.

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