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A continuous crystallographic approach to generate cubic lattices and its effect on relative stiffness of architectured materials

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ABSTRACT

This original work proposes to investigate the transposition of crystallography rules to cubic lattice architectured materials to generate new 3D porous structures. The application of symmetry operations provides a complete and convenient way to configure the lattice architecture with only two parameters. New lattice structures were created by slipping from the conventional Bravais lattice toward non-compact complex structures. The resulting stiffness of the porous materials was thoroughly evaluated for all the combinations of architecture parameters. This exhaustive study revealed attractive structures having high specific stiffness, up to twice as large as the usual octet-truss for a given relative density. It results in a relationship between effective Young modulus and relative density for any lattice structure. It also revealed the opportunity to generate auxetic structures at will, with a controlled Poisson ratio. The collection of the elastic properties for all the cubic structures into 3D maps provides a convenient tool for lattice materials design, for research, and for mechanical engineering. The resulting mechanical properties are highly variable according to architecture, and can be easily tailored for specific applications using the simple yet powerful formalism developed in this work.

1. Introduction

The important development of Additive Manufacturing (AM) processes and the potential capabilities that it offers for industrial applications, allows producing more complex three-dimensional parts. These opportunities highlight new ways to design optimal functional and lightweight structural parts. The use of lattice structures is also motivated by the requirements to reduce the costs inherent to the AM processes by decreasing material consumption and building time. The development of architectured porous materials is the ultimate step to achieve mass reduction on mechanical parts. Basically, this reduction consists in removing the fraction of the material that has a limited effect if any on the mechanical resistance. Hence, only the load-bearing material fraction is kept. To achieve this mass-reduction, two main strategies are emerging. The first approach relies on a topological optimization [1,2] using finite element computation [3,4] aimed at removing the needless part of the material (Fig. 1.1). This first strategy is efficient, but depends widely on the initial geometry of the considered part. In addition, topological optimization may result in multiple solutions, with numerical issues on the selection of the proper optimal structure. The second strategy aims at developing mesostructured metamaterials having controlled properties, which can fit a large range of application requirements [5,6,7]. Since the last decade, this strategy has been successfully explored by Ashby and Bréchet [8,9]. They developed hybrid multifunctional materials with appropriate properties providing an extension of the Ashby selection map compared to the initial properties of the bulk materials.

The lattice architecture is especially attractive for its capability to produce Functionally Graded Materials (FGM) with variable stiffness. Again, there are two main strategies: either the lattice density is modified, or the architecture is altered. These two distinct concepts are illustrated on Fig. 1.2 and .3: metal lattices were obtained by selective laser melting by using TA6V powder, with a laser power of 175W and a scanning rate of 775 mm/s. If the density is affected (Fig. 1.2), the part weight may become sub optimized. On the other hand, to adjust the stiffness gradient while preserving mass minimization (Fig. 1.3), it is necessary to produce architectures at will with a continuous procedure. It is also necessary to capture accurately the effective contribution of

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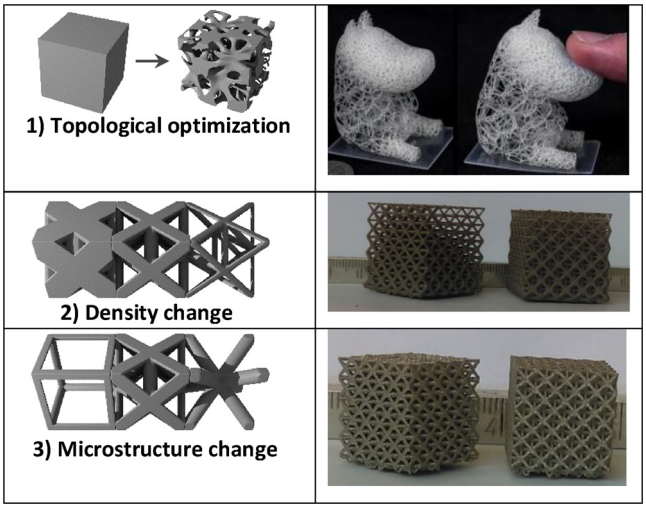

Fig. 1. The three main strategy to obtain porous materials 1) Topological optimization and a kind of application [1], 2) Graded density change and an graded porous materials obtain by SLM, 3) Microstructure change and a kind of periodic lattice product by SLM.

architecture to stiffness, independently of the density. As far as we know, up to now, there has not been any method reported in the literature for the continuous generation of lattice architectures. Information concerning the dependence of stiffness on density in a large cluster of continuous structures is also a missing piece of information. It would be very relevant and groundbreaking to set a method for the generation of architectures using crystallographic rules, and to compare them by evaluating the mechanical behavior. This paper proposes a continuous generation of cubic architectures and the investigation of the relationship between stiffness and density.

Periodic-cell and architectured structures have been extensively studied due to straightforward mathematical description [10,11]. The octet-truss lattice is an example of a structure which is commonly investigated. Fuller initially proposed this structure in 1961 [12]. Nayfeh focused on its elastic properties [13], while its plastic behavior has been studied by Deshpande et al. [14,15,16]. It is worth noticing that the octet-truss lattice is especially attractive because it fulfills the Maxwell criterion [17]:

$$b - 3j + 6 = s - m \quad (1)$$

where b is the number of struts, j is the number of joints, s and m are the number of states of self-stress and mechanisms. The octet-truss is therefore able to bear mechanical loading even in the case of frictionless rotation at joints [15]. The octet-truss symmetry corresponds to a face-centered cubic structure [13]. Many other structures with cubic symmetry have also been analyzed [7,10,18,19,20]. However, some of these cubic lattices were considered of lesser interest since they do not satisfy the Maxwell criterion. Indeed, they are assumed to exhibit significant stress level at nodes inducing an early collapse of the structure.

Nevertheless, any cubic lattice could possibly be attractive regardless of Maxwell's criterion. For instance, the primitive cubic structure [10] does not satisfy the Maxwell criterion, but is commonly adopted for simple mechanical structures. In itself, any lattice structure could be interesting due to specific elastic properties [7,10,19], or an unusual Poisson ratio [11,21,22,23], or again a high relative stiffness [11], or creep properties [24] with respect to specific application.

This study aims at exploring large numbers of geometrical configurations based on cubic lattices with crystallographic symmetry. First, the study will propose a continuous description of the architecture with reduced parameters. Next, the third section is devoted to the estimation of elastic properties using finite elements computations. Numerical results are then illustrated as performance surfaces by exploring the whole space of the architectural parameters. In the fourth section, the effect of the lattice architecture on the overall specific moduli is analyzed leading to the formulation of an explicit relationship. The latter clearly expresses the impact of relative density on elastic properties. The end of this section is dedicated to the Poisson ratio of cubic structures yielding to the identification of original auxetic structures for specific architectures and density ranges. The paper ends with some concluding remarks and provides some ideas for a future work.

2. Materials and Methods: New approach based on crystallography rules

At first sight, the mathematical description of lattices is complex since each beam location requires three position coordinates and three Euler angles. The description is made easier by considering only the joint nodes, having three coordinates only. It is common sense in crystallography to reduce further the mathematical description of nodes positions using symmetries. The minimal number of nodes to generate a 3D lattice can be reduced to a couple of points by proper use of all the isometric operations of a given space group. This approach using symmetries is innovative because it breaks with the habit of considering lattices as a huge complicated beams cluster. This new approach focuses on the minimalist architectural information of the lattice network. Any alteration of this information would lead to great modifications by moving continuously and slightly a single structural parameter. Such a method is ideal for mechanical engineering due to its simplicity and its versatility. The question arising at this point is: what is the minimal information required to properly describe cubic lattices?

In materials science, the three most common crystal structures are primitive cubic ($Pm\bar{3}m$), face centered ($Fm\bar{3}m$) and body centered ($Im\bar{3}m$). If the atoms in a crystal are replaced with vertices in the lattice, and chemical bonds are beams, then crystalline architectures can be directly applied to build porous materials. These three usual cubic structures have a common point: they share the same$m\bar{3}m$ point group. However, this $m\bar{3}m$ group contains only 10 well-known space groups, leading to 10 lattice structures already reported in literature. This panel would be very limited for producing FGM. To generate a larger number of structures, it is necessary to break the rules given by Bravais lattices, while preserving the symmetries of the point group. To distance ourselves from these rules, let us first consider the Bravais structures more closely. The Bravais cubic lattices are defined by two sets of nodes positions:

- One at the origin, defined by the vertex of the primitive cube,
- One located in the middle of the faces (FCC), or in the middle of the cube (BCC).

The first set of nodes must be preserved as is, because it is a mandatory condition for cubic structures. The second set of nodes is more interesting, because it is defined by changing geometric coordinates. If one considers the unit cube length to be equal to one, then the secondary point has the following coordinates:

- For a primitive cube, it does not exist at all. Still, one can attribute coordinates (0, 0, 0.5) to this node, and the resulting lattice will be equivalent to the primitive cube. The structure is actually a perovskite (ABX_3)-related structure with an empty A site [25]. If the structure is made of beams only, then the architecture can be considered as primitive-like.
- For a face-centered cube, the structure is set with a node at position (0, 0.5, 0.5)
- For a body-centered cube, the structure is set with a node at position (0.5, 0.5, 0.5)

By generalization, it is possible to set a continuous description of cubic structures for $Pm\bar{3}m$,$Fm\bar{3}m$ and $Im\bar{3}m$space groups by modifying the position of this secondary node. If the coordinates of the node are