Impact of Geometry on the Thermal and Mechanical Properties of Periodic Surface Structures: A Numerical Study

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Abstract. Periodic Surface Structures (PSS) fabricated via Additive Manufacturing (AM) have recently emerged as being appropriate candidates for high-value engineered structures. Among the many PSS designs, gyroid structures have demonstrated merits in mechanical properties and permeability compared to traditional lattice structures. Periodic surface structures are mathematically formulated by geometric factors: surface thickness, sample size, number of surface periods, or unit cells. These elements produce a continuous sur-face with specific topology. Numerical simulations of the effect of modulating these factors on overall thermal and mechanical properties require substantial computational resources and give a quite good qualitative assessment. Cubic P-surface ("Primitive"), D-surface ("Diamond"), and gyroid surface structures of various designs were simulated under load and heat transport using a numerical approach. The influence of geometric factors on thermal and mechanical behavior was determined qualitatively. The results show the impact of the number of cells and surface thickness on both thermal and strength modulus. The paper focuses on thermal and mechanical analysis of periodic surface structures. The study is conducted by solving the stress and heat equations using the Finite Element Method (FEM) and is achieved with the use of our authorial software. Our software module generates periodic surface structures and simulates stress and temperature distribution in it. The stress model is defined by dependence between stress and strain, it got from an experiment, and the correlation of strain and displacement got from geometric conditions. In the paper, we present calculations for three-dimensional systems in which we analyze the stress and temperature distribution depending on the geometric factors. The results presented allow estimation of the behavior of periodic surface structures under loads. It intends to evaluate the possibility of crack occurrence in complex structures based on the performed numerical simulations in future work.

1 Introduction

Periodic Surface Structures (PSS) have a locally minimized surface area that entwines in 3D space and typically separates the finite bounding volume into intimately interlaced domains filling the volume without wrapped closed voids (open structure). PSS have demonstrated advantages in their structural, mechanical efficiency over conventional solid mass structures. They are reaching increasing interest in the design community, including applications in high stiffness structures, impact energy absorbers, chemical catalysts, and medical bone implants [1-4]. Despite this interest, the characterization of the mechanical reaction of PSS remains an open research question.

The gyroid has been shown to display remarkable geometric and mechanical properties [5]. A team of researchers at MIT has designed one of the most durable lightweight materials known and has conducted the simulations with 3-D gyroid construction made from this matter. The results of tensile and compression tests presented that the construction could be ten times as strong as steel but much lighter. Their discoveries proved that the crucial aspect of performed tests has more to do with the unusual geometrical configuration than with the material itself. The researchers propose similar durable, lightweight materials that could be made from various matters by creating similar geometric features. The gyroid has circular and smooth struts with a spherical core. Its surface has no reflection symmetry nor straight lines giving the opportunity to reduce the effect of stress concentration within the structure and provides highly efficient mechanical properties compared to solid or lattice structures. The latest literature has demonstrated the potential for the gyroid in orthopedic bone-implant, and for more general thermal and mechanical applications that exploit energy absorption, liquid permeability, heat transfer, stress/strain distribution or mechanical response in mining, aerospace, chemical industries, et al. [6, 7]. These arising design opportunities are enabled by commercially reliable additive manufacturing technologies such as Selective Laser Melting (SLM). It allows the fabrication of high-definition metallic structures directly from a computer-aided design (CAD) data next converted to a stereolithography (STL) file. Such AM technologies in rapid prototyping radically increase the efficiency and cost-effectiveness connected with the production of complex geometries [8]. In the paper, numerical simulations are made with exemplary material properties for Al2%Cu alloy and are verified concerning the mechanical and thermal response of a full-size structure results. Based on this numerical model, the influence of the identified geometric factors: surface thickness, sample size, number of surface periods, or unit cells was investigated using authorial software.

In the paper, we use PSS, which are homogeneous, isotropic structures, preserving the same mechanical properties in each direction. Isotropy of PSS is very useful because there is no difference in the physical properties such as thermal expansion, heat conduction, electrical conductivity, refractive index, etc. regardless of the direction in which they are measured. In the paper, Cubic P-surface ("Primitive"), D-surface ("Diamond"), and gyroid surface structures of various designs were simulated under load and heat transport using a numerical approach. It is critical thought to know how new materials, structures, or models preserve under load. Therefore many researchers study the attained results of FEM analysis of stress and strain distributions to approximate the mechanical parameters of devices. That way, the models become useful for comparative analyses of different geometries, which - together with proper empirical verification studies - make it possible to develop useful structure. The influence of geometric factors on thermal and mechanical behavior was determined qualitatively.

The results show the impact of the number of cells and surface thickness on both thermal and strength modulus. The paper focuses on thermal and mechanical analysis of

periodic surface structures. The study is conducted by solving the stress and heat equations using the Finite Element Method (FEM) and is achieved with the use of our authorial software. Our software module generates periodic surface structures and simulates stress and temperature distribution in it. The stress model is defined by dependence between stress and strain, it got from an experiment, and the correlation of strain and displacement got from geometric conditions. The forces affecting the element increase stresses in it. Accumulation of stress may redound to locally exceeding of yield point and uncontrolled deformation of the element, and in extreme cases, rupture of the material's continuity. We present results for three periodic surface structures for which we analyze the temperature and stress distribution. We consider a static load case. The simulations showed to allow assessment of the dependence of the stress and temperature distribution on the geometric factors.

2 Methods

In literature, it was proved that the mean curvature of a minimal surface is zero at every point. Any infinitesimal region of such a surface has the least area of any region with the same boundary conditions [9]. Furthermore, the divergence of the unit normal vector n is zero throughout the minimal surface [10]. Periodic surface structures satisfy the requirements of minimal surfaces while self-tessellating infinitely in three mutually perpendicular coordinate directions [11]. In local Cartesian coordinates (X, Y, Z), we consider three mathematically defined periodic surface structures, the Primitive (P), Diamond (D), and Gyroid (G) structure:

$$\text{(P)}\quad \cos X + \cos Y + \cos Z = \delta \tag{1}$$

$$\textit{(D)}\quad \cos Z \sin(X+Y) + \sin Z \cos(X-Y) = \delta \tag{2}$$

$$\textit{(G)}\quad \sin X \cos Y + \sin Y \cos Z + \cos X \sin Z = \delta \tag{3}$$

where thickness δ is normalized, takes values from 0 to 1, and plays a significant role in the PSS topology and associated structural response. These implicit surfaces are defined as an iso-surface of some function f

$$f(X,Y,Z)=0 \tag{4}$$

The computer simulation of PSS structural behavior is based on efficiently generated, implicitly defined, and rapidly constructed finite element meshes. Finite element mesh for the bulk was generated with Gmsh software. The used version of Gmsh did not have the option of design NURBS surface, so mesh for PSS was created with our own software using the CGAL library (it contains procedures for describing the division of an area into finite elements). CGAL is a software project that provides easy access to efficient and reliable geometric algorithms in the form of a C++ library. CGAL is used in various areas that need geometric computation, such as geographic information systems, computer-aided design, molecular biology, medical imaging, computer graphics, and robotics [12].
Heat transfer simulation was based on the heat transfer equation:

$$\rho c\dot{T} - k\nabla^2 T = 0 \tag{5}$$

where ρ is density, c is specific heat, T is temperature, k is thermal conductivity. The Neumann boundary condition is used for description of heat flow into a calculation domain.

Stress analysis is a general term used to describe the quantities of stress and strains. It is also known as structural analysis. In terms of mechanical properties, the most crucial parameter concerning many structures are the elastic modulus and yield strength [13]. Increasing Young's modulus of the lattice structure ensures the improvement of mechanical properties necessary for counteracting high loading conditions [14]. The dependency of stress and strain characterizes the stress model, got from an experiment, and by the association of strain and displacement, got from geometric considerations. Stress is related to yield through the physical connection:

$$\sigma = C\epsilon \tag{6}$$

where σ is a stress tensor, C is a stiffness tensor, and ϵ is a tensor of elastic deformation. Physical properties that appear in elasticity tensor can depend on temperature. The relationship from Eqn. 6 is called generalized Hook's law. In turn, the strain is related to displacement through the Cauchy relations [15]:

$$\epsilon = \frac{1}{2}[(\nabla q) + (\nabla q)^T] \tag{7}$$

where q is the displacement vector. This work focuses on stress distribution in the three-dimensional case, so the stiffness tensor becomes:

$$\begin{bmatrix} \lambda+2\mu & \lambda & \lambda & 000 \\ \lambda & \lambda+2\mu & \lambda & 000 \\ \lambda & \lambda & \lambda+2\mu & 000 \\ & & 000\mu 00 & \\ & & 0000\mu 0 & \\ & & 00000\mu & \end{bmatrix} \tag{8}$$

where

$$\lambda = \frac{E\upsilon}{(1+\upsilon)(1-2\upsilon)} \tag{9}$$

$$\mu = \frac{E}{2(1+\upsilon)} \tag{10}$$

and E is Young's modulus, υ is Poisson's ratio.In this case, the stress tensor has the following structure:

$$\sigma^T = \{\sigma_x \sigma_y \sigma_z \tau_{xy} \tau_{xz} \tau_{yz}\} \tag{11}$$

While the tensor of elastic deformation is given by:

$$\epsilon^T = \{\epsilon_x \epsilon_y \epsilon_z \gamma_{xy} \gamma_{xz} \gamma_{yz}\} \tag{12}$$

where $\gamma_{xy} = 2\,\epsilon_{xy}$. And the displacement vector is equal:

$$\boldsymbol{q}^T = \{uvw\} \tag{13}$$

where x, υ, w are displacements in the direction of X, Y, Z axes, respectively.

3 Results

The article presents the results of the heat conduction and stress distribution simulations for a cube whose face has 0.04 [m] edge length and for the PSS inserted in the cube. The following physical properties were used in simulations: k - heat transfer coefficient 260 [W/(m·K)], ρ - density 2800 [kg/m3], c - specific heat 1000 [J/(kg·K)]. Such material properties are similar to those of aluminum alloys - material significant and often used in industry. The boundary condition is a heat flux established on one surface with a fixed value of 10 [kW/m2] (Neumann boundary condition). Mechanical properties as follow: Young's Modulus E = 6.9·1010 MPa, Poisson's ratio υ = 0.33, density ρ = 2700 [kg/m3]. All cubes had fixed bottom faces (all degrees of freedom were removed) and all cubes were subject to a load of value 10 MPa on the top face.
Table 1 presents different parameters used for generating the PSS, together with their volume fraction calculated as a ratio of volume used by a given structure to volume of the full cube.

Table 1. Parameters used for generating different periodic surface structures, together with their impact on volume of a specific structure.

Name	Number of cells [.]	Thickness δ [.]	Volume [m^3]	Volume fraction [.]
cube	-	-	$6.400 \cdot 10^{-5}$	1.0000
diamond (D)	2	0.5	$2.633 \cdot 10^{-5}$	0.4114
diamond (D)	2	0.8	$4.254 \cdot 10^{-5}$	0.6647
diamond (D)	4	0.5	$2.638 \cdot 10^{-5}$	0.4122
diamond (D)	4	0.8	$4.266 \cdot 10^{-5}$	0.6666
gyroid (G)	2	0.5	$2.069 \cdot 10^{-5}$	0.3233
gyroid (G)	2	0.8	$3.343 \cdot 10^{-5}$	0.5223
gyroid (G)	4	0.5	$2.071 \cdot 10^{-5}$	0.3235
gyroid (G)	4	0.8	$3.347 \cdot 10^{-5}$	0.5230
primitive (P)	2	0.5	$1.828 \cdot 10^{-5}$	0.2856
primitive (P)	2	0.8	$2.930 \cdot 10^{-5}$	0.4579
primitive (P)	4	0.5	$1.829 \cdot 10^{-5}$	0.2857
primitive (P)	4	0.8	$2.933 \cdot 10^{-5}$	0.4584

The results for the heat simulation are presented in Fig. 1, where temperature distribution is shown after 250 s of simulation time. It can be seen that the PSS in all configurations characterizes by regular temperature distribution and there are no overheated regions. Maximum achieved temperature is varied for different PSS and different configurations and this is because of different volume that each PSS has (it is also affected by the thickness δ).
The results for stress analysis are presented in Fig. 2 (total displacement) and Fig. 3 (von Mises stress distribution). It can be seen here that type of PSS has visible impact on total displacement. Moreover, for type D, increase in number of cells in cube lowers maximum total displacement. For other PSS, number of cells has less visible impact. We can also see that increasing thickness can affect total displacement. What is also interesting, for the stress distribution, we can observe the type D and G have some fragments in structure that do not participate in stress propagation, while for the type P all fragments participate. This results in much more uniform stress distribution for the type P structure.

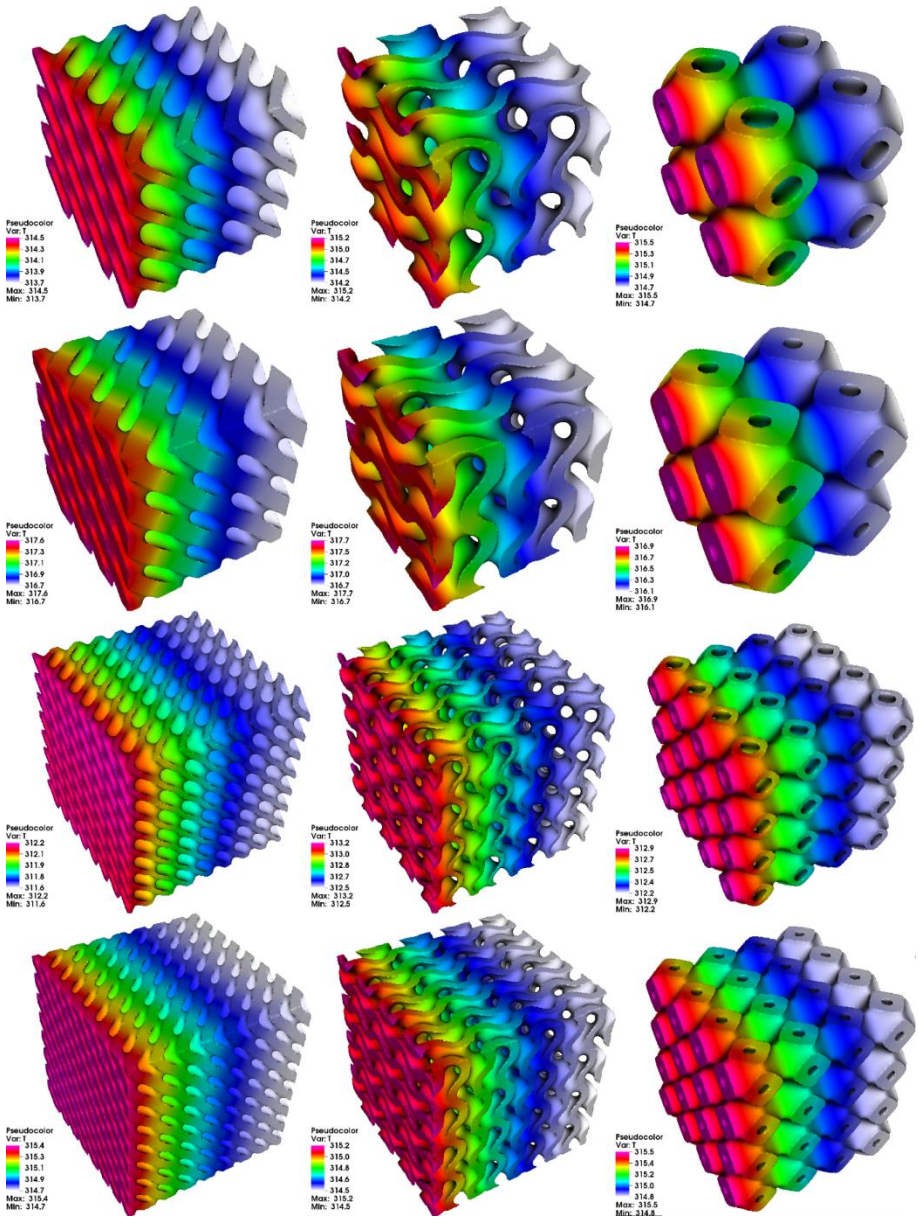

Fig. 1. The results of heat simulation after 250 s. Columns from left to right: Diamond (D) surface, Gyroid (G) surface, Primitive (P) surface. Rows from top to bottom: 2 cells, thickness δ=0.5; 2 cells, thickness δ=0.8; 4 cells, thickness δ=0.5; 4 cells, thickness δ=0.8.

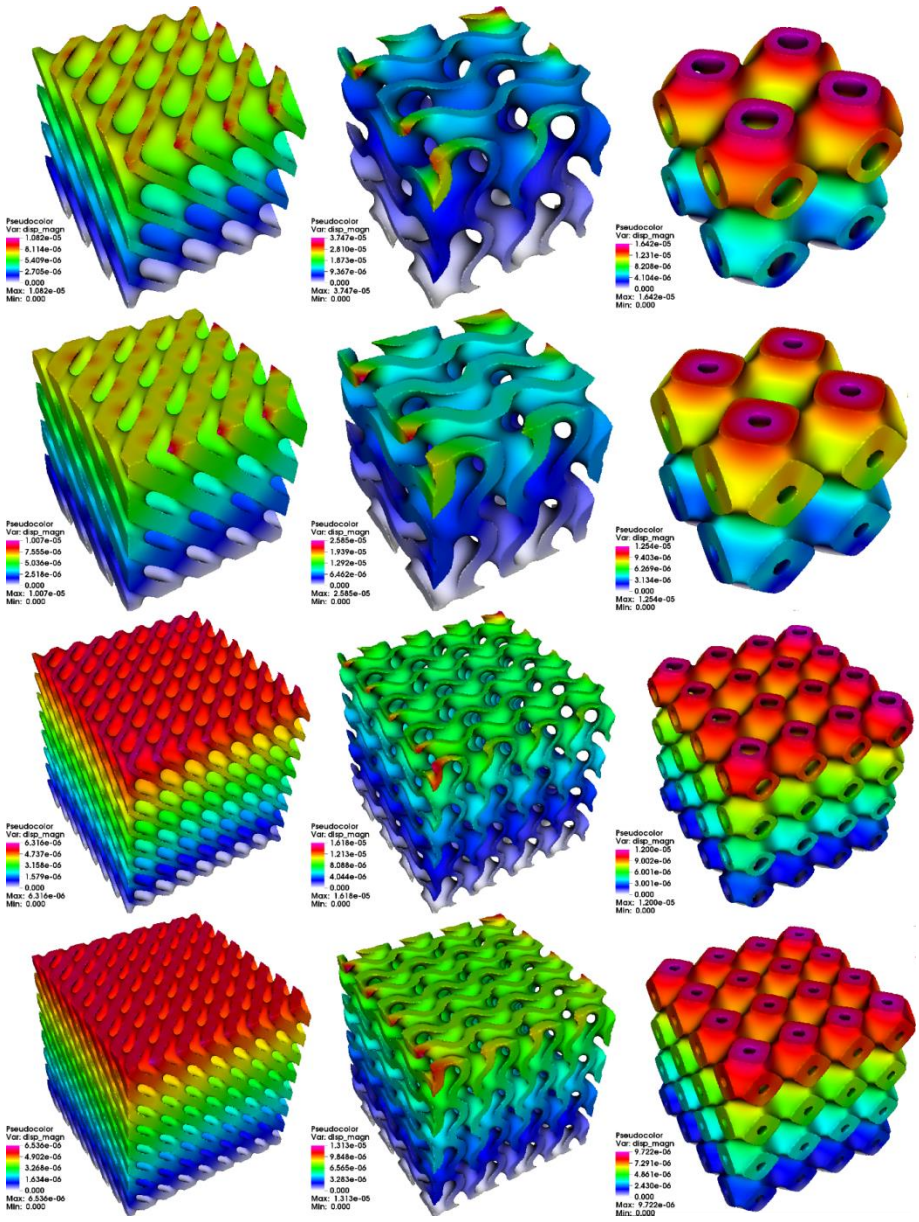

Fig. 2. The results of total displacement from stress analysis. Columns from left to right: Diamond (D) surface, Gyroid (G) surface, Primitive (P) surface. Rows from top to bottom: 2 cells, thickness δ=0.5; 2 cells, thickness δ=0.8; 4 cells, thickness δ=0.5; 4 cells, thickness δ=0.8.

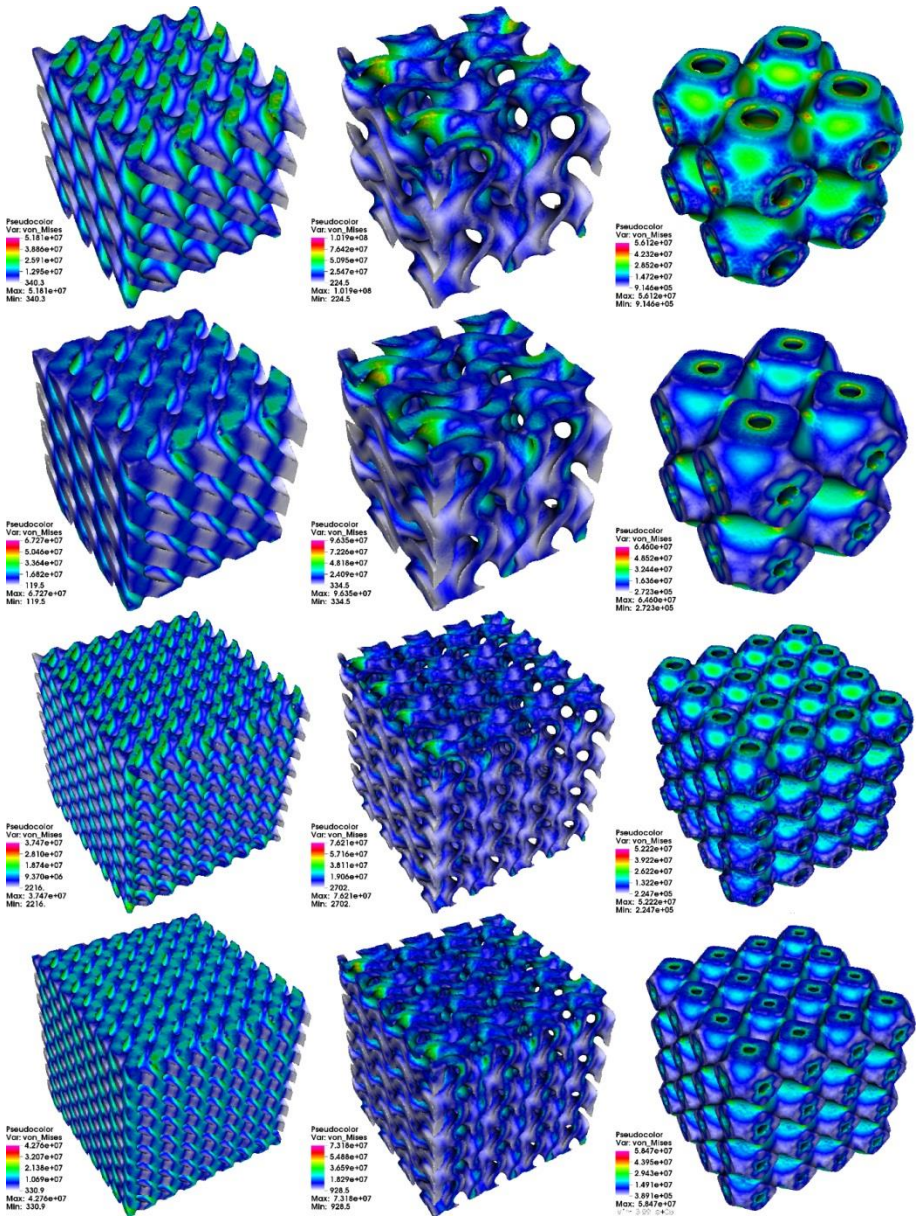

Fig. 3. Von Mises stress distribution in MPa. Columns from left to right: Diamond (D) surface, Gyroid (G) surface, Primitive (P) surface. Rows from top to bottom: 2 cells, thickness δ=0.5; 2 cells, thickness δ=0.8; 4 cells, thickness δ=0.5; 4 cells, thickness δ=0.8.

4 Summary

The paper presented different periodic surface structures and their behaviour in engineering calculations. The authors also explored potential influence of such factors like thickness or number of cells per unit cube on the results of simulations. Based on the results presented in paper, it can be observed that all presented in the paper structures can be interesting for engineers planning to use them, but eventual use should be preceded by careful analysis, because they have different properties.

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