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Finite element predictions of effective multifunctional properties of interpenetrating phase composites with novel triply periodic solid shell architectured reinforcements

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ABSTRACT

In this paper, new interpenetrating phase composites (IPCs) based on the mathematically-known triply periodic minimal surfaces (TPMS) are proposed. In these IPCs, different TPMS architectures are used as reinforcing solid shells to increase the effective multifunctional properties of IPCs. Several three-dimensional representative volume elements (RVEs) are generated and studied using the finite element method in order to predict the effective properties for various TPMS-based IPC architectures. The calculated properties are compared with some analytical bounds and conventional composites. The proposed IPCs have superiority against the conventional composites, and they possess effective properties close to the upper Hashin-Shtrikman bounds. Limited experimental validation of the computational prediction of effective conductivity is presented where the TPMS is made of conductive carbon nanostructured-based polymer composite.

1. Introduction

In recent years, a new type of composites, interpenetrating phase composites (IPCs), has been developed due to its superior mechanical and physical properties. As the name indicates, IPCs epitomize a kind of advanced engineering materials whose microstructure is characterized by three-dimensional continuous and interconnected phases. This category of composites has markedly different mechanical and physical properties from the conventional composites [1]. The IPCs are generally more complex than the conventional composites, but the rationale behind designing them is that the mechanical and physical properties of this new group of composites are usually superior to those of fiber-reinforced and particle-reinforced composites [2]. As mentioned above, the microstructure of the IPCs possesses a continuity in three-dimensions (3D), and this can lead to a noticeable enhancement in the effective properties in all directions. However, fiber-reinforced composites allow a major improvement in the direction of the fibers and slight improvement in the transverse directions. This is a crucial advantage which IPCs have over the fiber-reinforced composites. Compared to the particle-reinforced composites, IPCs have the advantage of continuous phases throughout the composite. Consequently, the characteristics of the reinforcing phase and the matrix are simultaneously preserved, and this leads to the best overall performance [3]. This advantage plays a vital role in enabling easy transport through the composite due to the period interconnectivity of the phases in 3D. In other words, the interconnectivities of the phases enhance the transport properties including the thermal conductivity, the electrical conductivity, and the fluid permeability [4]. In case of removal of one of the phases of the IPCs, the new structure will be a self-supporting open/closed-celled foam with certain fluid permeability [5]. The continuity of the phases makes the IPCs a multifunctional material [6]. In addition, based on the microstructural design, which is referred to here in this paper as the architecture, the IPCs can either be isotropic or anisotropic [4].

The behavior and the techniques to manufacture several IPCs have been investigated during the recent years. Tremendous number of IPC examples is available in the literature. Kim et al. [7] proposed a new synthetic route for metal-ceramic IPCs. Their proposed method eliminates the issue of low wettability between metal and ceramic phases and eliminates the problem of closed pores. Additionally, Poniznik et al. [4] provided a review on predicting the effective elastic properties (Young's modulus, Poisson's ratio, shear modulus, and bulk modulus) of IPCs. Besides that, they developed a finite element model in which the geometry is based on random voxels to study the behavior of the real Al_2O_3-Cu composite. Wegner et al. [5] listed several techniques for producing IPCs and summarized some of the techniques existing for modeling

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the coefficient of thermal expansion, elastic modulus, and the yield strength. They discussed the applicability of some of the available analytical models to evaluate the effective properties of IPCs. In addition, they developed a finite element model to study the properties mentioned above, where they considered an IPC with a hexagonal close-pack array of intersecting uniformly sized spheres. In their following paper [8], they investigated the thermo-mechanical properties of an IPC: a stainless-steel/bronze composite produced by three-dimensional printing process. They studied the behavior of this composite experimentally and numerically.

Recently, metal-ceramic IPCs attracted many researchers since they have superior properties compared to the conventional metal-ceramic composites. Li et al. [3] investigated the thermal conductivity and the coefficient of thermal expansion of SiC-Al composites where Al is the metallic matrix and SiC is the ceramic reinforcing phase. More specifically, Li et al. [3] performed a comparison between two types of microstructures, namely, the particle-reinforced microstructure and the three-dimensional interpenetrating, but random, network microstructure. They reported significant improvements in the effective properties when IPCs are tested. Moreover, they argued that this significant improvement in the effective thermal conductivity is due to the lower interfacial area between the two phases in the case of the IPC relative to the particle-reinforced one since a decrease in the interfacial area means a reduction in the thermal resistance.

Feng et al. [2] examined the relationship between the microstructure of the IPCs and the effective elastic modulus. They developed an analytical model to estimate the elastic modulus of an IPC in which each continuous phase is present in a unit cell as three mutually orthogonal branches with rectangular cross-sections. Their model also considers the effect of the disconnected inclusions besides the IPCs. They also developed a numerical model and compared its results with those of the analytical model they developed and the experimental results available in literature, and they found that the results of their analytical model agree well with the experimental results of [5] and the developed numerical model.

Generally, the effective properties can be quantified using analytical models, empirical equations, and/or numerical modeling. Most of the analytical models developed to predict the behavior of IPCs are based on the volume fractions and the material properties of the individual phases. However, there are other factors influencing the effective properties such as the topology of the phases and the thermal residual stresses [6]. For instance, the results of [8] showed a decrease in the effective elastic modulus of the stainless-steel/bronze composite due to the thermal residual stresses and the existence of the voids. Moreover, the architecture or morphology of the microstructure influences the effective properties including the ones related to the transport phenomena and the mechanical properties [9]. The focus of this paper is on investigating the role of novel architectures, the TPMS, on the effective thermal/electrical conductivity of IPC that are completely periodic.

In this paper, a cutting-edge type of microstructures of the IPCs is reconnoitered; the microstructures of the IPCs under study are three-dimensional geometries based on the mathematically-known triply periodic minimal surfaces (TPMS). Triply periodic indicates a repetition of the microstructures of the IPCs in 3D. Moreover, TPMS are infinite continuous smooth surfaces that separate the space into two intertwined complex regions [10]. Furthermore, TPMS are surfaces that are locally area minimizing, and they are defined as surfaces with zero mean curvature at each point on the surface [11,12]. Several TPMS were discovered in the last century, and they were discussed by several investigators [10,13–18]. Fig. 1 illustrates some of the commonly known TPMS, these surfaces are created as described in [13]. Brakke [13] developed the software *Surface Evolver* that generates the TPMS based on minimizing the energy of a surface subjected to constraints. The energy of a surface is proportional to its surface area [20]. The most common natural example of minimal surfaces is the soap films in which the surface tension minimizes the energy of the film; and consequently, minimizes its surface area [20]. TPMS are described in terms of a fundamental patch or asymmetric unit from which the whole minimal surface can be created by its symmetry elements [14].

Further studies on the TPMS structures have been conducted due to several potential applications in microstructure and nanostructure formation [12]. TPMS attracts many engineers, biologists, mathematicians, and physical scientists due to its geometric properties since the geometry of the TPMS strongly affects the physical properties of the materials [19]. Therefore, several investigators studied the behavior of TPMS. For instance, Melchels et al. [9] investigated the use of two TPMS; namely gyroid and diamond (different than the diamond in Fig. 1), in developing tissue engineering scaffold. Additionally, Kapfer et al. [10] studied the use of nine TPMS to obtain biomorphic scaffold designs. From the TPMS, Kapfer et al. created two types of one-phase scaffold architectures; namely, minimal surface network solids and minimal surface sheet solids. They developed a finite element model to predict the elastic properties of both types. They have shown that, sheet solids possess higher Young's and bulk moduli than the network solids at the same volume fraction.

Khaderi et al. [21] considered a gyroid lattice to study its mechanical properties (elasto-plastic response) under different loading conditions. In addition, they studied the feasibility of employing the gyroid as a thin film in electronic display applications, and they have obtained promising results. Furthermore, It was shown based on the topology optimization that Schwartz primitive and diamond TPMS creating IPCs, in which the TPMS are solid networks and not shell networks, can lead to an optimized multifunctional composite [20,22]. In other words, primitive and diamond TPMS are not only geometrically extremal but also provide extremal performance when there is a competition between two effective properties like electrical and thermal conductivities as discussed in [23] or transport properties and mechanical properties as argued in [20]. Chen et al. [12] argued that the bicontinuity and interface with nearly zero mean curvature are the key behind the enhanced transport properties.

In the present work, TPMS are utilized to create unique and novel IPCs and study their effective electrical and thermal conductivities. The prediction of the macroscopic effective conductivities is

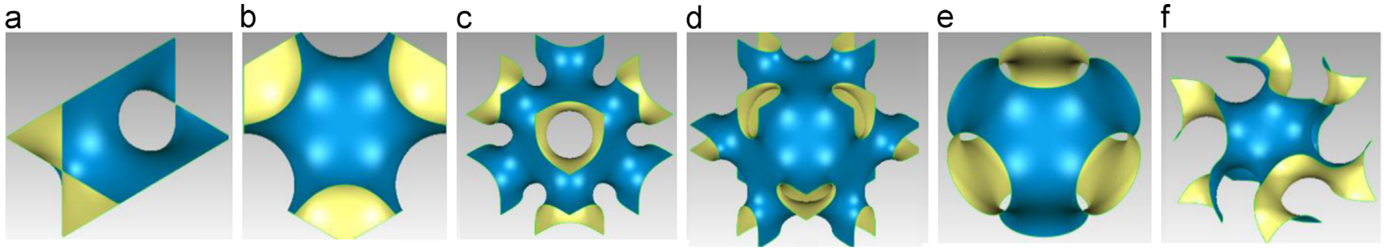

Fig. 1. Examples of TPMS, (a) crossed layers of parallels (CLP), (b) diamond in rhombic dodecahedron (diamond), (c) IWP, (d) neovius, (e) primitive, and (f) gyroid.