A closed-form orthotropic constitutive model for fused filament fabrication materials

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Abstract

We model two common fused filament fabrication mesostructures, square and hexagonal, using an orthotropic constitutive model and derive closed-form expressions for all nine effective elastic constants. The periodic void shapes are modeled using three and four point hypotrochoid curves with a single shape parameter that controls the sharpness of the points. Using the complex variable method of elasticity, we derive the in-plane elastic constants ($E_{xx}$, $E_{yy}$, $\nu_{xy}$, $G_{xy}$) as well as out-of-plane antiplane shear constants ($G_{zx}$ and $G_{zy}$). The remaining out-of-plane elastic constants ($E_{zz}$, $\nu_{zx}$, $\nu_{zy}$) are derived by directly solving the linearelasticity equations. We compare our results by conducting unit cell simulations on both mesostructures and at various porosity values. The simulations match the closed-form expressions exactly for $E_{zz}$, $\nu_{zx}$, and $\nu_{zy}$. For the remaining elastic constants, the simulation results match the closed-form expressions better for the square mesostructure than the hexagonal mesostructure. Differences between simulation and closed-form expressions are less than 10% for porosity values less than 6% (hexagonal mesostructure) and 10% (square mesostructure) for any of the nine elastic constants.

Keywords: fused filament fabrication, constitutive model, orthotropic, porosity, voids, homogenization

1 Introduction

Fused filament fabrication is an extrusion-based additive manufacturing technique that uses a heated nozzle and motor to melt thermoplastic filament feedstock and extrude the molten filament in a pre-defined set of print paths [1]. The technique is widely used for rapid prototyping [2]–[4], tooling [5], [6], production parts [7], and teaching [8]–[10]. However, widespread adoption of FFF for commercial production is still limited. Several limitations are theorized to be reasons driving down commercial demand: long print times [11], coarse surface finish [12], coarse geometric resolution [13], low interlayer bonding strength [14]–[16], and highly anisotropic behavior [17]–[21]. Nonetheless, there are certain applications where FFF is a better fit; for example, the International Space Station operates a FFF machine because it can work in microgravity, the feedstock is relatively nonhazardous, and the printed parts are recyclable [22], [23].

In order to design parts specifically for FFF, a detailed understanding of process parameters and how they affect part behavior is necessary. Prior work has shown that a variety of parameters, such as layer height [24], air gap [12], raster angle and pattern [19], infill pattern and density [25], [26], processing temperature [27]–[30], and even filament color [31] can all affect the overall mechanics of FFF parts. In this work, we isolate and look at how the void shape and the overall porosity of two common FFF mesostructures affect the overall effective compliance of the printed material. Although the void shape and porosity are a result of many of the aforementioned process parameters, we use the void shape and porosity as starting points, abstracting away any upstream causes. However, we will briefly talk about process parameters that may affect the compliance of a single extruded road compared to the filament feedstock.

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1.1 Outline

In Section 2, we will review prior literature on constitutive models for FFF materials as well as some relevant process parameters. In Section 3, we will define the mesostructures and material coordinate system that all subsequent analysis will use. In Sections 5.4, 5, and 6, we will derive all nine effective elastic constants with the aid of the complex variable method of elasticity. Finally, in Section 7, we compare our closed-form solutions for the nine elastic constants with finite element analysis on unit cells and talk about ranges of porosity values where our model matches well with simulation.

2 Literature review

2.1 Existing constitutive models

Methods for characterizing the apparent or effective stiffness of FFF materials are generally borrowed from techniques used in the composites industry. The rule of mixtures, first proposed by Voigt [32], is applicable for a variety of engineering material systems, including fiber-reinforced composites [33], honeycombs [34], [35], and FFF materials [36], [37]. In fact, the rule of mixtures yields an exact solution for the effective Young’s modulus of multiphase unidirectional material systems (like the ones previously mentioned) along the longitudinal material axis, as long as the Poisson ratio of all material phases are equal. However, the rule of mixtures makes poor predictions for transverse loading. Reuss [38] proposed an inverse rule of mixtures for transverse loading, but this yields a trivial result of zero stiffness in the case of materials with voids. Modifications to the rule of mixtures, such as adding empirical fit factors, measuring the effective area in different cross sectional planes, and re-formulating it as a power law have been used by several authors for FFF materials [35], [37], [39]. A comprehensive survey of empirical and semi-empirical models can be found in Choren’s work [40].

Due to a lack of closed-form models specifically for FFF materials, there has been significant interest in simulating the effective elastic constants using homogenization theory. Rodriguez simulated the as-printed void by converting cross section photographs into finite element meshes [37], resulting in a monoclinic constitutive model (due to asymmetries in the as-printed void). By assuming an ideal void shape, simpler orthotropic models have been simulated [41], [42]. These models are expensive to compute as they require modeling the void geometry and solving a finite element problem for every void geometry and mesostructure variation. Nonetheless, they can be highly accurate if the cross section geometry is known. While present-day computers make the computational expense less of a concern, there is still a need for closed-form solutions, especially for performance-critical applications. For example, topology optimization that takes mesostructure geometry into consideration can become prohibitively expensive without a closed-form effective stiffness model.

Closed-form solutions for non-ellipsoidal voids would be impossible if not for the complex variable method of elasticity developed by Muskelishvili [43], which enabled mapping complex void shapes into the complex unit circle. This technique was used by several authors to derive effective 2D elastic constants for elliptical [44], [45], polygonal [44], [46], [47], and arbitrary void shapes [48], [49]. In this work, we build on this line of work to develop an effective orthotropic constitutive model for FFF materials.

2.2 Process parameters that affect feedstock compliance

Before developing our model, we mention some process parameters that may affect the compliance of a single printed road, compared to the filament feedstock. Since all of the aforementioned methods require elastic constants of the bulk material (i.e. no voids) as an input, any process parameters that may change the bulk material properties are relevant.

Rodriguez [27] and Bellini [50] performed tensile tests on both feedstock filament as well as single extruded roads. Bellini’s results show almost no change in Young’s modulus, while Rodriguez’s results show a 4% decrease in Young’s modulus. The slight decrease noted by Rodriguez is theorized to be caused by thermally-induced randomization of the polymer chains in the extruded road. Apart from these two studies, there is scant literature on experiments comparing the feedstock and a single extruded road; most studies compare the feedstock directly with printed tensile specimens, which already incorporate voids and a particular
mesostructure. In this study, we simply assume isotropic material properties \( E \) and \( \nu \) are provided as input parameters. While we believe using values derived from experiments on a single extruded road may yield marginally better results, the difference seems to be small and will probably be dwarfed by more influential factors, such as void shape and porosity.

### 3 Material frame

We define a material aligned coordinate system, as shown in Figure 1. The \( z \)-axis is aligned with the direction of the extruded road. We will refer to properties in the \( xy \) plane as in-plane properties, and anything else as out-of-plane properties. We consider two mesostructure systems: the hexagonal mesostructure and the square mesostructure, which are named for the periodic arrangement of extruded roads (in works by Rodriguez, they are referred to as the skewed and aligned mesostructures [27], [36], [37]). When the extruded roads have perfectly circular cross sections, the voids formed by the gaps between adjacent roads form curved triangles and diamonds. In this article, we will interchangeably associate the hexagonal mesostructure with curved triangle voids and the square mesostructure with curved diamond voids.

### 4 Axial loading in \( z \)-direction

For this section only, we assume that the voids can take any shape, as long as the overall structure is prismatic (i.e. the cross section does not change along the \( z \)-direction and the front/back faces are flat). To find the effective elastic constants \( E_{zz} \), \( \nu_{zx} \), and \( \nu_{zy} \), we apply a known displacement to the front/back faces while keeping the side face traction free. We also assume no body forces. The boundary value problem at
Figure 2: A general prismatic solid containing voids. For deriving elastic constants using axial loading in the z-direction, the voids can take any shape.

Hand is given by Equation 1.

\[
\begin{align*}
\nabla \cdot \sigma &= 0 \quad \text{in } \Omega \\
u_z &= 0 \quad \text{on } S_1 \\
u_z &= u_0 \quad \text{on } S_2 \\
\sigma_{xx} &= \sigma_{yy} = 0 \quad \text{on } S_1 \\
\sigma_{xx} &= \sigma_{yy} = 0 \quad \text{on } S_2 \\
\sigma \cdot n &= 0 \quad \text{on } S_3
\end{align*}
\]

where \( \Omega \) is the material domain and surfaces \( S_1 \), \( S_2 \), and \( S_3 \) are defined in Figure 2. The solution to this problem is given by a constant stress field

\[
\sigma_{zz} = E \frac{u_0}{L}
\]

where \( E \) is the Young’s modulus of the filament material and \( L \) is the distance from \( S_1 \) to \( S_2 \). All other stress components are zero. We define the effective Young’s modulus \( E_{xx} \) as the constant of proportionality relating the average stress to the average strain (averaged over the volume). We also define a porosity ratio \( f \) as the ratio of the void volume to the total volume. The effective Young’s modulus can then be expressed as

\[
E_{zz} = \frac{\sigma_{zz}^{\text{avg}}}{\epsilon_{zz}^{\text{avg}}} = (1 - f) \frac{E u_0}{u_0 L} = (1 - f) E
\]

The result is the venerable rule of mixtures for a two phase material system, where one phase is the void itself. Similarly, we can define the effective major Poisson ratios \( \nu_{xx} \) and \( \nu_{yy} \) as

\[
\begin{align*}
\nu_{xx} &= -\frac{\epsilon_{xx}^{\text{avg}}}{\epsilon_{zz}^{\text{avg}}} \\
\nu_{yy} &= -\frac{\epsilon_{yy}^{\text{avg}}}{\epsilon_{zz}^{\text{avg}}}
\end{align*}
\]
For $\nu_{zx}$, we get

$$\nu_{zx} = -\frac{\nu E}{2\mu L} = \nu$$

(5)

where $\nu$ is the Poisson ratio of the filament material. Following the same approach for $\nu_{zy}$ yields $\nu_{zy} = \nu$.

These results are well known in linear elasticity theory and have been used to derive effective elastic constants for other prismatic porous structures such as honeycombs [35].

Finally, we mention that the results of this section are exact for any porosity ratio $f \in [0, 1]$. This will not be the case in subsequent sections.

5 In-plane loading in x- and y-directions

To derive closed form expressions for the effective elastic constants in the x-y plane, we break the problem into two parts. The first part involves solving for the stress and displacement fields around a single void of a known geometry embedded in an infinite media. This part can be solved exactly using the complex variable method of elasticity [43], [51], [52]. Once the stress and displacement fields are known, we find the effective elastic constants by equating strain energy in the void-containing material to a homogeneous, void-free material [44], [46], [47]. For low porosities, we can assume that the voids are non-interacting. This assumption allows us to calculate the strain energy of a material containing multiple voids by summing up the strain energy contribution of each individual void.

5.1 Mapping function

For fused filament fabrication, the hexagonal and square mesostructures produce periodic voids in the shape of curved triangles and diamonds, respectively. The shape of the voids can be approximated by hypotrochoid voids [53], [54]. Specifically, the curved triangle is approximated by the conformal map

$$m_t = \zeta + \frac{c_t}{\zeta^2}$$

(6)

and the curved diamond is approximated by

$$m_d = \zeta + \frac{c_d}{\zeta^3}$$

(7)

where $\zeta = \rho e^{i\phi}$ represents a coordinate in the complex $\zeta$-plane. These mapping functions transform the complex unit circle (given by $\zeta \rightarrow e^{i\phi}$ for $\phi \in [0, 2\pi]$) into a hypotrochoid void. The shape parameters $c_t \in [-\frac{1}{2}, \frac{1}{2}]$ and $c_d \in [-\frac{1}{3}, \frac{1}{3}]$ control the sharpness of the corners of the voids. When $c_t$ and $c_d$ are zero, the voids are circular; when they take their maximum allowable values, the voids contain cusps at the corners; when they take their minimum allowable values, the voids are the same shape as the maximum case, but rotated by $60^\circ$ and $45^\circ$, respectively. We can also write the void shapes in parametric form by taking the real and imaginary parts of Equations 6 and 7 to get

$$x_t = \cos \phi + c_t \cos 2\phi$$
$$y_t = \sin \phi - c_t \sin 2\phi$$

(8)

for the curved triangle and

$$x_d = \cos \phi + c_d \cos 3\phi$$
$$y_d = \sin \phi - c_d \sin 3\phi$$

(9)

for the curved diamond. A variety of voids are shown in Figure 3.
Figure 3: Curved triangle (top row) and curved diamond voids (bottom row) constructed from various shape parameter values.

5.2 Stress and displacement field around a single void

We consider a single void embedded in an infinite media, subject to an applied uniaxial stress far away from the void. The direction of loading will determine which elastic constant we solve for, but for now we will formulate it for the general in-plane loading case. The 2D boundary value problem at hand becomes

\[
\nabla \cdot \sigma = 0 \quad \text{in } \Omega
\]
\[
\sigma_{xx} = \sigma_{xx}^0 \quad \text{for } |r| \to \infty
\]
\[
\sigma_{yy} = \sigma_{yy}^0 \quad \text{for } |r| \to \infty
\]
\[
\sigma_{xy} = \sigma_{xy}^0 \quad \text{for } |r| \to \infty
\]
\[
\sigma \cdot n = 0 \quad \text{on } S
\]

(10)

where \( r^2 = x^2 + y^2 \) and \( S \) is the surface of the void.

To solve this boundary value problem, we use the complex variable method of elasticity. Here, we give a brief description of the method. More details of the procedure can be found in textbooks by Muskhelishvili, England, and Barber [43], [51], [52].

The complex variable method of elasticity involves finding two holomorphic functions \( \chi(\zeta) \) and \( \theta(\zeta) \), also known as the Kolosov-Muskhelishvili potentials. The potentials are related to stress and displacement fields by the following:

\[
\Theta = 2 \left( \frac{d\chi}{dm} \frac{d\zeta}{d\zeta} + \frac{d\chi}{dm} \frac{d\zeta}{d\zeta} \right)
\]
\[
\Phi = \frac{2}{dm} \left( m \left( \frac{d^2\chi}{dm} \frac{d\zeta}{d\zeta} - \frac{d\chi}{dm} \frac{d^2\zeta}{dm} \frac{d\zeta}{d\zeta} \right) + \frac{d\theta}{d\zeta} \right)
\]
\[
u = \frac{1}{2G} \left( \kappa \chi - m \frac{d\chi}{dm} \frac{d\zeta}{d\zeta} - \theta \right)
\]

(11)

where

\[
\Theta \equiv \sigma_{xx} + \sigma_{yy}
\]
\[
\Phi \equiv \sigma_{yy} - \sigma_{xx} + 2i\sigma_{xy}
\]
\[
u = u_x + iu_y
\]
\[
\kappa = \frac{3 - \nu}{1 + \nu}
\]

(12)
an overbar refers to the complex conjugate, and \( m \) is the mapping function. We note that \( \sigma_{xx}, \sigma_{yy}, \sigma_{xy}, \) and \( \Theta \) are all real-valued functions, but expressed in terms of the complex variable \( \zeta \). We can rewrite Equation 12 as

\[
\sigma_{xx} = \Theta - \Re \{ \Phi \} \\
\sigma_{yy} = \Theta - \sigma_{yy} \\
\sigma_{xy} = \Im \{ \Phi \}
\]

where \( \Re \{ \cdot \} \) and \( \Im \{ \cdot \} \) refer to taking the real and imaginary components, respectively.

To find \( \chi \) and \( \theta \), we can break up the problem into two pieces: finding the uniform stress solution with no void, then finding the perturbation solution that makes the void traction free. Thus,

\[
\chi = \chi_0 + \chi_1 \\
\theta = \theta_0 + \theta_1
\]

where 0-subscripts refer to the uniform solution and 1-subscripts refer to the perturbation solution. The uniform solution can be found by inspection by setting \( \sigma_{xx} = \sigma_{xx}^0, \sigma_{yy} = \sigma_{yy}^0 \) and \( \sigma_{xy} = \sigma_{xy}^0 \) in Equation 12. Noting that the expressions for \( \Theta \) and \( \Phi \) in Equation 11 can be re-written as

\[
\Theta = 2 \left( \frac{d\chi}{dm} + \frac{d\chi}{dm} \right) \\
\Phi = 2 \left( \frac{m^2 d\chi}{dm^2} + \frac{d\theta}{dm} \right)
\]

we find that

\[
\chi_0 = \frac{\sigma_{xx}^0 + \sigma_{yy}^0}{4} m \\
\theta_0 = \frac{\sigma_{yy}^0 - \sigma_{xx}^0 + 2i\sigma_{xy}^0}{2}
\]

To find \( \chi_1 \) and \( \theta_1 \), we first define a traction function on the void surface \( s = e^{i\phi} \in S \):

\[
\psi(s) = \chi(s) + m(s) \frac{d\chi}{dm} \bigg|_{\zeta = \frac{s}{m}} + \theta(s)
\]

This function can also be split up as \( \psi = \psi_0 + \psi_1 \) where the subscripts refer to the uniform solution and perturbation solution as before. Substituting in Equation 16 into 17 yields

\[
\psi_0(s) = \frac{\sigma_{xx}^0 + \sigma_{yy}^0}{2} m(s) + \frac{\sigma_{yy}^0 - \sigma_{xx}^0 - 2i\sigma_{xy}^0}{2} m(s)
\]

However, the void must be traction free (i.e. \( \psi = 0 \), so therefore,

\[
\psi_1 = -\psi_0 = -\frac{\sigma_{xx}^0 + \sigma_{yy}^0}{2} m(s) - \frac{\sigma_{yy}^0 - \sigma_{xx}^0 - 2i\sigma_{xy}^0}{2} m(s)
\]

Given \( \psi_1 \), we can find \( \chi_1 \) and \( \theta_1 \) by solving the following integro-differential equations [52]:

\[
\chi_1 = -\frac{1}{2\pi i} \oint_{\gamma} \frac{\psi_1(s)}{s - \zeta} ds + \frac{1}{2\pi i} \oint_{\gamma} \frac{m(s)d\chi_1(s)/ds}{dm(s)/ds(s - \zeta)} ds \\
\theta_1 = -\frac{1}{2\pi i} \oint_{\gamma} \frac{\psi_1(s)}{s - \zeta} ds + \frac{1}{2\pi i} \oint_{\gamma} \frac{m(s)d\chi_1/ds}{dm(s)/ds(s - \zeta)} ds
\]
To find $\chi_1$, we express $\chi_1$ and its derivative using a Laurent series with only the negative powers

$$\chi_1(\zeta) = \sum_{n=1}^{\infty} \frac{a_n}{\zeta^n}$$

$$\frac{d\chi_1}{d\zeta} = -\sum_{n=1}^{\infty} \frac{n a_n}{\zeta^{n+1}}$$

$$\frac{d^2\chi_1}{d\zeta^2} = -\sum_{n=1}^{\infty} \frac{n a_n}{\zeta^{n+1}}$$

Only the negative powers are included because we want the perturbation solution to disappear as $|\zeta| \to \infty$.

In addition, even though Equation 21, in general, has an infinite number of terms, there will only be a finite number of terms in the final solution due to simple form of the mapping functions given in Equations 6 and 7. After substituting Equation 21 along with a mapping function into the first equation in Equation 20, we can find the coefficients $a_n$ by comparing terms on both sides of the equation. Finally, after finding $\chi_1$, we can find $\theta_1$ by substituting our result for $\chi_1$ into the second equation in Equation 20. The contour integrals in Equation 20 can be solved by using Cauchy’s integral formula or the residue theorem. Once $\chi$ and $\theta$ are known, the stress, strain, and displacement fields can be calculated using Equation 11.

5.3 Strain energy equivalence

Once the stress, strain, and displacement fields around a single void are known, we can use strain energy equivalence to derive effective elastic constants. The strain energy of a single void under uniform stress far away from the void can be expressed using Eshelby’s formula [55]:

$$W = W_0 + W_1$$

$$W_0 = \frac{1}{2} \iiint_V \sigma_{ij}^0 \epsilon_{ij}^0 dV$$

$$W_1 = \frac{1}{2} \int_S \sigma_{ij}^0 n_j u_i dS$$

where $W$ is strain energy, $W_0$ is the strain energy contribution due to the uniform applied stress, $W_1$ is the strain energy contribution due to the presence of a single void, $V$ is the volume of the infinite media, $S$ is the void surface, $\sigma_{ij}^0$ and $\epsilon_{ij}^0$ are the uniform stress and strain far away from the void, $u_i$ is the displacement, and $n_j$ is the unit normal vector along the surface of the void.

We have to be very careful here, as $u_i(\zeta)$ and $n_j(\zeta)$ represent quantities in the $x$-$y$ plane, but expressed as functions of $\zeta$. Since we’re evaluating the line integral in Equation 22 along the void, $u_i$ and $n_j$ within the integrand are really functions of $s = e^{i\phi}$ (or equivalently, just $\phi$). We can define the void surface in the $x$-$y$ plane parametrically as a function of $\phi$:

$$x(\phi) = \Re\{m(\zeta)|_{\zeta \to e^{i\phi}}\}$$

$$y(\phi) = \Im\{m(\zeta)|_{\zeta \to e^{i\phi}}\}$$

This allows us to express the components of the unit normal as

$$n_x = \frac{\frac{dy}{d\phi}}{\sqrt{\left(\frac{dx}{d\phi}\right)^2 + \left(\frac{dy}{d\phi}\right)^2}}$$

$$n_y = -\frac{\frac{dx}{d\phi}}{\sqrt{\left(\frac{dx}{d\phi}\right)^2 + \left(\frac{dy}{d\phi}\right)^2}}$$

In addition, the quantity $dS$ becomes

$$dS = \sqrt{\left(\frac{dx}{d\phi}\right)^2 + \left(\frac{dy}{d\phi}\right)^2} d\phi dz$$
Using these relations, the term \( W_1 \) in Equation 22 becomes

\[
W_1 = \frac{1}{2} \int_0^t \int_0^{2\pi} \left( \sigma_{0x} u_x \frac{dy}{d\phi} - \sigma_{0y} u_y \frac{dx}{d\phi} + \sigma_{xy} \left( u_y \frac{dy}{d\phi} - u_x \frac{dx}{d\phi} \right) \right) d\phi dz
\]  

(26)

For periodic mesostructures in FFF materials that contain multiple voids, we assume that the voids are small and do not interact with each other, such that we can express the strain energy contribution of all the voids as a sum of the individual voids. Under these assumptions, we can set \( V \) to be the volume of a representative volume element (RVE) containing a single void. We define the porosity \( f \) as

\[
f = \frac{V_{\text{void}}}{V_{\text{RVE}}} = \frac{A_{\text{void}}}{A_{\text{RVE}}}
\]

(27)

where \( A \) refers to area and \( V \) refers to volume. To find the effective elastic constants, we equate the strain energy in the RVE with a single void to the strain energy of an effective homogeneous RVE (containing no void) subject to the same uniform loading condition to get

\[
W = W_0 + W_1 = \sigma_{ij}^{\epsilon ff} S_{ijkl}^{\epsilon ff} \sigma_{kl}^{\epsilon ff}
\]

(28)

where \( S_{ijkl}^{\epsilon ff} \) is the effective compliance matrix of the homogenized RVE. By applying stresses in particular directions, we can isolate and solve for the components \( E_{xx}, E_{yy}, \nu_{xy}, \) and \( G_{xy} \) embedded in the effective compliance matrix.

### 5.4 Axial loading in x-direction

The uniform loading far away from the void for this case is given by \( \sigma_{0x} = \sigma_0, \sigma_{0y} = \sigma_{xy} = 0 \). Evaluating Equation 20 for the case of a curved triangle void, we find the Kolosov-Muskhelishvili potentials to be

\[
\begin{align*}
\chi &= \frac{\zeta}{4} \sigma_0 + \frac{\sigma_0}{2} \zeta c_t \sigma_0 - \frac{c_t}{4} \sigma_0^2 \\
\theta &= \sigma_0 \left( \zeta^4 + \zeta^2 - 2(\zeta^2 - 1) c_t^2 - 2(\zeta^2 - 1) c_t \right) \\
&= \frac{\sigma_0}{4} \left( \zeta^4 + \zeta^2 - 2(\zeta^2 - 1) c_t^2 - 2(\zeta^2 - 1) c_t \right)
\end{align*}
\]

(29)

for the curved triangular void and

\[
\begin{align*}
\chi &= \sigma_0 \left( \frac{\zeta}{4} - \frac{1}{2(c_d - 1) \zeta} - \frac{c_d}{4 \zeta^3} \right) \\
\theta &= \sigma_0 \zeta \left( 1 - \zeta^2 - 3c_d \zeta^2 + 3c_d^2 \zeta^2 - \zeta^4 - c_d (3 + \zeta^2 + \zeta^4) \right) \\
&= \frac{\sigma_0 \zeta}{2} \left( 1 - \zeta^2 - 3c_d \zeta^2 + 3c_d^2 \zeta^2 - \zeta^4 - c_d (3 + \zeta^2 + \zeta^4) \right)
\end{align*}
\]

(30)

for the curved diamond void.

For the uniaxial loading case in the x-direction, Equation 22 simplifies to

\[
W = \frac{1}{2} \frac{\sigma_0^2}{E} A_{\text{RVE}} t + \frac{1}{2} \sigma_0 \int_0^t \int_0^{2\pi} u_x \frac{dy}{d\phi} d\phi dz
\]

\[
= \frac{1}{2} \frac{\sigma_0^2}{E} A_{\text{void}} t + \frac{1}{2} \sigma_0 t \int_0^{2\pi} u_x \frac{dy}{d\phi} d\phi
\]

\[
= \frac{1}{2} \frac{\sigma_0^2}{E} A_{\text{void}} t + \frac{1}{2} \sigma_0 t \int_0^{2\pi} u_x \frac{dy}{d\phi} d\phi = \frac{1}{2} \frac{\sigma_0^2}{E \sigma_{yy}} A_{\text{void}} t
\]

(31)

(32)

The void areas for the curved triangular void and curved diamond void are given by

\[
A_{\text{void}}^t = \pi \left( 1 - 2c_d^2 \right)
\]

\[
A_{\text{void}}^d = \pi \left( 1 - 3c_d^2 \right)
\]

(33)
Substituting $u_x$ for the curved triangular void into Equation 32, we get

$$\frac{E_{xx}'}{E} = 1 - \frac{2c_l^2}{2c_l^2 + 3f - 2c_l^2 + 1}$$

Doing the same for the curved diamond void, we get

$$\frac{E_d}{E} = \frac{(c_d - 1)(3c_d^2 - 1)}{(c_d - 1)(3c_d^2 - 1) - f(3c_d^3 - 3c_d^2 + c_d - 3)}$$

By argument of symmetry, for the curved diamond, $E_{xx} = E_{yy}$, so there is no need to repeat the exercise for loading in the $y$-direction. We will show in Section 5.7 that, for the curved triangle, $E_{xx} = E_{yy}$ as well. This is due to the fact that a regular triangular void (and all regular polygonal voids except for the square) is an isotropic shape [44]. Due to this, the “orthotropic” constitutive model we are deriving for the hexagonal mesostructure is in fact a transversely isotropic constitutive model.

### 5.5 Shear loading in y-z plane

We repeat the process with $\sigma_{xy}^0 = \sigma_0$, $\sigma_{xx}^0 = \sigma_{yy}^0 = 0$. The Kolosov-Muskhelishvili potentials for the curved triangle void are

$$\chi = i\frac{\sigma_0}{\zeta}$$
$$\theta = -\frac{i\sigma_0(\zeta^4 + 2c_l^2 - 2\zeta c_l + 1)}{2c_l - \zeta^3}$$

and for the curved diamond void are

$$\chi = i\frac{\sigma_0}{\zeta(c_d + 1)}$$
$$\theta = i\frac{\sigma_0\zeta(\zeta^4 + (\zeta^4 - 3)c_d + 1)}{\zeta^4 - 3c_d^2 + (\zeta^4 - 3)c_d}$$

Equation 28 simplifies to

$$\frac{1}{2} G \frac{A_{void}}{f} + \frac{1}{2} \sigma_0 t \int_0^{2\pi} \left( u_y \frac{dy}{d\phi} - u_x \frac{dx}{d\phi} \right) d\phi = \frac{1}{2} \frac{\sigma_0^2}{2G_{xy}} \frac{A_{void}}{f}$$

Substituting in $u_x$, $u_y$ for the curved triangle and rearranging yields

$$G_{xy}' = \frac{1 - 2c_l^2}{f(\kappa + 1) - 2c_l^2 + 1}$$

Doing the same for the curved diamond void yields

$$G_{xy}' = \frac{(c_d + 1)(1 - 3c_d^2)}{(c_d + 1)(1 - 3c_d^2) + f(\kappa + 1)}$$

### 5.6 Equibiaxial loading

We repeat the process with $\sigma_{xx}^0 = \sigma_{yy}^0 = \sigma_0$, $\sigma_{xy}^0 = 0$. The Kolosov-Muskhelishvili potentials for the curved triangle void are

$$\chi = \frac{\zeta\sigma_0}{2} - \frac{c_l\sigma_0}{2\zeta^2}$$
$$\theta = \frac{\zeta^2 (2c_l^2 + 1) \sigma_0}{2c_l - \zeta^3}$$
and for the curved diamond void are

\[
\chi = \frac{\zeta \sigma_0}{2} - \frac{c_d \sigma_0}{2 \zeta^3}, \quad \theta = \frac{\zeta^3 (3c_d^2 + 1) \sigma_0}{3cd - \zeta^4}
\]  

Equation 28 simplifies to

\[
\frac{1}{2} \frac{\sigma_0^2 (1 - \nu) A_{\text{void}}}{E_f} f + \frac{1}{2} \sigma_0 f \int_0^{2\pi} \left( u_x \frac{dy}{d\phi} - u_y \frac{dx}{d\phi} \right) d\phi = \frac{1}{2} \frac{\sigma_0^2 (1 - \nu_{xy}) A_{\text{void}}}{E_{xx}} f
\]  

Solving for \( \nu_{xy} \) for the curved triangle void yields

\[
\nu_{xy}^t = \frac{(1 - 2c_t^2) (f + \nu)}{f (2c_t^2 + 3) - 2c_t^2 + 1}
\]

and for the curved diamond void yields

\[
\nu_{xy}^d = \frac{\nu (-3c_t^3 + 3c_d^2 + c_d - 1) - f (3c_t^3 - 3c_d^2 + c_d + 1)}{f (3c_t^3 - 3c_d^2 + c_d - 3) - 3c_t^3 + 3c_d^2 + c_d - 1}
\]

### 5.7 Axial loading at an oblique angle

At this point, we have derived all of the four in-plane elastic constants. However, it is worth further investigating the effective Young’s modulus \( E_\eta \) when the mesostructures are uniaxially loaded at some arbitrary oblique angle \( \eta \) (as measured positive counterclockwise from the positive x-axis). We first transform our oblique angle uniaxial stress \( \sigma_\eta^0 = \sigma_0 \) into axis-aligned components:

\[
\begin{align*}
\sigma_{\eta xx}^0 &= \sigma_0 \cos^2 \eta \\
\sigma_{\eta yy}^0 &= \sigma_0 \sin^2 \eta \\
\sigma_{\eta xy}^0 &= \sigma_0 \cos \eta \sin \eta
\end{align*}
\]

The Kolosov-Muskheishvili potentials for the curved triangle void are

\[
\chi = \frac{\sigma_0 (\cos(2\eta) + i \sin(2\eta))}{2\zeta} + \frac{\zeta \sigma_0}{4} - \frac{c_t \sigma_0}{4 \zeta^2}
\]

\[
\theta = \frac{\sigma_0 (\cos(2\eta) (\zeta^4 - 2c_t^2 - 2\zeta c_t - 1) - i \sin(2\eta) (\zeta^4 + 2c_t^2 - 2\zeta c_t + 1) + i \zeta^2 (2c_t^2 + 1)))}{4c_t - 2\zeta^3}
\]

and for the curved diamond void, they are

\[
\begin{align*}
\chi &= \frac{\zeta \sigma_0}{4} - \frac{\sigma_0 ((c_d + 1) \cos(2\eta) - i (c_d - 1) \sin(2\eta))}{2\zeta (c_d^2 - 1)} - \frac{c_d \sigma_0}{4 \zeta^3} \\
\theta &= \frac{\zeta \sigma_0 ((c_d + 1) \cos(2\eta) (-\zeta^4 + (\zeta^4 + 3) c_d + 1))}{2 (c_d^2 - 1) (3c_d - \zeta^4)} \\
&+ \frac{\zeta \sigma_0 ((c_d - 1) (\zeta^2 (3c_d^2 + 3c_d^2 + c_d + 1) - i \sin(2\eta) (\zeta^4 + (\zeta^4 - 3) c_d + 1)))}{2 (c_d^2 - 1) (3c_d - \zeta^4)}
\end{align*}
\]

The Young’s modulus ratio for the curved triangle void is

\[
\frac{E_\eta^t}{E} = \frac{1 - 2c_t^2}{2c_t^2 + 3f - 2c_t^2 + 1}
\]

and for the curved diamond void is

\[
\frac{E_\eta^d}{E} = \frac{-3c_d^2 + 4c_t^2 - 1}{-3c_d^2 + 4c_t^2 - 1 + f (3c_d^2 - 2c_t^2 - 3) - 2fc_d \cos(4\eta)}
\]
Figure 4: Polar plot of the Young’s modulus ratio under oblique loading for a circular, cusped triangle ($c_t = 0.5$), and cusped diamond ($c_d = 0.33$) voids at a porosity value of $f = 0.1$. Both the circle and the curved triangle void shapes are isotropic.

We note that the results match those presented by Kachanov [44], and by setting $\eta = 0$, we recover the results presented in Section 5.4. We also note that, as briefly mentioned in Section 5.4, the curved triangle void is an isotropic shape, and this is evident by the fact that the result in Equation 49 is the same as Equation 34.

For the curved diamond void, the modulus ratio changes as a function of $\eta$. As shown in Figure 4, the ratio is largest (for any given porosity value $f$) for the 45° loading case and lowest for the 0°/90° cases. This implies that if the FFF mesostructure needs to be loaded in the x-y plane, the 45° direction offers the highest stiffness.

6 Shear loading in z-x and z-y planes

In Section 5, we used the complex variable method of elasticity to solve the 2D elasticity problems around a single void. In this section, we will use the same method to solve the antiplane shear problem [52]. The antiplane shear problem assumes that all displacements in the x-y plane are zero, and the displacement in the z-direction is a function of x and y only, i.e.

\[ u_x = u_y = 0 \]
\[ u_z = u_z(x, y) \] (51)

The stresses are given by

\[ \sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = 0 \]
\[ \sigma_{zx} = G \frac{\partial u_z}{\partial x} \]
\[ \sigma_{zy} = G \frac{\partial u_z}{\partial y} \] (52)
In the absence of body forces, the boundary value problem at hand becomes
\[
\nabla^2 u_z = 0 \quad \text{in } \Omega \\
\sigma_{zx} = \sigma_{zx}^0 \quad \text{for } |r| \to \infty \\
\sigma_{zy} = \sigma_{zy}^0 \quad \text{for } |r| \to \infty \\
\sigma \cdot n = 0 \quad \text{on } S
\]
\[\text{(53)}\]

The boundary condition on \(S\), expanded out, is
\[
\sigma_{zx} n_x + \sigma_{zy} n_y = 0
\]
\[\text{(54)}\]

Since both the real and imaginary parts of a holomorphic function independently satisfy Laplace’s equation, and since \(u_z\) is a real function, we can solve the boundary value problem by finding a holomorphic function \(h(m(\zeta)) = h_R + ih_I\) defined such that
\[
u_z = h_R
\]
\[\text{(55)}\]

where \(\zeta = \rho e^{i\phi}\) and \(m(\zeta) = x + iy\) is the mapping function as defined previously. Taking the derivative of \(h\) with respect to \(m\) gives us
\[
\frac{dh}{dm} = \frac{\partial h}{\partial x} \frac{dx}{dm} + \frac{\partial h}{\partial y} \frac{dy}{dm}
\]
\[= \frac{\partial u_z}{\partial x} - i \frac{\partial u_z}{\partial y}
\]
\[= \frac{\sigma_{zx}}{G} - i \frac{\sigma_{zy}}{G}
\]
\[\text{(56)}\]

which implies that
\[
\sigma_{zx} = G \Re \left\{ \frac{dh}{dm} \right\}
\]
\[= G \frac{\frac{dh}{dm} + \frac{\overline{dh}}{dm}}{2}
\]
\[\sigma_{zy} = -G \Im \left\{ \frac{dh}{dm} \right\}
\]
\[= -i G \frac{\frac{dh}{dm} - \frac{\overline{dh}}{dm}}{2}
\]
\[\text{(57)}\]

The normal components can be expressed as
\[
n_x = \frac{dy}{ds}
\]
\[= \frac{i}{2} \left( \frac{dm}{ds} - \frac{dm}{ds} \right)
\]
\[
n_y = -\frac{dx}{ds}
\]
\[= \frac{1}{2} \left( \frac{dm}{ds} + \frac{dm}{ds} \right)
\]
\[\text{(58)}\]

where \(s = e^{i\phi}\) is an arc length variable along the void surface. Substituting Equations 57 and 58 into Equation 54 yields
\[
0 = \frac{i}{2} G \left( \frac{dm}{ds} - \frac{dm}{ds} \right) \frac{dh}{dm} + \frac{\overline{dh}}{dm} - \frac{i}{2} G \left( \frac{dm}{ds} + \frac{dm}{ds} \right) \frac{dh}{dm} - \frac{\overline{dh}}{dm}
\]
\[= \frac{iG}{2} \left( \frac{dh}{dm} \frac{dm}{ds} - \frac{\overline{dh}}{dm} \frac{dm}{ds} \right)
\]
\[= \frac{iG}{2} \left( \frac{dh}{dm} \frac{dm}{ds} - \frac{\overline{dh}}{dm} \frac{dm}{ds} \right)
\]
\[\text{(59)}\]
This means that, to satisfy the traction boundary condition on the void, we need \( h - \overline{h} = 2ih_I = 0 \) (i.e., the imaginary part of \( h \) must be zero).

As before, we split the problem into finding a uniform solution and a perturbation solution due to the presence of a single void to get

\[
h = h_0 + h_1
\]  
(60)

where superscript (0) represents the uniform solution and (1) represents the perturbation. The uniform solution is given by

\[
h_0(\zeta) = \sigma_0 \left[ G m(\zeta) + i \sigma_0 \frac{m(\zeta)}{G} \right]
\]  
(61)

For the void to be traction free,

\[
\Im\{h_0(s) + h_1(s)\} = 0
\]  
(62)

As before, we will represent \( h_1 \) using a Laurent series with negative power terms

\[
h_1(\zeta) = \sum_{n=1}^{\infty} a_n \zeta^{-n}
\]  
(63)

Substituting Equations 61 and 57 into Equation 62 yields

\[
\frac{\sigma_0}{G} \Im\{m(s)\} + \frac{\sigma_0}{G} \Re\{m(s)\} + \sum_{n=1}^{\infty} \Im\{a_n e^{-i\phi}\} = 0
\]  
(64)

Given a mapping function, we can solve for the unknown constants \( a_n \) by matching coefficients in Equation 64. As before, only a finite number of coefficients will be nonzero due to the simple form of the mapping function given by Equation 6 and 7.

We start with finding \( G_{zx} \) by setting \( \sigma_0 = 0, \sigma_0 = 0 \). For both the curved triangle and diamond void, \( h \) is given by

\[
h = \frac{\sigma_0}{G} \left( \zeta + \frac{1}{\zeta} \right)
\]  
(65)

The effective modulus can be found by equating strain energies using Equation 22

\[
\frac{1}{2} \frac{\sigma_0^2 A_{\text{void}} t}{G f} + \frac{1}{2} \frac{\sigma_0 t}{f} \int_0^{2\pi} \left( u_z \frac{dy}{d\phi} \right) d\phi = \frac{1}{2} \frac{\sigma_0^2 A_{\text{void}} t}{G_{zx}}
\]  
(66)

The effective modulus ratios for the curved triangle and curved diamond are given by

\[
\frac{G'_{zx}}{G} = \frac{1 - 2c_t^2}{2f - 2c_t^2 + 1}
\]  
(67)

\[
\frac{G_{zy}}{G} = \frac{1 - 3c_d^2}{2f - 3c_d^2 + 1}
\]  
(68)

Due to symmetry in the curved diamond, \( G_{zx} = G_{zy} \). We also observe that \( G'_{zx} = G'_{zy} \) due to the \( xy \) plane being isotropic for the curved triangle.

7 Unit cell simulations

We simulate the effective elastic constants by conducting volume average homogenization on unit cells using the procedure described by Sun [56]. Circular, cusped triangle \( c_t = 0.5 \), and cusped diamond \( c_d = 0.33 \) voids are used. For computational efficiency, 2D simulations under plane stress conditions are used to find \( E_{xx}, E_{yy}, \nu_{xy}, \) and \( G_{zx} \). The remaining elastic constants are found using 3D simulations. Appropriate periodic boundary conditions are used in all cases. For material properties, \( E = 3500 \text{ MPa} \) and \( \nu = 0.33 \) are used, which represent the linear elastic material properties of polylactic acid (PLA), a commonly used FFF material. In the following plots, closed-form solutions are denoted by \( \text{cf} \) and simulation results are denoted by \( \text{sim} \) when appropriate.
Figure 5: Simulation results for $E_{zz}$ match the closed-form solution for all porosity values and void shapes.

Figure 6: Simulation results for $\nu_{zx}$ and $\nu_{zy}$ match the closed-form solution for all porosity values and void shapes.
Results for $E_{zz}$, $\nu_{zx}$, and $\nu_{zy}$ are shown in Figures 5 and 6. As expected, the numerical results match the closed-form solution exactly (apart from numerical error) for the entire range of porosity values.

Results for $E_{xx}$ and $E_{yy}$ are shown in Figure 7, and the relative difference between closed-form predictions and simulation results are shown in Figure 8. For the circular void, the closed-form solution is very accurate, differing by 10% for porosity value around 35%. For the triangle and diamond void, 6% and 17% porosity lead to 10% difference, respectively. This is a trend shown in all of the remaining elastic constants as well: the closed-form solution deviates from simulation faster than the diamond, which deviates faster than the circle. In addition, the stiffness ratio at a given porosity ratio is lowest for the triangle, followed by the diamond, with the circle having the highest stiffness ratio. Similar results have been observed by Jasiuk [47], who noted that the stiffness ratio is lower for polygonal holes with fewer sides.

Results for $\nu_{xy}$ are shown in Figure 9, and the relative difference is shown in Figure 10. The results for the diamond void are interesting in that the closed-form solution predicts $\nu_{xy}$ increasing slightly from an initial value of 0.33 and leveling off. This initial increase is captured by the simulation (see inset of Figure 9), but the simulations show that $\nu_{xy}$ decreases towards 0 as porosity is increased for all void shapes. Intuitively, this makes sense; at high porosity values, there is a thin narrow band within the unit cell along the direction of loading that is under stress, while most of the the unit cell is relatively stress free, causing very little displacement transverse to the loading direction. Under 10% of difference can be achieved by using porosity values less than 6%, 7%, and 15% for the triangle, diamond, and circular voids, respectively. However, we would like to note that in certain situations, such as uniaxial loading and bending of slender beams), the Poisson ratio plays a minimal role in the overall stress, strain, and displacement fields. In the aforementioned situations, having a less accurate Poisson ratio value may not matter.

The results for $G_{xy}$, $G_{zx}$, and $G_{zy}$ are given in Figures 11 and 13, with relative differences shown in Figures 12 and 14. The shear modulus results are similar to the Young’s modulus result: the triangle void still has the lowest ratio, and the closed-form solution diverges from the simulation fastest for the triangle void. To achieve under 10% difference for $G_{xy}$, porosity values less than 7%, 10%, and 11% should be used for the triangle, diamond, and circular voids, respectively. To achieve under 10% difference for $G_{zx}$ and $G_{zy}$, porosity values less than 8%, 14%, and 24% should be used for the triangle, diamond, and circular voids, respectively.
Figure 8: Relative difference between closed-form solution and simulation for $E_{xx}$ and $E_{yy}$.

Figure 9: Poisson ratio $\nu_{xy}$ as a function of porosity $f$ and void shape.
Figure 10: Relative difference between closed-form solution and simulation for $\nu_{xy}$.

Figure 11: Shear modulus $G_{xy}$ as a function of porosity $f$ and void shape.
Figure 12: Relative difference between closed-form solution and simulation for $G_{xy}$.

Figure 13: Shear modulus $G_{zx}$ and $G_{zy}$ as a function of porosity $f$ and void shape.
One reason the hexagonal mesostructure performs worse than the square mesostructure is because the extruded roads in the hexagonal mesostructure become fully disconnected from neighbors at a lower porosity. We can conduct a geometric analysis to determine at what porosity the extruded roads become disconnected. For the cusped triangle void, the distance from the center to the void to one of the tips is 1.5. The voids are arranged in a hexagonal array, with tips touching each other. The dimensions of the rectangular unit cell is $3\sqrt{3} \times 9$. Since there are the equivalent of four triangle voids per unit cell, the total void area in a unit cell (found using Equation 33) is $2\pi$. This means that the maximum porosity for the hexagonal mesostructure is

$$f_t^{max} = \frac{2\pi}{3\sqrt{3} \times 9} = 0.134$$

(69)

Similar analysis for the square mesostructure leads to

$$f_d^{max} = \frac{2\pi/3}{9} = 0.295$$

(70)

The close-pack nature of the hexagonal mesostructure essentially leads to worse stiffness-per-weight ratio than the square mesostructure. The only exception is loading in the $x$-direction, in which case they both perform the same for any porosity value. While these upper bounds on porosity assume ideal mesostructures and void shapes, real world parts printed with porosity values near (or exceeding) the upper bounds are expected to have many intersecting voids and bond defects—all of which lead to significantly degraded mechanical performance.

The sharpness of the voids also has a significant effect on the effective stiffness, with rounded corners (lower absolute values of $c_t$ and $c_d$) leading to higher modulus values. One method to round out the void shapes is to increase the negative gap between extruded roads, causing the material to overflow and fill in the voids. There is a limiting point: at very high negative gaps, the geometric distortion can be extreme and the as-printed part geometry may differ significantly than the original input geometry [36], [57], [58].
Table 1: Summary of effective elastic constants.

<table>
<thead>
<tr>
<th>Elastic constant</th>
<th>Curved triangle</th>
<th>Curved diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{E}{G}$</td>
<td>$1-f$</td>
<td>$1-f$</td>
</tr>
<tr>
<td>$\nu_{xx}$</td>
<td>$\nu$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$\nu_{yy}$</td>
<td>$\nu$</td>
<td>$\nu$</td>
</tr>
<tr>
<td>$\nu_{xy}$</td>
<td>$\frac{1-2c^2}{f(2c^2+3f-2c^2+1)}$</td>
<td>$\nu\left(\frac{1-2c^2}{f(2c^2+3f-2c^2+1)}\right)$</td>
</tr>
<tr>
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</tr>
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</tr>
<tr>
<td>$\nu_{zy}$</td>
<td>$1-2c^2$</td>
<td>$1-2c^2$</td>
</tr>
</tbody>
</table>

8 Conclusion

We have derived closed-form expressions for all nine effective elastic constants for two mesostructures: hexagonal and square. The effective elastic constants depend on the void shape, porosity, and material properties of the bulk material. Simulation results for several void shapes match the closed-form expressions very well at low porosity values, with the largest error coming from the $\nu_{xy}$ prediction.

A summary of effective moduli ratios as a function of porosity, shape parameters, and material Poisson ratio is given in Table 8.

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Conflicts of Interest

The authors declare no conflict of interest.

References


