

Mechanical modeling based on numerical homogenization of an $\text{Al}_2\text{O}_3/\text{Al}$ composite manufactured via binder jet printing



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ABSTRACT

The present research work takes advantage of a recently published numerical homogenization implementation in MATLAB to find the elasticity tensor of a ceramic–metallic composite (CMC) system to be compared to an experimental data. Numerical homogenization is an efficient way to determine effective macroscopic properties of a composite material. This technique represents an effective means to model a two-phase composite. In this work, an extension of a previously published numeric homogenization code was investigated in order to model the compressive elastic modulus of the ceramic–metallic composites. The extension to the numerical code makes use of physical micrograph images to accurately describe the phase distribution of the composite. Multiple micrographs were taken from each sample, to subsequently better represent the actual microstructure of the composite as a whole. The composites were created using a binder jet 3D printing technology, where a ceramic precursor material was initially assembled, followed by a molten metal infiltration process. It was found that the studied numerical homogenization yielded an elastic modulus approximately 11.5% lower than the experimental data, suggesting a reliable modeling technique for predicting the elastic tensor of CMCs.

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1. Introduction

The microstructure and mechanical properties of ceramic–metallic composites (CMCs) have been extensively studied over the last 20 years. CMCs can be manufactured through a large variety of techniques, including reactive metal penetration (RMP) [1], directed metal oxidation (DIMOX) [2], and pressure assisted infiltration [3]. The composition of CMCs can be made based on a wide variety of ceramic and metal materials. The most commonly studied CMC system is based on a $\text{Al}_2\text{O}_3/\text{Al}$ composite which was originally patented by Breslin [1], who used a RMP process to produce a co-continuous ceramic–metal composite (C4). In the RMP process, a silica ceramic preform is reactively infiltrated with molten aluminum to create the final composite. A reduction reaction between the molten aluminum and silica creates the final $\text{Al}_2\text{O}_3/\text{Al}$ composite. Typically the ceramic precursor materials are made by a slip or squeeze casting techniques. These manufacturing techniques can be limited by the complexity of the part design. In order to overcome the geometrical constraints associated with the manufacturing of complex parts, the use of additive manufacturing

seems to be a feasible alternative. Binder jet process is a layer-by-layer building approach which was originally established at MIT [4]. In this process, a binder is physically deposited onto an evenly spread powder bed following the design of a predetermined CAD model. A fresh layer of powder is then laid on top of the previous layer and the process is repeated until the design is accomplished (see Fig. 1).

After the printing process, the binder is cured in order to harden and glue the piece together. Subsequently, the binder is burned off during the sintering cycle. The burning off of the binder creates a natural porosity in the final part, which prevents the final part from achieving highly dense parts. Yoo et al. [5] reported that they were able to achieve a final density of 62.5%, without post processing, for binder jet printed alumina. Although the porosity is not always a desired feature on bulk ceramics, it may be beneficial for the creation of infiltrated CMCs. In fact, most of the research groups have used additive manufacturing to assemble a ceramic backbone for subsequent metal infiltration, to create a multiphase composite [6–17]. However, no previous studies on AM for producing multiphase composites have reported the use of the aforementioned RMP infiltration technique. This represents an opportunity to explore the combination of AM with RMP to yield unique interpenetrated composites. Hence, the present paper will investigate

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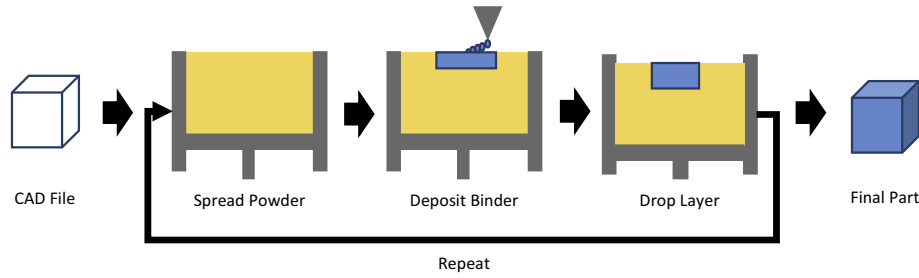


Fig. 1. Schematic for the binder jet printing process.

and model the elastic properties of an interpenetrating ceramic–metal $\text{Al}_2\text{O}_3/\text{Al}$ composite manufactured by binder jet printing and infiltrated via RMP, using a numerical homogenization technique. Here, the predicted elastic properties will be compared to the experimental data to evaluate the reliability of the aforementioned technique.

1.1. Modeling of composite materials

There are many models and methods that have been studied to simulate the physical properties of CMCs and interpenetrating phase composites (IPCs); such as the Voigt and Reuss bounds [18], and the rule of mixtures [19]. More unique methods of creating unit cells have been studied by Wegner and Gibson [20] and Feng et al. [21]. However, all these previously mentioned methods do not account for random geometries. Alternatively, a modeling based on finite element analysis, which divide an interpenetrating phase composite (IPC) into cubic “voxels”, seems to initially represent a suitable modeling approach, since the phase distribution of the materials can be assigned with the corresponding properties. However, such “voxels” approach does not take into account the randomness of the microstructure [22]. Agarwal et al. [23] used an effective mesh free method to describe IPCs. Kaminsky and Kleiber [24] modeled the randomness of an IPC using a two-step homogenization method. Although some of the methods can describe an IPC’s material properties accurately, they require a lot of computing time. On the other hand, Andreassen and Andreassen [25] have offered a MATLAB code based on a homogenization technique which is computing friendly. Hence, the present study uses this MATLAB code, with additional modifications to accurately model the elastic tensor of a 3D printed $\text{Al}_2\text{O}_3/\text{Al}$ composite.

1.2. Homogenization background

Materials like composites, solid foams, bone, and ceramic matrix composites consist of multiple, distinct phases. Each of these phases has their own individual physical and mechanical properties, and it is the sum of these phases, that form a heterogeneous material. Most heterogeneous materials, CMC’s included, exhibit a random arrangement of phases throughout its continuum structure. Prediction of the mechanical properties of these materials can be performed through the micro-mechanics theory. This typically makes use of a representative volume element (RVE), or a statistical volume element (SVE). A RVE is the smallest volume of a structure which still represents the macroscopic properties of the structure, while a SVE is smallest volume of a structure that statistically represents the macroscopic properties of the structure [26,27]. It should be noted that a RVE and SVE are very similar in theory, where both intend to capture the macroscopic properties, but only the mechanism differs between them. Additionally, the authors suggest an addendum to the definition of the RVE; the

RVE is the smallest volume of a structure which contains the required information under the chosen numeric scheme to represent the macroscopic properties of the structure. In heterogeneous materials, forming a RVE for all phases within the continuum is the process of homogenization. A main benefit of homogenization is that the physical and the mechanical properties can be determined analytically without need to test the material. This is especially important in composites materials, since statistically relevant testing of the numerous variables applicable to composites would be onerous and expensive.

While there exist many techniques for homogenization of a multiphase composite, the method of cells, or unit cell method, and Hashin spheres are two prominent homogenization methods. Hashin and Shtrikman [28] used a variational approach and multi-layer spheres to model particles in a multiphase material. These spheres then form the RVE for this multiphase material. The unit cell method, depending on which definition is taken, is synonymous of the RVE approach, and in practice, the two concepts are interchangeable. Both of these methods discretize a material into a periodic repeating structure, and therefore the quality of the result of homogenization is directly tied to the quality of the RVE. The authors find that the unit cell approach of Andreassen and Andreassen [25] to be advantageous due to the ability to incorporate micrographs into the homogenization. This allows for the creation of multiple, but not necessarily unique unit cells, which will discretize the domain.

According to the theory of homogenization, the macroscopic elasticity tensor for two distinct periodic phases is given by Eq. (1) [27];

$$C_{ijkl}^H = \frac{1}{|V|} \int_V C_{pqrs} \left(\varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^{(ij)} \right) \left(\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^{(kl)} \right) dV \quad (1)$$

where V is the volume of the unit cell, C_{ijkl}^H is the homogenized elasticity tensor, and C_{pqrs} , which is a function of position, is the local elasticity tensor. Here, C_{pqrs} can be obtained by

$$C_{pqrs}(\mathbf{x}) = C_{pqrs}^{\text{mat.1}} \beta^{\text{mat.1}}(\mathbf{x}) + C_{pqrs}^{\text{mat.2}} \beta^{\text{mat.2}}(\mathbf{x}) \quad (2)$$

where $\beta(\mathbf{x})$ is an indicator function to determine the phase (mat.1 = material 1 and mat.2 = material 2) for a given position, and $\varepsilon_{pq}^{0(ij)}$ is the macroscopic strain field. Here, $\varepsilon_{pq}^{(ij)}$ represents the local strain fields and it is given by

$$\varepsilon_{pq}^{(ij)} = \frac{1}{2} \left(\frac{\partial u_p^{(ij)}}{\partial \mathbf{x}_q} + \frac{\partial u_q^{(ij)}}{\partial \mathbf{x}_p} \right) \quad (3)$$

Therefore, Eq. (1) can be found by solving the elasticity equation,

$$\int_V C_{ijpq} \varepsilon_{ij}(v) \varepsilon_{pq}(u^{kl}) dV = \int_V C_{ijpq} \varepsilon_{ij}(v) \varepsilon_{pq}^{0(kl)} dV \quad (4)$$

where v is a virtual displacement within the unit cell, which is calculated by weighted residuals or finite element techniques.

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