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Finite Element Analysis of Filler Shape in Photopolymerization Additive Manufacturing Using the Fusion RSA-RVE Algorithm

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ABSTRACT

Photopolymerization-based additive manufacturing has become a key technology due to its advantages, such as low energy consumption and rapid processing. However, optimizing the mechanical properties of composite materials produced through this process remains a challenge. The impact of filler geometry on the mechanical performance of photopolymerized composites has not been fully explored. Shrinkage stresses during polymerization, especially in acrylate-based materials, can lead to brittleness and cracking, limiting their structural integrity and industrial application. This study aims to investigate the influence of different filler shapes and densities on the tensile strength, strain, and stress distribution of composite materials fabricated through photopolymerization. A Finite Element Representative Volume Element (FE-RVE) approach was employed, integrating ABAQUS scripting with Random Sequential Adsorption (RSA) for filler modelling. Non-linear dynamic tensile simulations were conducted to analyse the mechanical behaviour of composites with three filler shapes: sphere, prism, and polyhedron. Experimental validation was performed using ASTM D-638 tensile tests to ensure the accuracy of the simulations. The study anticipates that filler geometry significantly influences the mechanical performance of composites. Polyhedron-shaped fillers are expected to exhibit the highest tensile stress due to their superior stress distribution capabilities, while prism fillers may demonstrate enhanced flexibility. These findings aim to provide valuable insights into designing optimized composites for industrial applications, such as automotive and high-performance engineering.

Keywords: Photopolymerization; FE-RVE; RSA-RVE; ABAQUS; additive manufacturing

INTRODUCTION

Photopolymerization has recently gained considerable attention as a highly effective and efficient method for fabricating advanced materials. This process, integral to several additive manufacturing (AM) techniques, particularly in stereolithography (SLA) and digital light processing (DLP), involves the use of light to initiate polymerization, resulting in rapid polymer network formation. One of the significant advantages of photopolymerization is its low energy consumption, which contributes to reduced operational costs and environmental impact. Additionally, its ability to precisely control the polymerization process makes it attractive for producing materials with complex geometries and fine details. However, despite these advantages, several challenges persist, limiting the broad applicability of photopolymerization in more demanding industrial applications.

A key limitation of photopolymerization is the issue of shrinkage stress, particularly in acrylate-based materials. During the polymerization process, shrinkage occurs as the monomers are converted into a polymer network, resulting in internal stresses. These stresses can lead to brittleness, cracking, and a reduction in the overall durability of the final product. This is a significant drawback, particularly in applications requiring high mechanical performance. Acrylate-based materials, while popular for their fast-curing times and high resolution, are particularly prone to this issue. As a result, the development of composite materials by incorporating fillers has emerged as a promising solution to mitigate the effects of shrinkage stress and improve the mechanical properties of photopolymerized materials (Ligon-Auer et al. 2015; Liska 2007).

In the context of three-dimensional printing (3DP), which relies heavily on photopolymerization, there is also an increasing concern about the environmental impact of the materials used. Many commonly used 3DP materials, such as Acrylonitrile Butadiene Styrene (ABS), are petroleum-based and contribute to environmental pollution. In response, biodegradable alternatives like polylactic acid (PLA), derived from renewable resources, have gained popularity. PLA offers an eco-friendly solution; however, its mechanical properties are often inferior to those of petroleum-based polymers. It is frequently modified through composite formulation to enhance PLA's mechanical performance, which introduces complexities in optimizing factors such as matrix-to-fiber ratio, filler shape, orientation, and volume fraction (Figiel, 2018; McKeown & Jones, 2020). These parameters must be carefully balanced to achieve specific applications' desired strength, stiffness, and durability.

One of the most effective methods for analyzing and optimizing the mechanical properties of photopolymerized composites is Finite Element Analysis (FEA). FEA allows researchers to perform detailed microstructural analysis of composite materials by simulating their behavior under various conditions. The Finite Element Representative Volume Element (FE-RVE) approach is beneficial. By creating a representative volume of the composite material that includes both the matrix and the fillers, the FE-RVE method enables researchers to investigate how different filler shapes, sizes, distributions, and volume fractions affect the material's mechanical performance. This approach provides valuable insights into key composite parameters, such as stress-strain behavior and failure points, while maintaining a balance between computational efficiency and accuracy (Schwarze, 2018).

Incorporating fillers into photopolymerized materials significantly impacts their mechanical properties, including tensile strength, stress distribution, and overall structural integrity. Filler shape, density, and volume fraction are critical factors that determine the performance of these composites, and small variations in these parameters can lead to substantial differences in material behavior. For example, certain filler shapes may enhance tensile strength but reduce flexibility, while others may improve elongation at break but compromise overall strength. Therefore, predicting the mechanical properties of photopolymerized composites at the microscale before physical production is essential for ensuring the optimal performance of a specific material (Babaei & Farrokhabadi 2020; Pinto 2017).

The current research seeks to address these challenges by investigating the mechanical properties of photopolymerized composites using a multiscale FE-RVE approach. This study focuses on three different filler shapes; sphere, prism, and polyhedron and examines how these geometries influence the composite materials' tensile strength, strain, and stress distribution. By combining the Random Sequential Adsorption (RSA) formulation in computational FE-RVE with experimental data, this research aims to develop a comprehensive understanding of how varying filler shapes and densities influence the mechanical properties of composite materials produced through photopolymerization.

Despite the growing interest in photopolymerized composites, limited studies have systematically investigated the influence of filler geometry on their mechanical properties. Previous research primarily focuses on general composite performance, leaving a critical gap in understanding how specific filler shapes and distributions affect stress distribution, tensile strength, and flexibility at the microstructural level.

The Random Sequential Adsorption-Finite Element Representative Volume Element (RSA-RVE) method addresses this gap by enabling precise modelling of filler placement and its effects on material behaviour. Recent studies have demonstrated that RSA-RVE enhances computational efficiency while maintaining high accuracy in simulating composite microstructures with various particle shapes and distributions (Tian et al. 2021; Zhang et al. 2024). These advancements are particularly valuable in industrial contexts such as aerospace, automotive, and biomedical engineering, where the design of high-performance materials with tailored properties is crucial. For instance, RSA-RVE facilitates the optimization of mechanical properties like tensile strength and durability, making it a cost-effective and reliable tool for composite design in additive manufacturing. This study contributes to bridging the identified research gap by applying RSA-

RVE to analyse the impact of filler shapes and densities on photopolymerized composites, providing insights for advancing industrial applications.

METHODOLOGY

FINITE ELEMENT REPRESENTATIVE VOLUME ELEMENT (FE-RVE) APPROACH

In this study, a macro-scale Representative Volume Element (RVE) tensile model with spherical-shaped, polyhedron-shaped and hexagonal-prism-shaped fillers was developed using the Random Sequential Addition (RSA) approach (Tian et al. 2015). The selection of filler shapes was guided by their industrial relevance, geometric diversity, and proven significance in influencing the mechanical performance of composites. Spheres were chosen for their isotropic stress distribution properties, ease of manufacturing, and widespread use in composites as a baseline geometry (Tian et al. 2021). Prisms were selected to represent elongated and angular fillers that can provide directional strength or flexibility, essential in structural applications (Zhang et al. 2024). Polyhedrons, with their complex geometry, were included for their superior ability to distribute stress uniformly and enhance structural integrity, making them suitable for high-performance applications in industries such as aerospace and automotive (Tian et al. 2015). Together, these shapes encompass a broad spectrum of geometrical configurations, allowing for a comprehensive evaluation of their impact on tensile strength, stress distribution, and elongation at break. This selection supports the study's objective of optimizing composite design and aligns with existing research highlighting the critical role of filler geometry in composite material performance.

The process of Representative Volume Element (RVE) tensile model involves the systematic generation of a statistically representative filler microstructure embedded within the RVE domain as in Figure 1. The process ensures that the filler placement adheres to collision avoidance rules and periodic boundary conditions while achieving the desired filler volume fraction (Pütz et al. 2020).

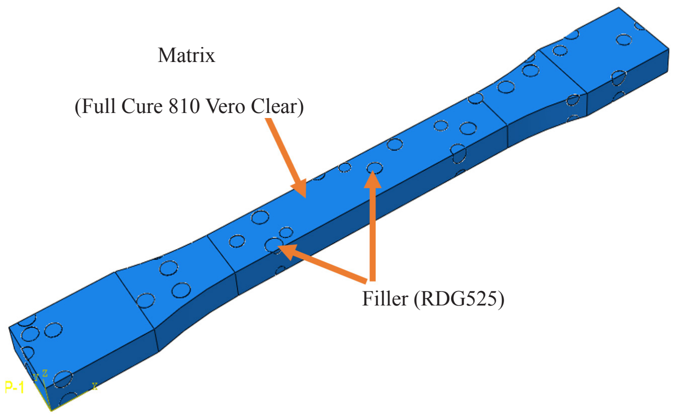

FIGURE 1. 3D RSA-RVE specimen model generated in ABAQUS

The RVE geometry was defined as a 3D model based on the ASTM D638 Type I tensile specimen, characterized by a gauge section, transition sections with fillets, and wider end sections (Tian et al. 2015). The total length of the specimen (L_{total}) is 165 mm, with a width of 19 mm and a thickness of 3 mm. The central gauge section has a length (L_{gauge}) of 57 mm, and the transition sections are defined by a fillet radius (R) of 76 mm. The length of each end section (L_{end}) was calculated as $L_{end} = \frac{165-115}{2} = 25$ mm. The total volume of the RVE (L_{RVE}) was computed as:

$$V_{RVE} = W \cdot t \cdot L_{gauge} + 2 \cdot (W \cdot t \cdot L_{end}) + V_{fillets} \tag{1}$$

where W=19 mm is the width, t = 3 mm is the thickness, and $V_{fillets}$ represents the volume of the curved fillets, which was approximated using CAD tools for precise geometric accuracy.

The spherical fillers were characterized by their radius (r) and corresponding volume (V_f), expressed as:

$$V_f = \frac{4}{3}\pi r^3 \tag{2}$$

For the Polyhedron filler, the volume (V_f) is given by:

$$V_f = \frac{1}{3}\sum_{f=1}^{N_f} A_f \cdot h_f \tag{3}$$

where N_f is the number of faces of the polyhedron. A_f is the area of the f-th face, h_f is the perpendicular height from the centroid of the f-th face to a reference point or the projection axis.

As for the hexagonal-prism filler, the volume (V_{f})is given by:

$$V_f = \frac{3\sqrt{3}}{2}a^2 \cdot h \tag{4}$$

Where a is the side length of the hexagonal base and h is the height (or length) of the prism.

To ensure a statistically accurate microstructure, the target filler volume fraction (V_f^{target}) was set as a design parameter. At each iteration, the current filler volume fraction ($V_f^{(i)}$) was calculated as:

$$V_f^{(i)} = \frac{\sum_{n=1}^{N} V_f}{V_{\mathbf{RVE}}} \tag{5}$$

where N is the number of fillers placed in the RVE. The RSA approach was used to iteratively add fillers while ensuring no overlap between the fillers. For each filler, the potential collision time (t_c) was calculated to prevent overlaps and respect the periodic boundary conditions. The collision time between two fillers (t_c^{ij}) was determined by:

$$t_c^{ij} = \frac{r_i + r_j - d_{ij}}{\|\mathbf{v}_i - \mathbf{v}_j\|} \tag{6}$$

where d_{ij} is the distance between the centers of fillers i and j, and v_i, v_j are their velocities.

Similarly, the collision time with the RVE boundaries (t_c^{ib}) was calculated as:

$$t_c^{ib} = \min\left(\frac{r_i - (x_i - 0)}{|v_i^x|}, \frac{r_i - (L_x - x_i)}{|v_i^x|}, \ldots\right) \tag{7}$$

The minimum collision time for a filler (t_{min}) was then obtained as:

$$t_{\min} = \min\left(t_c^{ij}, t_c^{ib}\right) \tag{8}$$

Based on t_{min}, the fillers were moved to their new positions, ensuring they remained within the RVE boundaries and adhered to periodicity. The new position for each filler was updated as:

$$\mathbf{x}_i^{(t+t_{\mathrm{mm}})} = \mathbf{x}_i^{(t)} + \mathbf{v}_i t_{\min} \tag{9}$$

If a collision occurred, the velocities of the fillers were updated using conservation of momentum:

$$\mathbf{v}_i^{\mathrm{new}} = \mathbf{v}_i + \Delta\mathbf{v} \tag{10}$$

To enforce periodic boundary conditions, any filler crossing the RVE boundaries was repositioned using:

$$x_i \to x_i - L_x \text{ (if } x_i > L_x), \; x_i \to x_i + L_x \text{ (if } x_i < 0) \tag{11}$$

This iterative process continued until the current filler volume fraction ($V_f^{(i)}$) met or exceeded the target volume fraction (V_f^{target}). Once the macro RVE Tensile model with filler microstructure was generated, the RVE was used to simulate a tensile test in the macroscale model. Then, the complete algorithm was converted into Abaqus/Python scripting for generating a 3D solid model. A uniaxial tensile load was applied along one axis of the RVE, while the opposite face was fixed to prevent rigid body motion. The interaction between the matrix and the spherical fillers was modeled using general contact with predefined interaction properties. The finite element simulation was performed in Abaqus/CAE using a dynamic explicit solver. The results included stress-strain curves, filler-matrix interaction behavior, and the evolution of failure mechanism The flow of the tensile model generation is depicted in Figure 2.

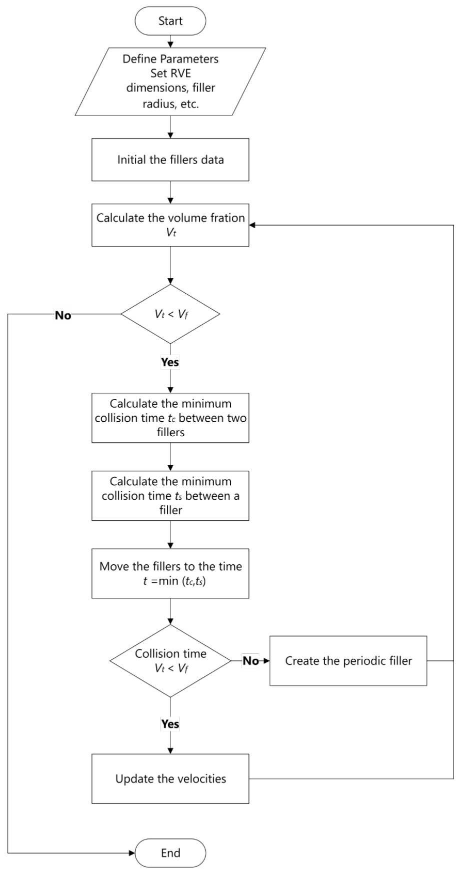

FIGURE 2. Algorithm generation flowchart for the periodic random packing of fillers

MATERIALS USED

The matrix material selected for this research was FullCure 810 VeroClear, a widely used photopolymer in additive manufacturing known for its transparency and mechanical properties. The filler material chosen was RDG525, with a fixed volume fraction of 15%. These materials were selected based on their prevalence in industrial applications and their suitability for photopolymerization-based additive manufacturing processes. The material properties of the material are tabulated in Table 1.

TABLE 1. Material Properties

Property	Young's Modulus (MPa)	Poisson's Ratio	Tensile Strength (MPa)	Yield Stress (MPa)	Density (kg/m³)	Flexural Strength (MPa)
Full Cure 810 Vero Clear	3000	0.35	55 MPa	41 MPa	1180	85 MPa
RGD525 (High-Temperature Material)	3200	0.35	80 MPa	60 MPa		130 MPa

MESHING AND SIMULATION SETUP

To accurately simulate the mechanical behavior of the composite material, the FE-RVE models were meshed using C3D10, a 10-node tetrahedral element well-suited for capturing the detailed geometry of filler shapes (Shen et al. 2018). The global mesh size was set at 0.02 mm, while a finer mesh size of 0.015 mm was applied to critical areas where stress concentrations were anticipated. This meshing strategy ensured a balance between computational efficiency and the accuracy of the results, allowing for precise analysis of stress distribution and deformation in the composite material. The meshing is illustrated in Figure 3.

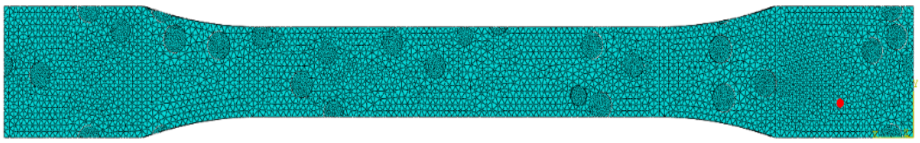

FIGURE 3. The meshing of the model

The mechanical behavior of the composite materials was simulated using a non-linear dynamic explicit analysis (Hsu & Cheng 2012). Boundary conditions were applied to replicate tensile loading, with the left face of the model fully constrained and the right face allowed to displace along the X-axis as shown in Figure 4 (Xue et al. 2003). This setup mimicked the conditions of a standard tensile test, enabling the detailed observation of stress distribution, deformation, and material failure. Additionally, element deletion was employed in the model to simulate material failure, allowing for the removal of elements as they reached their failure criteria. The simulation was prescribed to run for 1 minute, during which the complete stress-strain behavior of the composite under tensile loading was observed (Saykin et al. 2017).

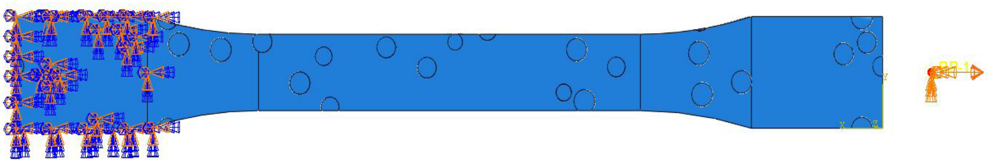

FIGURE 4. The boundary condition prescribed on the model

EXPERIMENTAL VALIDATION

In order to validate the simulation results, the FE-RVE models were printed using a Stratasys Object30 Prime photopolymerization 3D printer. Tensile tests were conducted on printed specimens using a Universal Testing Machine (UTM) as in Figure 5 at a constant 2 mm/min loading rate. This rate was chosen based on ASTM-D638, a standard for measuring the tensile properties of plastics (Cerda-Avila et al.2017.). The experimental data collected included key mechanical properties such as yield strength, ultimate tensile strength, and modulus of elasticity.

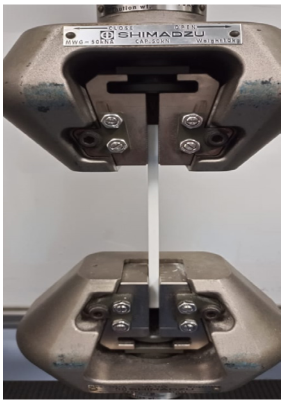

FIGURE 5. Tensile Test

RESULTS AND DISCUSSION

SIMULATION RESULTS AND FILLER SHAPE INFLUENCE

The finite element analysis of photopolymerized composites reinforced with sphere, polyhedron, and prism fillers was conducted using the Fusion RSA-RVE algorithm, with a consistent volume ratio of 15% for all filler models. The Fusion RSA-RVE algorithm enabled the accurate representation of filler placement and orientation within the matrix, particularly capturing the random angular orientations of the asymmetrical prism fillers through a RSA and PBC-based method. Symmetrical fillers, such as spheres and polyhedrons, were assigned uniform random orientations, reflecting their isotropic behavior. The computational predictions were validated using experimental tensile test, which confirmed the spatial alignment and distribution of fillers in mechanical strength, demonstrating the reliability of the algorithm in modeling realistic microstructures.

The tensile strength results revealed a strong dependence on filler geometry. Polyhedron-filled composites exhibited the highest average tensile strength of 62 MPa, attributable to the polyhedron's ability to distribute stress uniformly across the matrix, thereby minimizing localized stress concentrations and delaying failure. Sphere-filled composites recorded a lower tensile strength of 55 MPa, with stress localization at the filler-matrix interface contributing to earlier failure (Pan et al. 2008). Prism-filled composites exhibited an intermediate tensile strength of 58 MPa but showed greater variability due to their random angular orientations, which influenced stress distribution and mechanical response (Shen et al. 2018). The stress-strain curves presented in Figure 6 highlight these differences, with the prism-filled composites displaying a wider range of mechanical responses compared to the consistent behavior observed for the sphere- and polyhedron-filled composites. The Fusion RSA-RVE algorithm effectively captured these orientation-dependent effects, showcasing its robustness in modeling asymmetrical fillers.

The failure mechanisms of the composites varied based on filler geometry. Polyhedron fillers showed uniform stress distribution, leading to delayed failure progression, while sphere and prism fillers exhibited localized stress concentrations that accelerated failure (Hsu & Cheng, 2012; Saykin et al. 2017). Figures 7 illustrate the example of failure progression for sphere-filled composites tensile FE-RVE model, where cracks initiated and propagated around regions of high stress. The superior tensile strength observed for polyhedron-shaped fillers aligns with findings by (Tian et al. 2021), who reported that complex filler geometries improve stress distribution and reduce localized stress concentrations. Prism fillers, due to their random orientations, showed more heterogeneous failure patterns, with localized stress regions influencing crack development (Cerda-Avila et al. 2017.). These results were validated by experimental tensile tests conducted at a loading rate of 2 mm/min, which closely aligned with the simulation data, demonstrating an average error of 3.6%. The experimental results also highlighted the influence of filler geometry on elongation at break, with prism-filled composites achieving the highest elongation of 22%, followed by polyhedron fillers at 19%, and sphere fillers at 17%. This enhanced flexibility of prism-filled composites underscores their suitability for applications requiring energy absorption and ductility, while polyhedron fillers provide superior load-bearing capacity (Shen et al. 2018). The enhanced flexibility exhibited by prism-shaped fillers is consistent with (Zhang et al. 2024), who demonstrated the role of angular fillers in directional flexibility improvements.

The study's findings underscore the critical role of filler geometry and orientation in determining the mechanical performance of photopolymerized composites (Babaei & Farrokhabadi, 2020). The consistent 15%

volume ratio across all filler types allowed for direct comparisons of their geometric effects on tensile strength and failure behavior. Polyhedron fillers, with their superior tensile strength and uniform stress distribution, are ideal for applications requiring high load-bearing capacity, such as aerospace and automotive components. Prism fillers, offering enhanced flexibility, are better suited for impact-absorbing materials, while spherical fillers, despite lower tensile strength, provide cost-effective solutions for less demanding applications. The Fusion RSA-RVE algorithm, by accurately modeling both symmetrical and asymmetrical filler shapes and orientations, has proven to be a reliable predictive tool for optimizing composite design. The effectiveness of the RSA-RVE methodology in simulating composite behaviour with high accuracy is supported by Schwarze et al. (2018), who emphasized its computational efficiency for microstructural analysis of composites. The close agreement between experimental and simulation results validates the effectiveness of this approach.

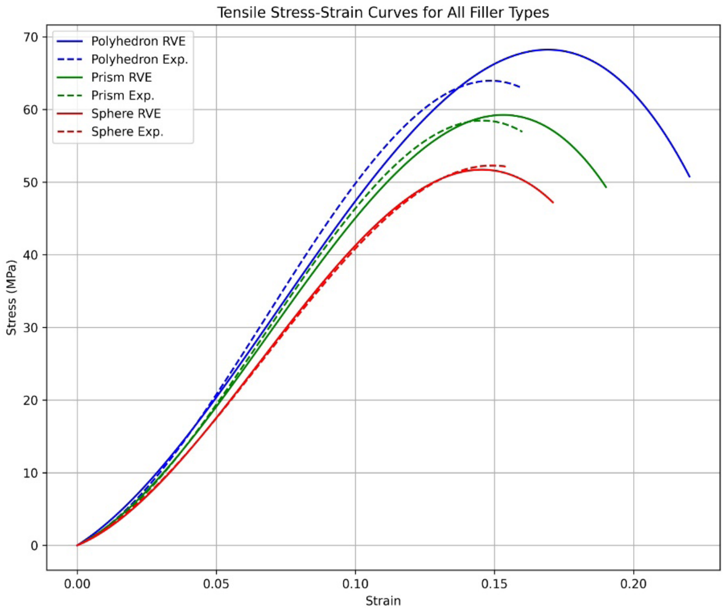

FIGURE 6. Tensile stress-strain curve for all types of fillers compares between simulation and experiment

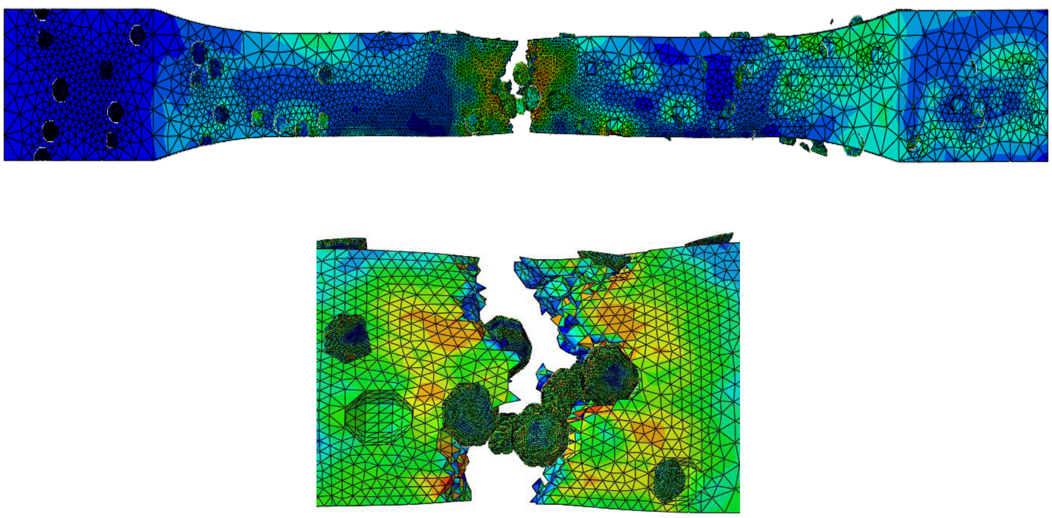

FIGURE 7. Example of failure damage in sphere filler shape in tensile FE- RVE model.

CONCLUSION

This research successfully analyzed the mechanical properties of photopolymerized composites using a Random Sequential Adsorption (RSA) formulation combined with the Finite Element Representative Volume Element (FE-RVE) method. By employing both finite element simulations and experimental validation, the study aimed to understand how different filler shapes affect photopolymerized composites' tensile strength and flexibility. The primary materials used in this study were FullCure 810 VeroClear as the matrix and RDG525 as the filler material, with a fixed 15% volume fraction. The study focused on three distinct filler shapes—sphere, prism, and polyhedron—to determine their impact on the mechanical performance of the composite.

The simulations and experimental work provided valuable insights into how filler geometry influences material behavior. Polyhedron-shaped fillers outperformed both prism and sphere fillers regarding tensile strength and elongation at break. The polyhedron fillers achieved the highest tensile strength, averaging 62 MPa, while prism fillers reached 58 MPa and sphere fillers 55 MPa. In addition to tensile strength, the polyhedron fillers demonstrated the best elongation at break, reaching 22%, compared to 19% for prisms and 17% for spheres. The superior performance of the polyhedron fillers can be attributed to their ability to distribute stress more uniformly within the composite material, minimizing localized stress concentrations and thereby delaying material failure. This more uniform stress distribution helped enhance the load-bearing capacity of the composite, making the polyhedron filler particularly effective for high-performance applications.

The alignment between the simulation and experimental results was remarkably close, with only a 3.6% error, further validating the accuracy of the FE-RVE method in predicting composite behavior. This strong correlation highlights the reliability of the FE-RVE approach, proving it to be an effective tool for simulating the mechanical properties of composite materials before physical testing. Such predictive capabilities are precious in additive manufacturing, where optimizing material properties for specific applications is critical.

The findings of this study emphasize the importance of filler shapes in composite design for additive manufacturing applications. The results suggest that polyhedron fillers should be prioritized in situations where both high tensile strength and flexibility are required. Their ability to maintain structural integrity under stress while still offering some degree of flexibility makes them ideal for aerospace, automotive, and biomedical engineering applications, where strength and durability are crucial.

Overall, this research demonstrates the effectiveness of the FE-RVE method in providing accurate predictions of composite behavior. By integrating RSA formulation and finite element analysis with experimental validation, the study offers a comprehensive framework for optimizing the mechanical properties of photopolymerized composites. The ability to predict and enhance these properties through detailed simulations will enable the development of more advanced, high-performance materials for industrial applications. This study also underscores the critical role that filler geometry plays in optimizing the mechanical performance of composites, providing a clear pathway for future research and innovation in additive manufacturing.

While this study provides valuable insights into the influence of filler shapes on the mechanical properties of photopolymerized composites, several areas warrant further investigation. Future work could explore the following directions:

1. Dynamic Loading Conditions: Investigate the performance of composites with different filler shapes under dynamic and cyclic loading to simulate real-world applications more accurately.
2. Thermal and Environmental Effects: Study the impact of varying thermal and environmental conditions, such as temperature fluctuations and humidity, on composite behavior.
3. Optimization of Filler Volume Fraction: Extend the RSA-RVE methodology to optimize filler volume fractions for specific applications, balancing mechanical performance with material efficiency.
4. Alternative Filler Materials: Evaluate the effect of using alternative filler materials, such as carbon-based or bio-based fillers, to enhance sustainability and performance.
5. 3D Printing Process Parameters: Incorporate process parameters, such as printing speed, layer height, and curing time, to assess their influence on the mechanical properties of the composites.

These future directions aim to build upon the findings of this study and expand its applicability to broader industrial and environmental contexts.

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DECLARATION OF COMPETING INTEREST

None.

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