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Research Paper

Construction of Porous Multiscale Heterogeneous Microstructures using Statistical Correlation Functions and Minimal Surfaces

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ABSTRACT

Design multiphase heterogeneous structures in order to provide multifunctional properties has many applications in the field of material design. In this research, a new method for construction multiscale heterogeneous microstructure is presented. Using statistical correlation function, specifically, two-point correlation functions, bicontinuous two-phase structure is constructed that has solid and void phases. In order to construction the heterogeneous media, an exponentially decreasing sine function is used as autocovariance function. Then based on Schwartz P minimal surface the porous media structure, is divided into two parts; porous solid phase and void phase. From the point of view of continuity, the phases are investigated and it is observed both phases of the constructed microstructure are connected throughout the media. Using this method it is possible to construct bicontinuous multiscale microstructures that are solid and void phase in coarse scale and the solid phase can be constructed as void and solid phase in fine scale.

Keywords : Heterogeneous microstructure; Statistical correlation function; Minimal surface; Multiscale modeling.

1 INTRODUCTION

TODAY, with the emergence of new needs, research on multifunctional structures that can perform multiple tasks simultaneously has received much attention [1]. Large groups of these materials, known as heterogeneous materials, have microstructures with two or more phases, in which each phase performs its own task. Heterogeneity occurs when there are at least two different states (called here phase) in a given volume such as void and solid phases in porous media or polycrystalline microstructures with grains with different orientations. These materials include, but not limited to, natural structures such as wood and body bones and synthetic items such as composites and honeycomb structures. It is possible to achieve excellent properties such as being ultralight and multifunctionality by engineering and optimization the phase distribution of heterogeneous microstructures [2].

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Solid oxide fuel cell cathode and bone implant microstructures are practical cases for engineered heterogeneous microstructure. Assuming multiscality, more capabilities are provided for optimizing and manipulating the microstructure. For example, by controlling the distribution of phases on the fine scale, the desired properties such as anisotropy can be controlled on the coarse scale [3].Determination of mechanical properties, thermal conductivity, diffusion coefficient and other properties of these materials has a long history and has been highly regarded by researchers [4]. Given that there is a close relationship between the geometry of the structure and its properties, the discovery of this relationship and in the next step, the optimization of microstructure in order to achieve optimal or predetermined properties, is an important goal in the field of materials engineering [5]. It should be noted that microstructure in the context of material design refers to a scale that is relatively finer than a coarse scale and it does not necessarily mean micrometers or very small dimensions. Therefore structures such as bone, concrete and sandstone are also called microstructure in this context [4]. In addition, mostly the classical continuum mechanics equations are used to evaluate intended properties for heterogeneous microstructures [1,6-10]. However, there are cases in which the classical continuum mechanics is incapable of explaining their behavior. For example, doublet mechanics that is a micromechanical theory has demonstrated better prediction of behavior of particulate materials [11,12]. In this theory, materials are assumed to be discrete and represented by an array of points with finite distances [13], therefore in some cases it is possible to predict mechanical behavior such as stress fields [12] or natural frequency [14] with more confidence. The geometry of heterogeneous structures can be randomly [15,16] or they can be repeated periodically [17,18]. In randomly modeled cases, no repetitive patterns in the structure can be detected, and mostly such structures are constructed using statistical functions [19]. The first step in construction a heterogeneous microstructure is to choose a suitable statistical method for expressing and describing it. Common methods of statistical description of microstructure are: N-point correlation function, cluster functions, lineal path method, etc., which have been studied in detail by Torquato [4]. The method used in this research is N-point correlation functions in general and two-point in particular. Due to the two-way relationship between geometry and properties in N-point correlation functions, these functions have also been used by researchers to investigate a variety of structural properties, such as the work of Beran [20], Kröner [21], Rémond et al. [22] and Hasanabadi et al. [23]. In the periodic cases, the unit cell must first be optimized using functions that relate the required properties of the microstructure to its geometry, and then the structure can be easily replicated to the desired size by repeating this cell [17]. One of the unit cells that has recently received attention in the engineering and biological fields is the use of minimal surfaces [24]. These surfaces are two hundred years old and were first proposed in Lagrange research. He sought to answer the question of what a surface with the smallest area would look like for a closed border [25]. The answer to this question leads to the formation of some differential equations that should be solved. For the first time, Schwarz provided examples of these surfaces [26]. Schwarz introduced five examples of these surfaces, the most famous of which is the Schwarz P minimal surface.

In this paper, firstly a bicontinuous structure is constructed based on Schwarz *P* minimal surface. This structure is a two-phase media composed of void and solid phase. Secondly the solid phase of constructed microstructure in turn, is divided into void and solid phase in smaller scale. This is done using exponentially decreasing sinusoidal autocovariance function that is usually used for bicontinuous structure. The resulted porous structure is appropriate for designing heterogeneous media such as artificial bone implants [27,28] and solid oxide fuel cell cathode [29].

2 MINIMAL SURFACES

The minimal surface, according to Fig. 1, is which at each point on it, the average of the two principal curvatures, which are also perpendicular to each other, is zero. Obviously, these surfaces must be saddled at any point so that sum of the two curvatures are equal to zero. The minimal surface used in this research is Schwartz *P* minimal surface (Fig. 2). If a unit cell is considered, this surface divides the cell into two parts, which can be solid and void space, or both solid space. Each of these two parts is called a phase. The Schwarz *P* surface has the property of phase symmetry, which means that if two phases have equal volume fraction, by changing the position of the two phases, there is no change in geometry and properties. Therefore, the proposed unit cell will create an optimal structure for the cases where each phase is nonconductive to what passes through the other phase, for example, one phase conducts heat and the other phase conducts electricity separately. In other words, in applications like this, the best structure that can be achieved, is the same structure that is periodically created by the Schwartz *P* unit cell [7]. This structure is bicontinuous, which means that each phase is connected to the whole structure from one side to the other side.

Fig.1
An example of minimal surface.

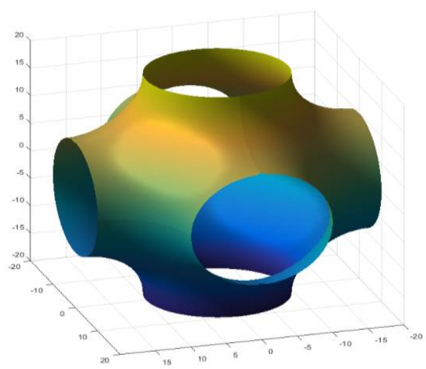


Fig.2
Schwarz *P* minimal surface.

There are various method proposed by researcher for construction minimal surfaces [30]. In this research, another method is used that is proposed by author [31]. For this purpose, the edges of the surface are first created by arcs with equal radius according to Fig. 3 and then using the method provided by Coons [32], these edges are turned into a surface using a suitable Matlab code according to Fig. 4.

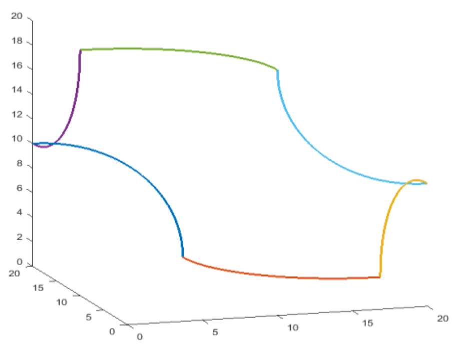


Fig.3
Arcs are used as boundary of the surface patch.

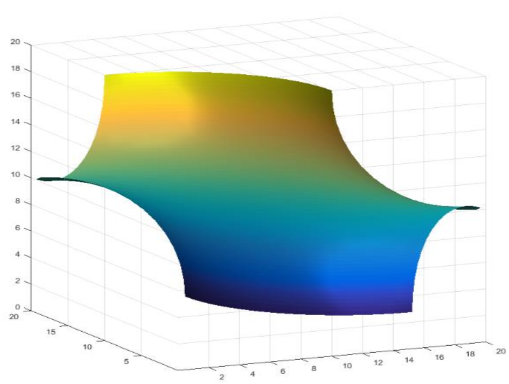


Fig.4
Surface constructed using Coons blending method.

3 CONSTRUCTION OF HETREOGENEOUS STRUCTURE

To create a microstructure, using statistical methods, a descriptor must first be introduced to describe the microstructure. This descriptor should have the ability to record its geometric properties to an acceptable extent. Among various microstructure descriptor, two-point correlation functions are used in this research to describe the microstructure due to their ease of calculation and compatibility with the phase recovery algorithm [33]. Correlation functions are expressed statistically, and in vector. One method of calculation is the use of Monte-Carlo-like methods [34] in which to calculate two-point functions, a large number of vectors are thrown on the space and then the value of the probability function is obtained by dividing the number of vectors whose beginning and end are in the desired phases by the total number of thrown vectors. For a two-phase structure such as Fig. 5, if the gray phase is considered as phase 1, four possible correlation functions are assumed to be expressed as, $C_2^{11}(r), C_2^{22}(r), C_2^{12}(r)$ and $C_2^{21}(r)$. Of the above four, only one is independent and the rest can be achieved according to it. $C_2^{11}(r)$ is the probability of placing the beginning and end of an arbitrary vector r in the gray phase, which will be obtained by dividing the number of red vectors by the number of all green and red vectors, according to Fig. 5 and do the same for the rest of the $C_2^{22}(r), C_2^{12}(r)$ and $C_2^{21}(r)$ functions.

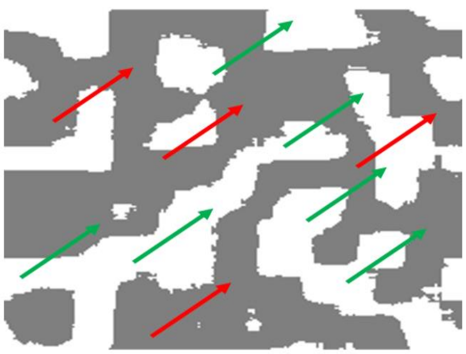


Fig.5
Calculation of correlation function for a two-phase microstructure.

Based on the correlation function a scaled function is defined as autocovariance function [35] that is expressed for phases 1 as;

$$f(r) = \frac{C_2^{11}(r) - v_1^2}{v_1(1-v_1)}, \tag{1}$$

where v_1, is the volume fraction of phase 1. It should be noted that for isotropic microstructure, the direction of vector r is unimportant and it is sufficient to consider only the value of it as r in Eq. (1). The autocovariance function used in this research is an exponentially decreasing sinusoidal function, which is expressed as Eq. (2):

$$f(r) = \exp\left(-\frac{r}{b}\right)\frac{\sin(qr)}{qr}, \tag{2}$$

In Eq. (2), q and b are positive parameters that controls the amount of oscillations and decreasing respectively. This function was first used by Cule and Torquato to reconstruct porous structures [15]. This function can be used for a wide range of volume fractions and creates suitable bicontinuous microstructures. Bicontinuity means that similar to the gray phase of Fig. 5, which is interconnected throughout the structure both phases are interconnected in three-dimensional mode throughout the structure. To construct the microstructure, first the values of the autocovariance functions are calculated in terms of values q and b , using Eq. (2), and then the two-point correlation function is determined using Eq. (1). The microstructure is then constructed using the phase recovery algorithm [33]. The details of microstructure construction based on the existing two-point correlation functions and the phase recovery method are explained in detail in [33].

4 RESULTS AND DISCUSSION

For $v_1 = 0.5, b = 3$ and $q = 5$, the porous microstructure (Fig. 6) is constructed using Eq. (1) and (2) and phase recovery algorithm [33]. The Schwarz *P* surface (Fig. 2) is then used to remove part of the previous porous media according to Fig. 7. According to Fig. 6, it can be seen that both of void and solid phase are a single connected cluster throughout the microstructure. For a cluster of a phase, it is possible to connect two arbitrary point on it through a path without crossing other phase. By developing algorithm proposed by Hoshen and Kopelman [36] the connectivity of each phases is checked using cluster multiple labeling technique [37].

Half of the structure of Fig. 7 is depicted in Fig. 8 (a). By sectioning the resulted structure, demonstrated in Fig. 8 (b), gradual changes in the geometric arrangement of the two phases can be clearly seen. Half of the structure volume of Fig. 6 is void phase therefore by removing half of it by Schwarz *P* surface, shown in Fig. 2, the constructed microstructure in Fig. 7 will eventually have approximately 75% void phase and 25% solid phase.

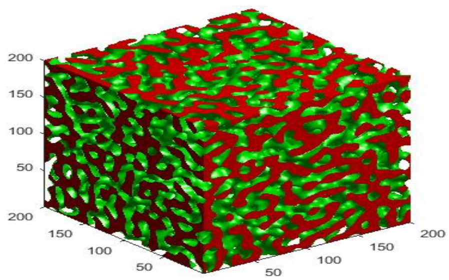


Fig.6
Construction the porous media for $v_1 = 0.5, b = 3$ and $q = 5$, void phase is the transparent one.

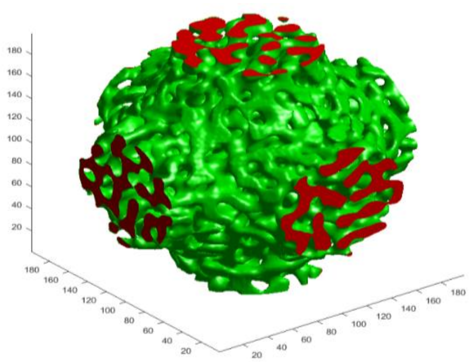


Fig.7
Superimposing the Schwarz *P* surface for construction multi-scale porous media. The transparent region is the void phase.

(a) (b)

Fig.8
(a)Half of structure of Fig. 7, (b) sectioning of the structure of Fig. 7 in pixel 1, 26, 51, 76 and 101 from left to right and from top to down respectively by equidistant planes. The black region is the void phase.

Since the volume fraction of a phase and its geometric arrangement will simultaneously affect the resulting properties, to determine the appropriate values of the volume fractions in different stages, it is necessary to use the objective function in each case and then optimize it. For example for $v_1 = 0.4$ (volume fraction of solid phase), and $q = 10$ and using the Schwarz P with volume fraction of solid phase equal to 0.14, the resulted microstructure is demonstrated as Fig. 9. This microstructure has volume fraction equal to 0.05 for solid phase and at the same time, it is interconnected throughout its structure. It is possible to repeat the unit structure to construct a large structure of desired extent according to Fig. 10. Due to the rapid advances in 3D printing technologies, designed structures can be turned into reality and used in applications such as artificial bone design [27,38] or fuel cells [39].

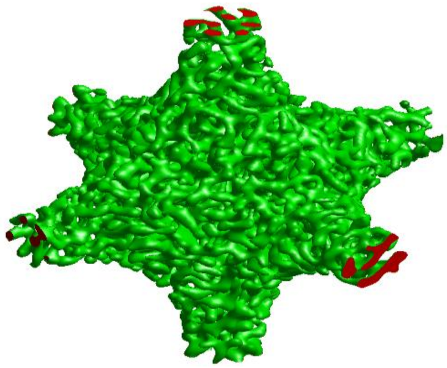


Fig.9
A fine and interconnected microstructure with volume fraction of 0.05 for solid phase.

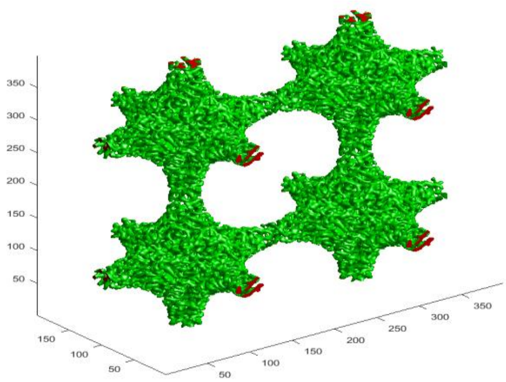


Fig.10
By repeating the unit cell, the structure can be designed to any size desired.

In order to evaluate the mechanical properties of the microstructure obtained in Fig. 7, the values of the effective thermal conductivity of each microstructure and phase are examined. Effective thermal conductivity is defined as the relative conductivity of a two-phase cube compared with a fully solid cube. Therefore if the conductivity of a fully solid cube is equal to 1, the effective conductivity of a porous cube must be between zero and 1. One side of the cube is assigned a high temperature and the other side is assigned a low temperature (see Fig. 11). It is assumed that no heat passes through the other four faces of the cube and then the heat flux value is obtained using the finite volume method. By dividing the amount of flux by the temperature difference between the two sides, the value of the effective thermal conductivity is determined.

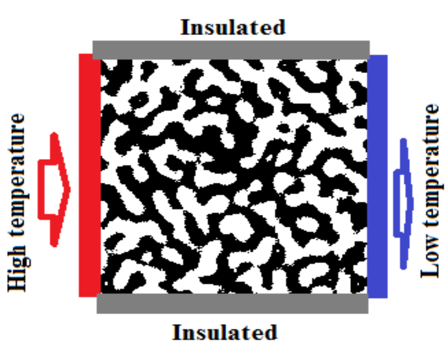
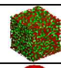
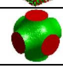
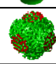
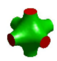


Fig.11
Boundary conditions applied to calculate effective thermal conductivity.

The results of the effective thermal conductivity for various structures are summarized in Table 1. It is observed that the effective thermal conductivity of two-scale microstructure, presented in this research is slightly lower than Schwarz *P* minimal surface with volume fraction of solid phase equal to 0.25. However, it should be noted that the surface-to-volume ratio is much higher in two-scale microstructure, a feature that is very important in cases such as solid oxide fuel cell [40] where a chemical reaction or exchange of heat, ions and electrons takes place on the surface.

Table 1
Effective thermal conductivity for various structures.

structure	appearance	Volume fraction of void phase	Volume fraction of solid phase	Effective thermal conductivity for void phase	Effective thermal conductivity for solid phase
Constructed using Eq. (2)		0.5	0.5	0.27	0.25
Schwarz *P* (with equal phases)		0.5	0.5	0.33	0.33
Two-scale microstructure		0.75	0.25	0.59	0.08
Schwarz *P* (with unequal phases)		0.75	0.25	0.65	0.10

5 CONCLUSION

In this research, a new method was presented for multi-scale modeling of porous structure based on random heterogeneous design and minimal surfaces. The porous microstructure was constructed using two-point correlation functions and phase recovery algorithm. In another stage, Schwarz *P* minimal surface was created based on boundary curve and Coon's blending method. By superimposing Schwarz *P* minimal surface on random heterogeneous structure a completely bicontinuous porous structure was created in two scale. Such structures are suitable for designing items such as artificial bone and fuel cell cathodes that require low weight and high area-to-volume ratio.

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