Representative volume element analysis in material coextrusion

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Abstract

Multi-material additive manufacturing enables the opportunity to combine multiple materials within the same part, allowing for an expanded range of properties that can gradually change inside the design space.

This category of materials is commonly referred to as functionally graded materials (FGMs). However, FGMs currently face several limitations and challenges in terms of design and manufacturing, such as compatibility, distribution design, and prediction of mechanical properties. Furthermore, when dealing with parts possessing complex micro/meso-structures, finite element simulation often becomes a costly and time-consuming process.

Among various additive manufacturing technologies, fused filament fabrication allows the combination of multiple thermoplastic materials within the same nozzle during the deposition process, thereby creating FGMs.

This process, known as coextrusion, enables the gradual deposition of materials adjacent to each other while changing their fractions. Moreover, the deposition direction shapes the distribution of materials within each deposited layer, influencing the material structure and the resulting mechanical properties. A recent study proposes a preliminary model describing the deposition mechanism, which has been confirmed by experimental tests. This model delineates the section of the material deposited based on the tool path and process parameters, such as layer thickness and hatching space.

To expand upon these findings, this paper applies a homogenization approach based on finite element analysis to the deposition model. This approach enables the description of material mechanical properties based on the material fractions, tool path, and other process parameters. Additionally, this study presents a methodology to tailor the mechanical properties according to the printed part's orientation around the print bed.

Keywords: Representative Volume Element, RVE, Homogenization, Multi-material coextrusion, Fused Filament Fabrication, FFF, functionally graded materials, FGM.

1 Introduction

With the advent of new manufacturing techniques, the field of materials science has witnessed a transition from conventional materials to advanced composites and smart materials. In this context, a new class of composite materials known as functionally graded materials (FGMs) has garnered significant attention from the scientific community due to their programmable mechanical performance [1,2].

FGMs are characterized by gradual variations in composition and structure within their volume, resulting in corresponding changes in material properties.

Recently, this kind of materials can be achieved by additive manufacturing (AM), a well-known technology able to produce parts layer by layer. By strategically controlling the addition of materials throughout the volume, as well as the geometry and arrangement of the phases, it becomes possible to tailor the overall functions and properties of FGM components.

Multi-material additive manufacturing (MMAM) technologies enable the incorporation of multiple materials within a single component, and even within a single deposition [2]. In the context of MMAM for FGMs, there is a focus on improving the interfacial bond between dissimilar materials, where gradual transitions between phases can enhance the properties if compared to distinct material boundaries [3].

However, these advancements face challenges due to limited design knowledge and application. The bottleneck lies in the design tools, both for the part itself and the deposition process [3,4]. Over the past decade, Computer-Aided Design/Manufacturing (CAD/CAM) software utilizing a volumetric approach has been developed. These software tools primarily focus on the design, functional analysis, and simulation of homogeneous FGMs, where density gradients can be strategically modulated by changing the microstructure or morphology of lattice structures throughout the volume [5]. Software for multi-material design commonly employs voxel data structures, where each voxel can hold different information such as material properties. However, these tools are still limited and require further improvements to become more effective, such as Autodesk Monolith.

In a previous study [2], two compatible pairs of materials were investigated by varying the material fractions in the coextrusion process. Models describing the deposition mechanism and mechanical properties were proposed and partially confirmed through preliminary experimental tests. The results demonstrated that material properties change according to the extrusion direction and the material mixing fraction.

By employing homogenization techniques, it is possible to derive the stiffness matrix of repetitive structures, assuming they consist of homogeneous materials, with the Representative Volume Element (RVE) representing the repeating element. This approach allows for the replacement of complex material distributions with an equivalent material, reducing simulation efforts.

Ferretti et al. [6] constructed linear RVE models to predict the macroscopic behavior of fused filament fabrication (FFF) manufacts, taking into account the typical voids resulting from the deposition process. They observed anisotropic behavior due to the presence of voids between layers. Hasanov et al. [7] designed and fabricated FGM dogbone samples using a voxelization approach and subsequently used homogenization to predict the effective material properties of FFF FGMs. They found that the homogenized mechanical properties of the flat-oriented dogbones closely matched the experimental tests. Tian et al. [8] evaluated the effective mechanical properties of composites with complicated microstructures by employing RVE and periodic boundary conditions (PBC). They demonstrated that implementing PBC ensures stress and strain continuity, as well as the uniaxial deformation constraint of the RVE, leading to an accurate evaluation of effective elastic properties and elastoplastic responses of composites with complex microstructures.

In this work, RVE analysis is applied to study the linear elastic mechanical properties of multilateral coextrusion printed parts, based on a previously proposed deposition model [9]. This model describes the section of the material deposited according to material fractions, tool path, and process parameters such as layer thickness and hatching space.

2 Material and Methods

The material properties used in this study refer to a Polylactic Acid and Thermoplastic Polyurethane (PLA-TPU) as described in the previous investigation [9] and summarized in Table 1.

Table 1. Material mechanical proprieties.

Material	Tensile modulus [MPa]	Poisson ratio	Density [g/cm^3]
PLA	3425.00	0.33	1.24
TPU	161.60	0.45	1.23

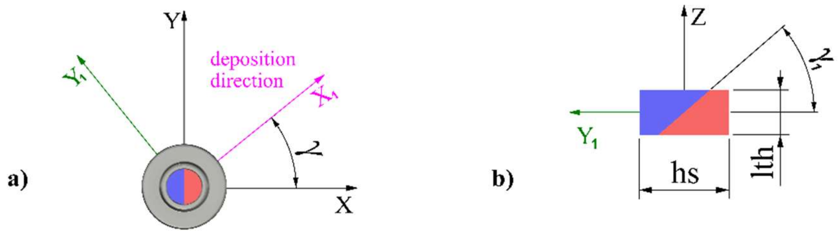
2.1 Material modeling

In order to determine the geometry of the elementary volume element that describes the cross-section of the layer perpendicular to the path of the nozzle, the following assumptions have been made:

- Within the nozzle, the selected pairs of materials are arranged side by side in a reciprocal position, divided by the YZ plane (see Fig. 1a);
- The deposition angle γ is defined as the angle between the X-axis and X_1-axis, where X_1 represents the deposition direction, i.e., the direction of the nozzle path (see Fig. 1a);
- The materials interface plane is assumed to be parallel to the deposition direction X_1 (see Fig. 1a);
- The materials interface plane is inclined at an angle γ_1 in the Y_1Z plane, as demonstrated in the literature [9];
- The cross-section is a rectangular shape with a base dimension referred to as "hatching space" (hs) and a height dimension known as "layer thickness" (lth) (see Fig. 1b).

The following figures depict the PLA material in blue and the TPU material in red.

When the nozzle moves along the Y-axis, the material in the left channel is deposited on the left side, while the material flowing in the right channel is deposited on the right side. On the other hand, when the nozzle moves in the positive X-direction, the material on the right is deposited below the material on the left. Conversely, when the nozzle moves in the negative X-direction, the material flowing on the left is deposited beneath the material on the right.



$$\gamma 1 = arctan(tan(\gamma) * lth/hs)$$

Fig. 1. a) The main and the deposition coordinate systems, b) The reference frame for the material distribution modeling.

Under this assumption, a series of unitary volume elements can be described by the sections shown in Figure 2, adopting the following parameters:

- *lth* = 0.2 mm and *hs* =0.4 mm;
- Material fraction *MF* varying the percentual of TPU: 25%, 50%, and 75%;
- γ from 0° to 360°, with 15° steps.

Looking at Figure 2, it is evident that the elements ranging from 90° to 180° are mirrored by the elements ranging from 0° to 90° along the Z-axis. Additionally, the elements ranging from 180° to 360° are mirrored by the 0° to 180° elements along the Y_1-axis. Therefore, it is sufficient to study the elements ranging from 0° to 90°.

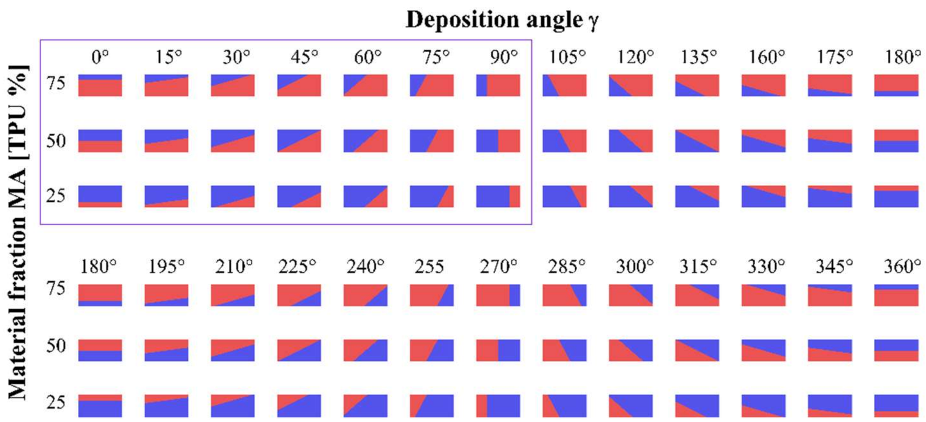


Fig. 2. Volume element as a function of deposition angle and material fraction.

2.2 Mechanical characterization

The material behaves as a composite, exhibiting varying mechanical properties along the three Cartesian directions (X_1, Y_1, Z_1). Numerical simulations were conducted to predict the mechanical properties of RVE. Two sets of RVE were with one set representing 100% grid infill and the other set representing the perimeter of the FFF process.

In 3D printing, the perimeters are described by the contour of the manufactured part and assume different deposition angles according to the local tangent.

To study the mechanical properties of the perimeter, the RVE is simply defined by the elementary volume element according to the local tangent, i.e., the deposition angle (see Fig. 2).

For the RVE of the infill path, which consists of a grid pattern, it is obtained by considering two adjacent elementary volume elements with opposite deposition directions overlapped on a pair of orthogonal identical elements (as depicted in Figure 3a). Additionally, the RVE is adjusted by translating the volume element by a quarter along the X-, Y-, and Z-axes to ensure coincident topologies at the shared interfaces, i.e., the same mesh nodes. This adjustment facilitates the application of periodic meshing and Periodic Boundary Conditions (PBC) (as illustrated in Figure 3b).

Assuming an orthotropic material hypothesis, the necessary mechanical properties to define the stiffness matrix K of the homogenized material are the elastic moduli E_x, E_y, E_z, the shear moduli G_{xy}, G_{xz}, G_{yz}, and the Poisson's ratios υ_{xy}, υ_{xz}, υ_{yz}.

The homogenization process was performed using Ansys Material Designer 2022, a SpaceClaim tool within Ansys Workbench (Ansys, Inc., USA). Material Designer assumes that the constituent materials in the RVE model are linear elastic and perfectly bonded at the interface. The meshing settings utilized involve a conformal mesh with periodic meshing, employing SOLID 187 mesh elements with a maximum size of 0.02 mm (as shown in Figure 3c).

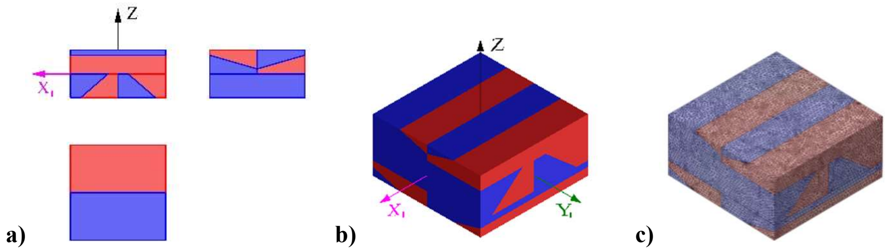


Fig. 3. a) Infill RVE of MF=50% and γ = 30°-120°,
b) RVE adjusted for the periodic meshing process required for the PBC, c) RVE meshed.

3 Results and Discussion

The results of the simulations defined in the previous sections are displayed in the graphs of Figure 4. For each path, the graphs are subdivided into 3 groups based on: elastic modulus, shear modulus, and Poisson ratio in the 3 directions referred on the X_1-Y_1-Z coordinate system.

The elastic and shear modulus exhibit distinct behavior for the infill and perimeter elements.

Regarding the perimeters, this behavior can be explained through the concept of parallel and series springs [9].

Along the deposition direction, the material distribution runs parallel to the X_1-direction and acts as parallel springs, resulting in a constant E_{X1}.
In the other directions (E_{Y1}, E_Z), the behavior transitions from parallel to series springs. For instance, E_{Y1} behaves as parallel springs at γ=0° and as series springs at γ=90°. A continuous variation within these limits can be observed within the 0°-90° range.

In the case of infill, due to the complex arrangement of materials involving two layers of perimeters orthogonally stacked in the vertical direction, the behavior can no longer be simplified as a combination of springs, leading to a more complex distribution of mechanical properties. Comparatively, the values of E_Z in the infill exhibit a narrower range, potentially due to a mitigating effect resulting from the orthogonal distribution of materials.
Similar patterns can be observed for G and ν based on the aforementioned explanation. Furthermore, for the infill, the behavior along the deposition angle mirrors at 90° for E_{X1}, E_{Y1}, G_{Z1X1}, and G_{Y1Z1}, while for the perimeter, it occurs at 180° for E_{Y1}, E_Z, and G_{X1Y1}, and G_{ZX1}. This behavior can be attributed to the symmetry of the material. Additionally, G_{X1Y1} for the infill and G_{Y1Z} for the perimeter reach their maximum values around 45°.

As noted in other studies, even in the case of metamaterials and lattice structures, the Poisson ratios can exceed 0.5 [9]. Similarly, for the present study, the Poisson ratios demonstrate a specular relationship, with ν_{ZX1} and ν_{Y1Z} for the infill at 90°, and ν_{X1Y1} and ν_{ZX1} for the perimeter at 90°, respectively.

To obtain the results in the main coordinate system X-Y-Z, a rotation matrix is required to rotate each RVE compliance matrix. This rotation can be achieved using the following equation [10]:

$$[C_1] = [T]^{-1}[C][T] \tag{1}$$

Where C represents the compliance matrix, T denotes the rotation matrix, and c and s in equation 2 represent the cosine and sine of the deposition angle γ:

$$[C] = \begin{bmatrix} \frac{1}{E_x} & -\frac{v_{yx}}{E_y} & -\frac{v_{zx}}{E_z} & 0 & 0 & 0 \\ -\frac{v_{xy}}{E_x} & \frac{1}{E_y} & -\frac{v_{zy}}{E_z} & 0 & 0 & 0 \\ -\frac{v_{xz}}{E_x} & -\frac{v_{yz}}{E_y} & \frac{1}{E_z} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{yz}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{zx}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{xy}} \end{bmatrix} ; \quad [T] = \begin{bmatrix} c^2 & s^2 & 0 & 0 & 0 & 2cs \\ s^2 & c^2 & 0 & 0 & 0 & -2cs \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & s & 0 \\ 0 & 0 & 0 & -s & c & 0 \\ -cs & cs & 0 & 0 & 0 & c^2 - s^2 \end{bmatrix} \tag{2}$$

By employing this approach, the compliance matrix behavior of each RVE, excluding the one at 0°, undergoes a transition from orthotropic to anisotropic behavior.

Through the proposed methodology it is possible to verify the behavior of the coextruded components. Based on the obtained results, it becomes possible to strategically orient the deposition of the infill and the MF through an optimization process. This enables the achievement of programmed or tailored properties in the final product.

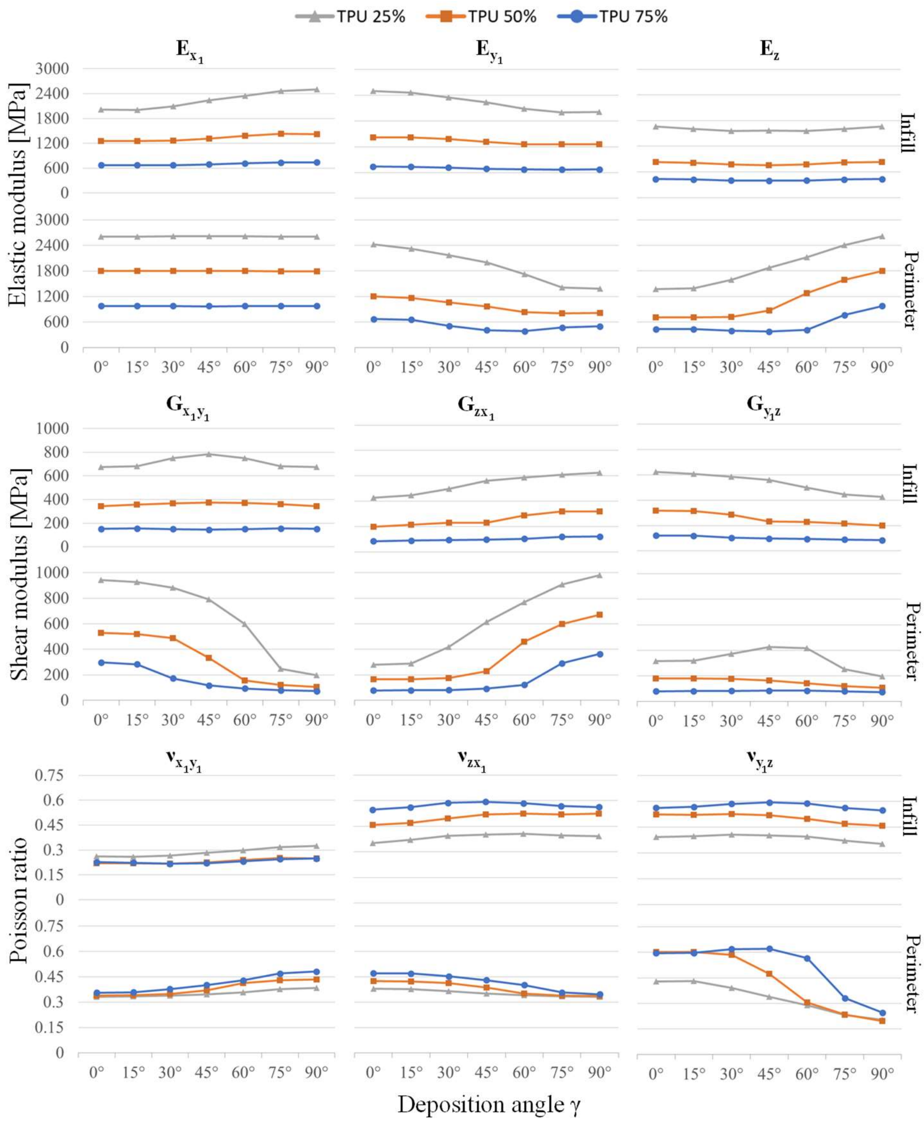


Fig. 4. The homogenization results are presented as a function of the deposition angle and are divided into infill and perimeter paths. The results pertain to the elastic moduli, shear moduli, and Poisson ratio, according to the variation of the TPU material fraction.

4 Conclusion

This study provides significant insights for designing the shape and mechanical properties of coextruded components, taking into consideration the feeding system and print bed orientation. The analysis involved the development of a linear RVE model to predict the macroscopic behavior of 3D printed coextrusion geometries. The deposition angle, infill or perimeter path, and material fraction were considered variables in the model. The mechanical properties of the coextruded components are highly influenced by the deposition angle and exhibit variations based on the type of deposition employed. In numerical simulations, it is crucial to distinguish between the properties associated with the infill and perimeter regions. While the properties of the infill can be directly associated, the properties of the perimeters need to be discretized into multiple zones based on their orientation angles.

Future developments will focus on conducting experimental tests to validate the models.

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