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Improving Uniform Dispersion in Ti-6Al-4V + Graphene-SLM through an Agglomeration Factor: Multiscale Simulation and Experimental Study

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Abstract

The integration of graphene into Ti-6Al-4V alloys via Selective Laser Melting (SLM) presents a promising pathway to enhance the mechanical and functional properties of metal matrix composites. However, achieving uniform dispersion remains a challenge due to graphene agglomeration in the base material. This study introduces an Agglomeration Factor (AF) as a quantitative metric to assess graphene clustering as a result of variation in laser power during the SLM process. In this study, a hybrid methodology is used, which combines Multiscale Multiphysics Simulation Modeling (MMSM) using Ansys, with experimental validation through SEM-based image analysis. Five specimens were simulated and fabricated using laser powers of 200, 250, 300, 350, and 400 W, respectively, while maintaining all other process parameters, including scanning speed and powder bed temperature, constant. Results demonstrated a strong inverse correlation between laser power and AF in both experimental and simulated environments, with the lowest AF observed at 400 W, which indicates optimal dispersion. While the highest AF was observed at 200 W. This demonstrates that an increase in laser power, translates in improved graphene dispersion in the Ti-6Al-4V matrix. Furthermore, it was observed that the MMSM's predictive accuracy deviates from experimentation by 5.71%. This study establishes AF as a reliable dispersion metric and demonstrates the critical role of laser power in mitigating graphene clustering. This study provides a framework for optimizing SLM-based nanocomposite fabrication.

Keywords
Ti-6Al-4V + Graphene, Selective Laser Melting, Multiscale Multiphysics Simulation Model, Agglomeration Factor

Introduction
The integration of graphene into titanium alloys, particularly the widely used Ti-6Al-4V alloy, offers a promising pathway toward the development of next-generation materials for high-performance applications. Ti-6Al-4V provides enhanced mechanical properties, including high strength, low weight, and biocompatibility, making it ideal for industries such as aerospace, medical implants, and automotive (Pegues et al. 2016). When combined with graphene, a material with high tensile strength (~130 GPa) as well as high electrical and thermal conductivity, the resulting composite indicates significant enhancements in wear resistance, fatigue strength, and overall structural integrity. This combination can revolutionize applications requiring high performance and lightweight structures under extreme conditions (Sun et al. 2021).

Additive Manufacturing (AM), particularly Selective Laser Melting (SLM), is a transformative technology that enables the creation of complex geometries and the precise control of microstructural features in metal matrices, rendering it ideal for the fabrication of parts using Ti-6Al-4V + graphene composites. However, uniform dispersion of graphene within the titanium matrix remains a major challenge due to its tendency to agglomerate. The high surface energy and Van der Waals interactions of graphene promote clustering, leading to non-uniform reinforcement, and degraded mechanical properties (Fang et al. 2009).

To address the challenge, this study introduces an Agglomeration Factor (AF) aimed at quantifying and controlling the clustering of graphene during the SLM process. By regulating this factor, this study aims to achieve uniform dispersion of graphene within the Ti-6Al-4V matrix, thereby enhancing the mechanical properties of the composite. To identify the optimal SLM parameter for effective dispersion, a MMSM is employed. While several printing parameters such as laser power, scan speed, powder bed temperature, and hatch spacing influence the quality of the printed output, this study solely focuses on regulating the laser power to achieve optimal graphene dispersion. Previous researches have shown that laser power is the most influential parameter in determining the output quality in Ti-6Al-4V-SLM process. The MMSM results are used serve as guidelines for refining the printing process, which are then experimentally validated to ensure that the ideal dispersion parameters are realized in practice. The following sections outline the structure of this study: Data and Materials, Methods, Results, Discussion, and Conclusion.

1.1 Objectives

This study aims to enhance uniform dispersion in Ti-6Al-4V + Graphene composites fabricated through SLM. This is achieved through the following objectives:

a. To define an AF to measure graphene clustering in Ti-6Al-4V **+ G**raphene SLM outcomes.
b. To Simulate Ti-6Al-4V + Graphene SLM process using MMSM to identify optimal laser power parameters for uniform dispersion.
c. To fabricate physical specimens under the simulated conditions to validate the predictive accuracy of the MMSM model.
d. To characterize graphene dispersion through microstructural analysis to quantify the AF in simulated and fabricated specimens.
e. To validate simulated results to evaluate the reliability and predictive performance of the MMSM.

2. Literature Review

Uniform Dispersion

Overview

Uniform dispersion refers to the homogeneous distribution of reinforcement particles such as graphene within a base material such as Ti-6Al-4V to ensure consistent mechanical, thermal, and electrical properties throughout the composite (Kumar et al. 2019). As poor dispersion can lead to localized stress concentrations, weak interfacial bonding, and reduced mechanical performance (Sun et al. 2021 & Fan et al. 2021).
Pegues et al. (2016) argue that uniform dispersion is crucial to prevent graphene agglomeration in SLM process.

Agglomeration is defined as a clustering of nanoparticles due to Van der Waals forces, electrostatic interactions, and insufficient wetting of reinforcement particles in the base material matrix. In Ti-6Al-4V + Graphene SLM, agglomeration occurs when graphene sheets stack together, forming large clusters instead of remaining evenly dispersed within the Ti-6Al-4V matrix (Wang and Zhang 2023). This may compromise material integrity by causing inhomogeneous reinforcement, phase separation, and defect formation (Pegues et al. 2016). The following have been identified as the consequences of Agglomeration in SLM process:

a. Weakened Mechanical Properties: Agglomeration creates defects that serve as fracture initiation points, reducing fatigue life, and tensile strength of printed parts (Martinez and Gomez 2022).
b. Inhomogeneous Microstructure: Agglomeration causes uneven reinforcement, which leads to variable material performance across different regions of the printed part (Wang and Zhang 2023).
c. Thermal and Electrical Inconsistencies: Agglomeration reduces heat dissipation efficiency and lowers conductivity, which is crucial for aerospace and biomedical applications (Sun et al. 2021).

2.1 Formation of Agglomeration in the SLM Process

SLM process involves rapid melting and solidification, which can either enhance dispersion or exacerbate agglomeration, depending on process parameters (Wang and Zhang 2023 & Becker et al. 2022). Figure 1 depicts a step-by-step formation of agglomeration in SLM process. The following key mechanisms have been identified as key contributor to Agglomeration in SLM - These factors are summarised in Table 1 below:

a. Powder Bed Inhomogeneity (Martinez and Gomez 2022):
   - Uneven graphene distribution in the powder bed can lead to localized clustering before melting.
   - Graphene's low density compared to Ti-6Al-4V causes it to segregate unevenly in the powder mixture.

b. Insufficient Laser Energy Input (Chang et al. 2023):
   - Low laser power results in partial melting, leading to poor graphene integration within the Ti-6Al-4V matrix.
   - Incomplete wetting causes graphene sheets to stack, forming large agglomerates instead of dispersing uniformly.

c. Melt Pool Dynamics and Thermal Convection (Priarone et al. 2017):
   - High surface energy of graphene prevents complete mixing in the molten Ti-6Al-4V pool.
   - Weak Marangoni flow leads to non-uniform redistribution, which traps graphene clusters in specific regions.

d. Rapid Solidification and Phase Segregation (Kumar & Taylor 2023):
   - During fast cooling, graphene re-solidifies unevenly, which may lead to inhomogeneous reinforcement.
   - Clusters remain isolated, which may reduce interfacial bonding and mechanical strength.

Table 1. Summary of key Agglomeration factors in SLM

Agglomeration Factors	Cause	Effect on Material
Uneven Graphene Distribution	Poor powder mixing	Causes localized reinforcement which leads to inhomogeneous properties
Low Laser Power	Insufficient melting	Results in power nanoparticle wetting, which increases clustering
Weak Thermal Convection	Melt pool instability	Prevents effective dispersion, which leaves aggregates in certain regions
Rapid Solidification	Phase separation	Leads to segregated nanoparticle pockets, which reduces mechanical strength

2.2 Agglomeration Factor (AF)

The Agglomeration Factor (AF) is defined as a quantitative measure of clustering in the composite matrix. According to Wofl and Pöschel (2023), a high AF indicates severe agglomeration ($x > 0$), while a low AF suggests even distribution ($x < 0$). The AF is mathematically described as follow:

$$AF = \frac{\sum_{i=1}^{N} \quad A_i}{A_{Total}} \#(1)$$

Where:

A_i represents the area of nanoparticle cluster.

A_{Total} is the total nanoparticle area within the composite.

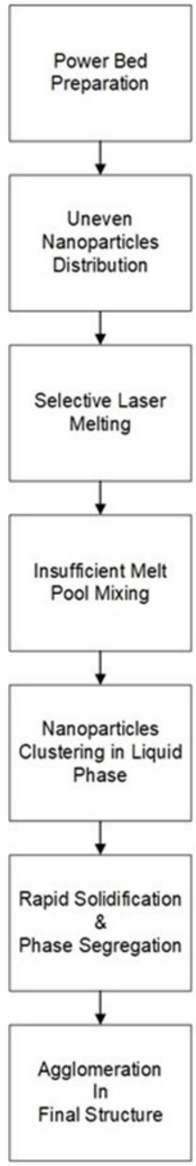

Figure 1. A step-by-step agglomeration formation in SLM process – Adapted from (Wang and Zhang 2023; Martinez and Gomez 2022; Priarone et al. 2017 & Kumar and Taylor 2023)

2.3 Effect of agglomeration on Ti-6Al-4V + Graphene SLM

2.3.1 Overview

Agglomeration mainly affects mechanical, thermal, and electrical properties of the composite (Wang & Zhang, 2023). This section explores the effect of agglomeration on these properties.

Influence of Agglomeration on Mechanical Properties

Agglomeration in Ti-6Al-4V + Graphene composites lead to localized stress concentrations, which cause premature crack initiation under mechanical loads. Studies indicate that graphene clusters act as fracture nucleation sites, significantly reducing tensile strength and fatigue resistance (Martinez and Gomez 2022). Additionally, the weak interfacial bonding between graphene agglomerates and the Ti-6Al-4V matrix further reduces load transfer efficiency, which compromises overall mechanical integrity (Wang and Zhang 2023).

Effect on Thermal and Electrical Conductivity

Graphene is known for its high thermal and electrical conductivity; however, agglomeration disrupts these properties when incorporated into the Ti-6Al-4V matrix. Studies have shown that isolated graphene clusters create non-uniform thermal conduction pathways, which reduce heat dissipation efficiency and increase residual stresses within the printed part (Kumar et al. 2019). The resulting thermal distortions may lead to warping and structural instability, particularly in high-temperature applications (Priarone et al. 2017). Similarly, agglomeration negatively affects electrical conductivity, as isolated graphene clusters disrupt electron transport, reducing the composite's effectiveness in functional applications requiring high conductivity (Sun et al. 2021).

Microstructural Defects and Porosity Formation

Agglomeration introduces microstructural defects such as pores, voids, and non-uniform grain structures. During the SLM process, graphene clusters inhibit proper fusion between Ti-6Al-4V particles, which leads to increased porosity and inconsistent grain growth. These defects weaken the overall structural reliability of the composite, which makes it prone to failure under cyclic loading conditions (Wang and Zhang 2023). Furthermore, rapid solidification rates in SLM exacerbate phase segregation, which results in a heterogeneous distribution of reinforcement throughout the composite (Wofl and Pöschel 2023).

2.4 SLM Laser Power parameters and Agglomeration

2.4.1 Overview

This section examines the correlation between laser power and agglomeration. It provides a brief analysis how variations in laser power influence the dispersion and clustering of graphene within the Ti-6Al-4V matrix.

2.4.2 Effect of SLM Laser Power in Agglomeration Control

To mitigate the adverse effects of agglomeration, researchers emphasize the importance of SLM process parameters such as laser power, scan speed, hatch spacing, and powder bed temperature (Kumar and Taylor 2023). Experimental studies have shown that higher laser power improves graphene wettability; thereby, promoting its homogeneous integration within the molten Ti-6Al-4V matrix and reducing clustering. However, excessive laser power may cause overheating, which leads to graphene vaporization and altering the composite's mechanical and thermal properties (Wang and Zhang 2023). Furthermore, Kumar and Taylor (2023) argue that adjusting SLM parameters such as laser power may foster a level of control over agglomeration; thereby preventing or maintaining agglomeration to a minimum.

2.5 MMSM Environments

2.5.1 Overview

Due to the complexities of real-time graphene dispersion analysis, researchers increasingly rely on Multiscale Multiphysics Simulation Models (MMSM) to predict and mitigate agglomeration effects before experimental fabrication. Computational models allow researchers to analyze melt pool behavior, thermal gradients, and nanoparticle interactions within the composite matrix.

MMSM is a computational framework that integrates multiple physical phenomena across different length and time scales to accurately model complex systems such as SLM process. Multiscale modelling enables the coupling of microscale interactions (I.e., material phase transformations, heat transfer at the particle level) with macroscale behaviors (I.e., mechanical properties, structural performance) (Priarone et al. 2017).

By incorporating multiple physics such as thermal dynamics, fluid mechanics, electromagnetism, and mechanical stresses, Multiphysics Modelling provides a comprehensive understanding of the interactions of various factors within a system. In the context of SLM, the MMSM simultaneously considers laser-material interaction, heat dissipation, molten pool dynamics, and phase changes to investigate the impact of process parameters on the final output (Priarone et al. 2017).

2.5.2 Optimum MMSM Environment

Mukalay et al. (2024) conducted a comprehensive study to determine the optimal Multi-scale Multiphysics Simulation Environment (MMSM) for holistic Ti-6Al-4V-SLM process simulation. The findings indicate that Ansys Additive Print, Flow-3D, Comsol Multiphysics, ESI Additive Manufacturing, Genoa 3DP, Amphyon, Simufact Additive, Autodesk Netfabb, and Simulia have been the most widely utilized MMSM environments over the past decades – See Figure 2. This review is limited to simulation tools with a minimum usage ratio of 1%, as per the available literature.

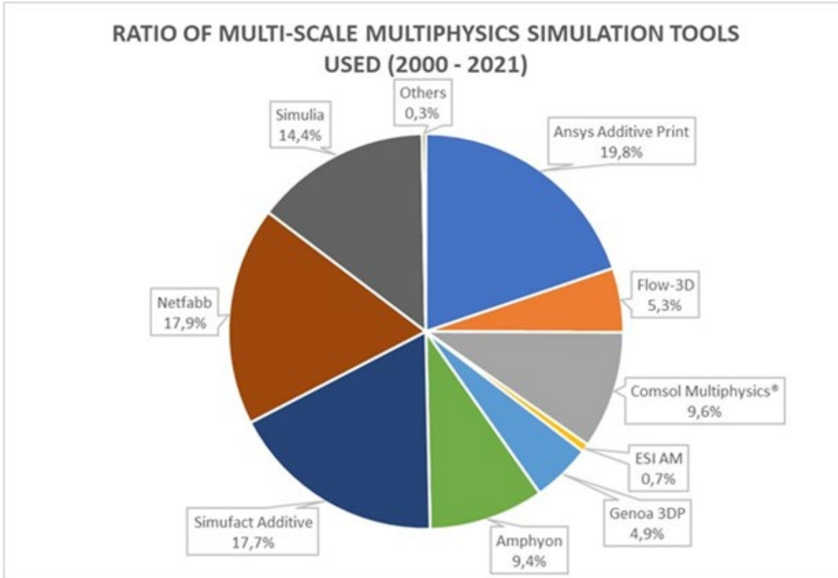

Figure 2. Utilization of Multi-scale Multiphysics SLM Simulation Environments through Existing Literature (Mukalay et al. 2024)

The study employed a two-phase methodology comprising a SWOT-ANP analysis (theoretical phase) and experimentation (validation and verification phase) to systematically evaluate the capabilities of these simulation environments. The theoretical phase involved two steps. First, a comprehensive literature review assessed each environment's Strengths, Weaknesses, Opportunities, and Threats (SWOT) with respect to five critical AM simulation modelling capabilities: modelling and simulation, design, materials, build process, and post-processing. Figure 3 describes the performance of each environment based on the defined capabilities. The theoretical analysis demonstrated that Ansys Additive Print, Autodesk Netfabb, Simulia, Genoa 3DP, Simufact Additive, and Comsol Multiphysics are the most effective MMSM environments, respectively. Secondly, standardized simulation models were executed in each environment under identical process parameters and run conditions to quantify variations in geometric deviation as a result of laser power variations across the outputs.

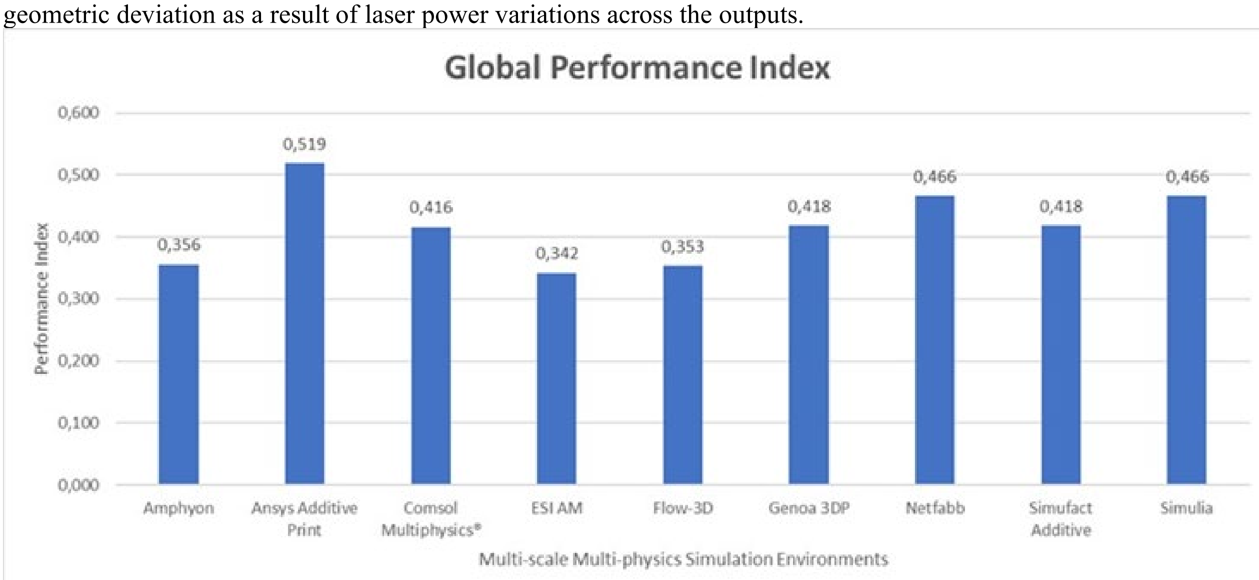

Figure 3. Benchmarking of Multi-scale Multiphysics SLM Simulation Environments Global Performance Indices (Mukalay et al., 2024)

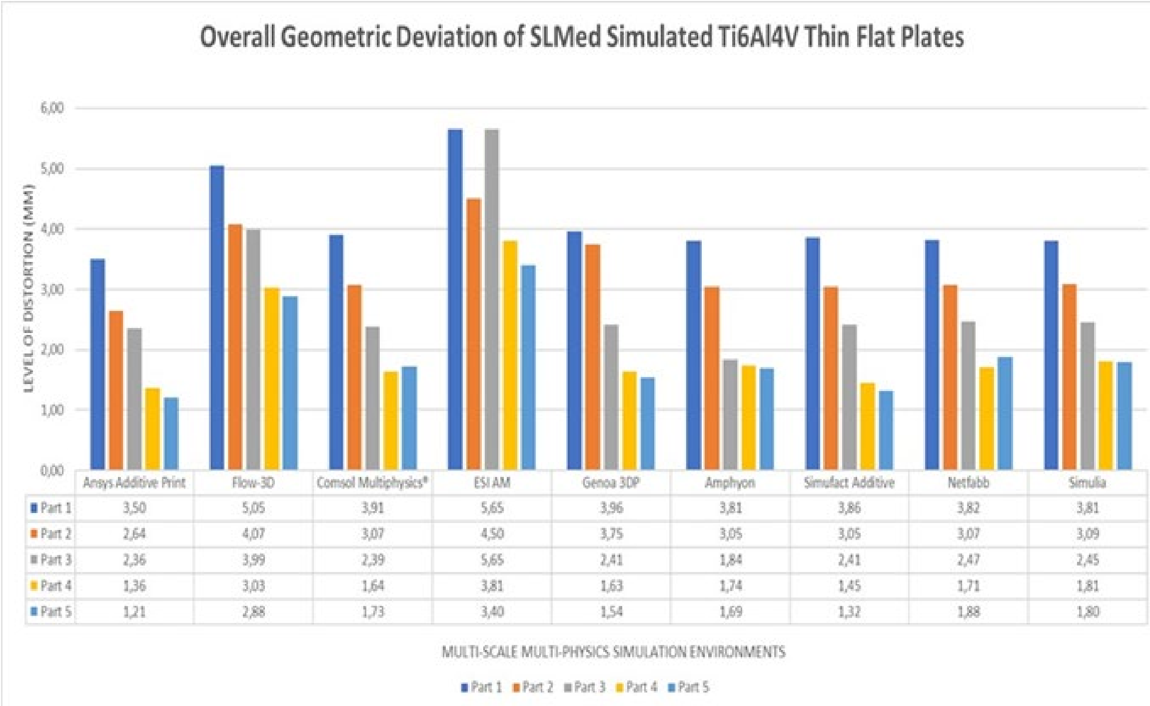

Figure 4. Overall Geometric Deviation of SLMed Simulated Ti6Al4V-Thin Flat Plates (Mukalay et al., 2024)

Based on results presented in Figure 4, Ansys Additive Print, which exhibited the most robust capabilities and the lowest level of deviation, was selected as the MMSM environment for this study.

2.6 Summary

From the literature review, it has been described that Agglomeration in SLM refers to the clustering of nanoparticles within the base material matrix. This phenomenon occurs due to Van der Waals interactions, poor powder bed mixing, weak thermal convection in the melt pool, and rapid solidification. The inability to achieve uniform dispersion results in inhomogeneous material properties, which leads to reduce effectiveness of graphene reinforcement.

As a consequence, agglomeration negatively impacts the mechanical performance, thermal stability, and overall structural integrity of the printed composite. The presence of graphene clusters creates stress concentration points, which significantly reduce tensile strength and fatigue resistance, making the material more susceptible to premature failure under mechanical loads. Additionally, poor dispersion leads to inefficient heat dissipation, increasing residual stresses and thermal distortions within the printed part. Structurally, non-uniform reinforcement causes weak zones, compromising the load-bearing capacity of the component. These defects highlight the necessity of optimizing process parameters, particularly laser power, to regulate graphene dispersion and prevent clustering.

To mitigate these issues and ensure uniform dispersion, MMSM serve as an essential cost-effective predictive tool before experimental fabrication. Studies have demonstrated that Ansys Additive Print is the most robust MMSM environment for Ti-6Al-4V SLM process. This simulation tool is to be used to determine the optimal laser power parameters to achieve uniform dispersion to mitigate the need for extensive experimental trials. The following section described the methodology adopted to achieve the aim of this study.

3 Methods

3.1 Research Approach

This research employs a hybrid approach, integrating both computational simulations and experimental validation to analyze agglomeration in the Ti-6Al-4V + Graphene SLM process. The first step involves defining the Agglomeration Factor (AF) variables, as represented in Equation 1. Next, a simulation model is developed and executed in Ansys, using predefined SLM process parameters. The third step involves fabricating physical specimens via SLM using the predefined process parameters used in the simulation model. Following fabrication, the specimens undergo microstructural characterization, where dispersion is analyzed using Scanning Electron Microscopy (SEM). Finally, a comparative analysis is conducted between simulation predictions and experimental results, assessing the any discrepancies between the two approaches. Figure 5 provides a comprehensive overview of the research workflow.

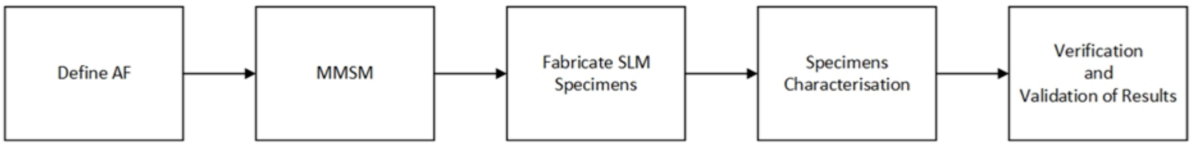

Figure 5. Research Approach Process Flow

3.2 Materials and Sample Preparation

This section outlines the base material, namely, Ti-6Al-4V and the nanoparticles, namely, graphene. Specifications of the Ti-6Al-4V powder used in this study are presented in Table 2.

Table 2. Specifications of Ti-6Al-4V Powder

Property	**Specification**
Powder Morphology	Spherical
Production Method	Plasma-atomized or Gas-atomized
Particle Size Distribution	30 µm
Chemical Composition	Ti (90 wt.%), Al (6 Wt.%), V (4 Wt.%)
Oxygen & Nitrogen Content	≤ 0.13 wt.% O, ≤ 0.03 wt.% N

Graphene serves as the reinforcement phase to enhance the Ti-6Al-4V matrix. The specifications of the Graphene used in this study are presented in Table 3.

Table 3. Specifications of Graphene Nanoparticles (GNPs)

Property	**Specification**
Type	Few-Layered Graphene (FLG)
Lateral Size	~ 500 nm
Thickness	~ 5 nm

3.3 SLM Process and Parameters

This section outlines the SLM equipment, process parameters, and the method for quantifying the Agglomeration Factor (AF), in both simulated and fabricated samples, used in this study.

3.3.1 SLM Equipment

The SLM system used in this study is the EOS M 290. Specifications of the EOS M 290 SLM Printer are presented in Table 4.

Table 4. Printer Parameters

Parameter	Values
Laser Source	Ytterbium Fiber Laser
Laser Power	400 W
Spot Size	~100 µm
Scan Speed	Up to 7.0 m/s
Build Volume	250 × 250 × 325 mm
Layer Thickness	20–40 µm
Atmosphere Control	Argon/Nitrogen for oxidation prevention

3.3.2 SLM Process Parameters

To assess graphene dispersion and minimise agglomeration in the base material, the following SLM process parameters, as presented in table 5, are used:

Table 5. SLM Process Parameters for Ti-6Al-4V + Graphene Printing

Process Parameters	Unit	Specimen 5	Specimen 4	Specimen 3	Specimen 2	Specimen 1
Laser Power	W	200	250	300	350	400
Scanning Speed	mm/s	700	700	700	700	700
Laser Spot Diameter	µm	80	80	80	80	80
Hatch Distance	mm	0.1	0.1	0.1	0.1	0.1
Heat Transfer Coefficient	$W/(m^2.K)$	20	20	20	20	20
Dynamic Velocity	Pa.s	0.002	0.002	0.002	0.002	0.002
Melting laten heat	$J.kg^{-1}$	3.7×10^5	3.7×10^5	3.7×10^5	3.7×10^5	3.7×10^5
Layer Thickness	µm	30	30	30	30	30
Initial Baseplate Temperature	ºC	200	200	200	200	200
Specimen Dimensions	mm	35 x 15 x 2 (L x W x H)				

The laser power is set at a minimum of 200 W to maintain a high energy density in each run to completely melt the powder ($x > 74$ J/mm^3) (Wang et al. 2018). This is to ensure fully formed specimens per run.

3.4 MMSM Workflow

MMSM is used in this study to predict the optimal laser power parameter at which Ti-6Al-4V + Graphene composites achieve uniform dispersion or minimum agglomeration. Table 6 describes the simulation modelling workflow.

Table 6. MMSM Workflow

Phase 1: Melt Pool Simulation	Phase 2: Graphene Dispersion Simulation
Tool: Ansys Additive Print 2023 R1	**Tool:** Ansys Fluent 2023 R1 (Support tool)
Inputs: ● Geometry: SolidWorks-developed specimen ● Matrix: Ti-6Al-4V ● Reinforcement: Graphene (0.4 wt.%) ● Process parameters: As per Table 5	**Inputs:** ● Temperature field ● Melt pool dynamic
Process: End-to-end SLM process simulation. The model is run 100 times for each specimen.	**Process:** Modelling particle motion via Discrete Phase Model (DPM) and applying User-Defined Function (UDF) for agglomeration (Eq. 1)
Outputs: ● Melt pool dynamic ● Time-dependent temperature field	**Outputs:** ● Agglomeration Factor (AF) data

3.5 Assumptions

The following assumptions were made during the study:

a. Pre-mixed Ti-6Al-4V + Graphene Powder Composition – See Table 7
- The research team did not participate in the powder mixing process.
- It is assumed that the graphene reinforcement was homogeneously distributed in the powder prior to the SLM.
- Any inconsistencies in graphene dispersion in the initial powder state are beyond the control of this study.

Table 7. Specifications of Ti-6Al-4V + Graphene Composite

Property	**Specification**
Graphene Content	0.4 wt.% GNPs
Powder Mixing Method	Ball Milling

b. Consistency in SLM Processing Conditions
- The SLM machine (EOS M 290) operated under stable environmental conditions, ensuring that laser power, scan speed, and other parameters remained constant throughout fabrication.
- It is assumed that no external disturbances (i.e., oxygen contamination, unexpected recoater blade deviations) influenced the powder bed.

c. Simulation Model Validity
- The computational model does not account for potential deviations in actual powder morphology, assuming that Ti-6Al-4V and graphene interact as idealized particles.

d. Graphene cluster size
- For this study a graphene cluster is characterized by a radius (r_c) equals or longer than 5 micrometers ($r_c \leq 5\ \mu m$) (Wang et al. 2023).

4 Data Collection and Analysis

As previously mentioned, the AF quantifies the degree of graphene clustering in both simulated and physical SLM-printed specimens.

4.1 AF Quantification in Simulated Samples (MMSM)

As outlined in Table 6, the simulated AF data were obtained in two phases. In Phase One, melt pool dynamics and time-dependent temperature fields were extracted from Ansys Additive Print. These outputs were then used as inputs in Ansys Fluent during phase two to quantify the AF for each simulation run. Table 8 describes the analysis process of simulated data.

Table 8. Simulated AF Quantification

Function	**DPM (Discrete Phase Model)**	**UDF (User-Define Function)**
Collecting particle motion data	Tracks graphene movement in melt pool	Encodes physics interactions
Analyzing clustering behavior	-	Maps agglomeration
Quantifying AF	Records particle positions	Compute Equation 1 in real time

4.2 AF Quantification in SLM Specimens

For printed specimens, the AF is experimentally determined using image processing techniques applied to SEM data. Table 9 present the steps involves in collecting and analyzing experimental data.

Table 9. Experimental data collection and analysis workflow

Phase 1: Microstructure Data Collection	**Phase 2: Image Segmentation and Cluster Identification**	**Phase 3: Quantification of AF**
Tool: SEM - Hitachi TM4000 Plus	**Tool:** ImageJ (Fiji)	**Tool:** MATLAB
Inputs: ● Printed Specimens: S1-5 ● Imaging parameters: 1000× magnification	**Inputs:** ● SEM images ● Cluster size criterion	**Inputs:** ● Cluster regions ● Equation 1
Process: Graphene distribution imaging	**Process:** ● Grayscale thresholding ● Segment and label regions based on pixel intensity and area (red dots in Fig. 12)	**Process:** Quantify AF for each specimen
Outputs: ● SEM images	**Outputs:** ● Clustered regions	**Outputs:** ● Statistical summary

4.3 Statistical Analysis and Validation

Statistical methods are used to evaluate AF and assess the reliability of the simulated results.

a. Descriptive Statistics:
- Mean and standard deviation (σ) of simulated AF values is computed to assess data consistency.
- A 95% confidence interval is used to determine the range of expected simulated AF values for the impact of laser power variation on dispersion for both.

b. Error Analysis:
- Root Mean Square Error (RMSE) is used to quantify the difference between simulated and experimental AF values:

$$RMSE = \left(\sqrt{\frac{1}{n}\sum_{i=1}^{n} \quad (y_i - \hat{y}_i)^2}\right)\%\#(4)$$

Where;
- y_i: Experimental AF value
- $\hat{y}_i$: Simulated AF value
- n: Number of observations

Results and Discussion

4.4 Results

The findings are derived from both computational simulations using MMSM and experimental microstructural analysis using SEM. The objectives of this section are to quantify the AF in simulated and experimentally printed samples, to determine the optimal laser power parameters, and validate the predictive capability of the simulation model.

4.4.1 Simulation Results from MMSM

Following the simulation process, it has been observed an inverse correlation between graphene dispersion and laser power. Figures 6 – 10 describe the patterns uncovered from the simulated data. From Figure 6, AF of the specimens simulated at 200 W ranges from 0.283 to 0.455, with a mean value of 0.368 and a standard deviation of 0.023. The distribution indicates a relatively low variability, as the AF values are tightly clustered around the mean.

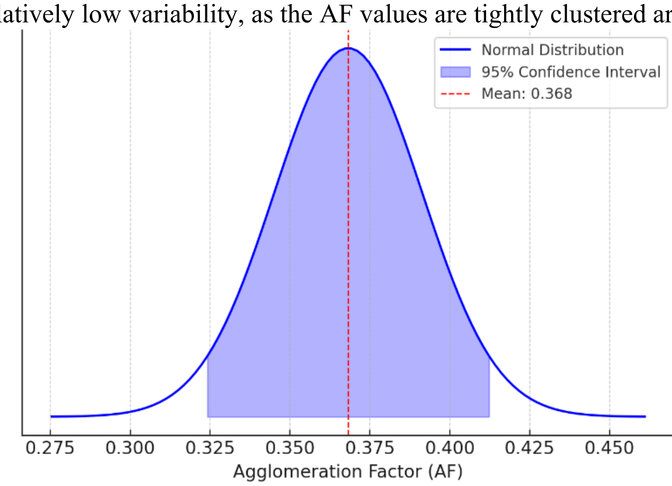

Figure 6. AF output data at 200 W

From Figure 7, AF of the specimens simulated at 250 W ranges from 0.170 to 0.322, with a mean value of 0.246 and a standard deviation of 0.019. The distribution indicates a relatively low variability, as the AF values are tightly clustered around the mean.

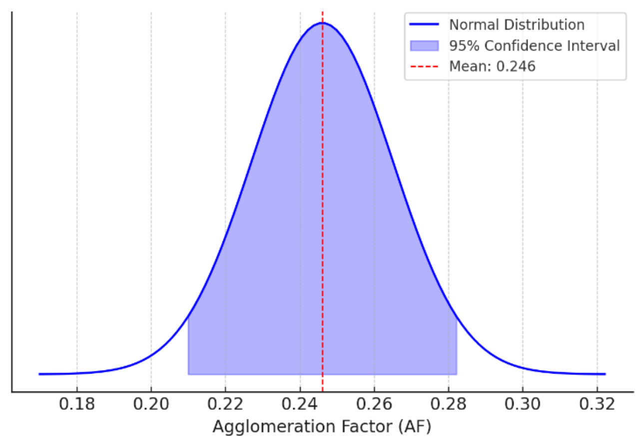

Figure 7. AF output data at 250 W

From Figure 8, AF of the specimens simulated at 300 W ranges from 0.118 to 0.252, with a mean value of 0.168 and a standard deviation of 0.016. The distribution indicates a relatively low variability, as the AF values are tightly clustered around the mean.

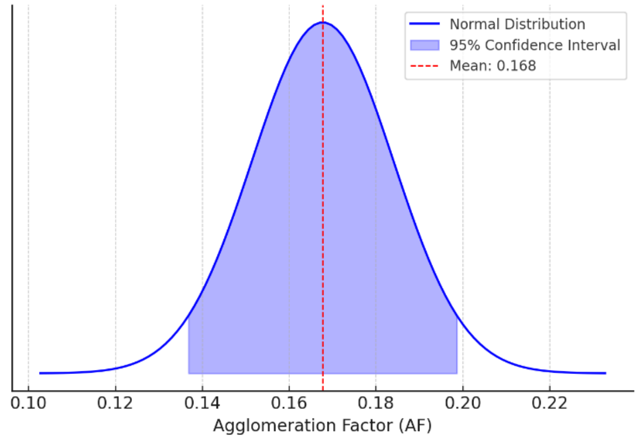

Figure 8. AF output data at 300 W

From Figure 9, AF of the specimens simulated at 350 W ranges from 0.043 to 0.163, with a mean value of 0.103 and a standard deviation of 0.014. The distribution indicates a relatively low variability, as the AF values are tightly clustered around the mean.

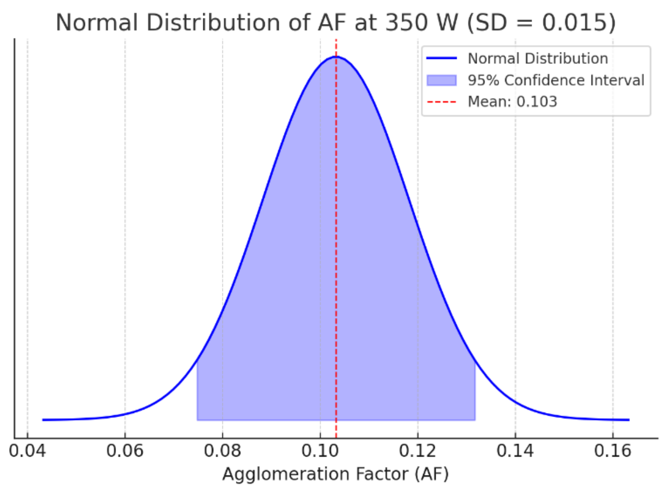

Figure 9. AF output data at 350 W

From Figure 10, AF of the specimens simulated at 400 W ranges from 0.026 to 0.122, with a mean value of 0.074 and a standard deviation of 0.012. The distribution indicates a relatively low variability, as the AF values are tightly clustered around the mean.

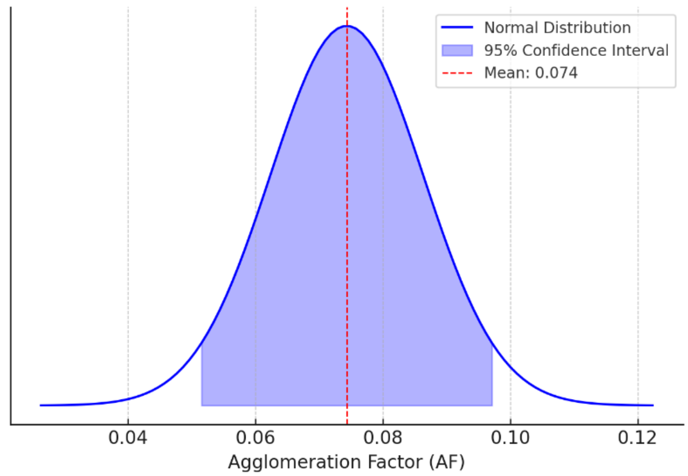

Figure 10. AF output data at 350 W

4.4.2 Experimental Results from SEM Microstructural Analysis

Following the fabrication process, the correlation between graphene dispersion and laser power was also observed. From Figure 11, it is evident that the Specimen 5 which was fabricated using the lowest laser power 200 W demonstrated the most clusters ($x > 5$ µm).

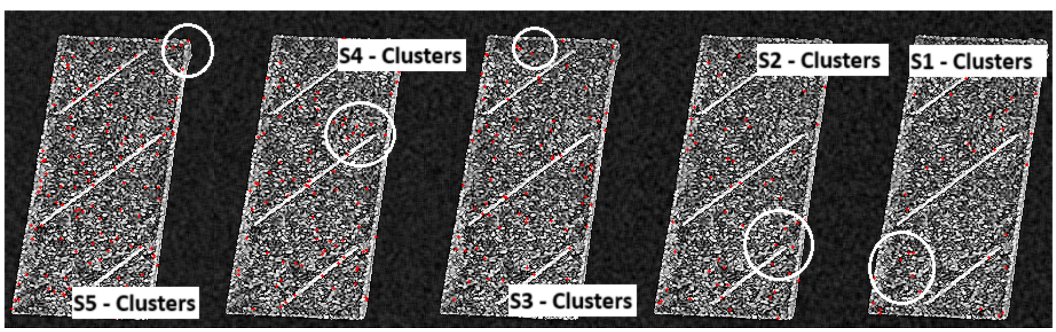

Figure 11. Graphene Clusters in Printed Specimens (Phase 2)

From Figure 12, it is observed that Specimen 5 exhibits the highest graphene cluster rate at 0.437, followed by Specimen 4 at 0.329, and Specimen 3 at 0.215. In contrast, Specimens 2 and 1 achieved the lowest clustering rates of 0.082 and 0.029, respectively. This trend was also observed in the simulation data.

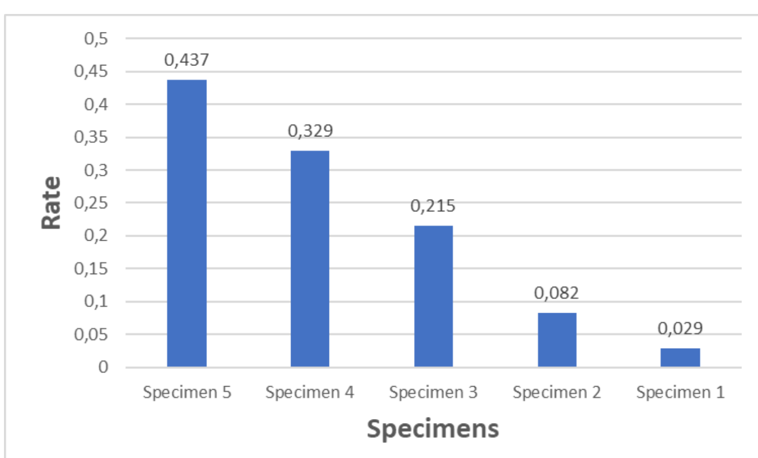

Figure 12. Clustered Graphene Rate

4.5 Validation

Although, a similar trend was observed in both experimental and simulation data with respect to the correlation of graphene dispersion and laser power. It is evident, as presented in Figure 13, that the simulation model does not accurately predict the physical outcome. The calculation of the RMSE shows that the simulated data deviates from the experimental results by 5.71%.

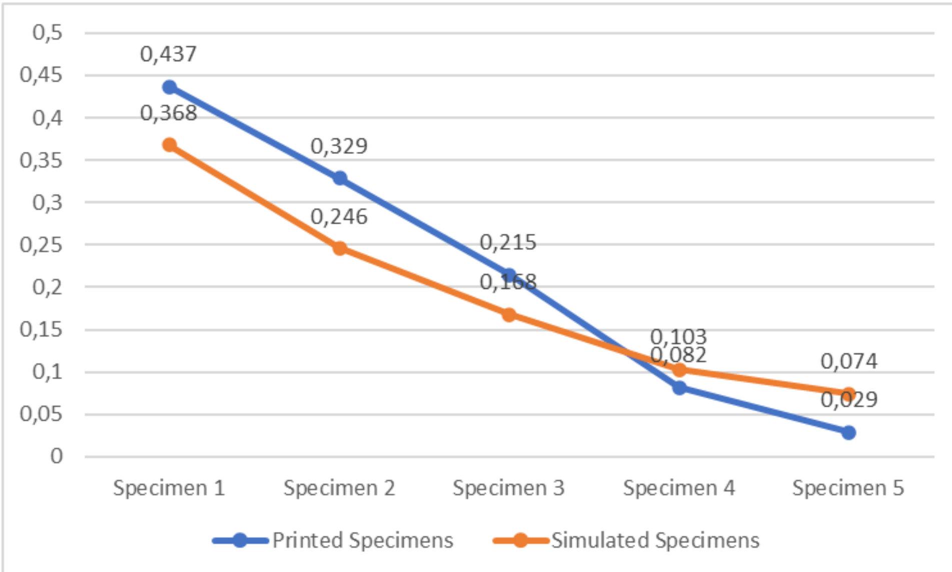

Figure 13. Comparison of Experimental and Simulation Trend

4.6 Discussion

The analysis of the simulated AF across pre-defined laser power levels (200 W to 400 W) reveals a clear trend of decreasing AF values and variability as power increases. At 200 W, AF exhibits the widest range (0.283 to 0.455) and the highest mean value (0.368, SD = 0.023), indicating significant graphene clustering. As power increases to 250 W, 300 W, and 350 W, the AF values progressively decline with reduced standard deviations, suggesting improved graphene dispersion. The narrowest range (0.026 to 0.122) and lowest mean AF (0.074, SD = 0.012) occur at 400 W, which demonstrates minimal agglomeration and a more homogeneous graphene distribution. This trend highlights the strong inverse correlation between laser power and AF, which reinforces the effectiveness of higher power levels in enhancing nanomaterial dispersion within the melt pool. According to the AF hypothesis, minimal AF was achieved in all simulated specimens since the highest recorded AF value is 0.368 at 200 W, which remains within the acceptable threshold ($x > 0$). This suggests that graphene dispersion is well-regulated under the simulated process conditions.

In the experimentation phase, it was observed that specimens 5 - 3, which were fabricated at using laser powers 200, 250, and 300 W, respectively, have presented the highest degree of graphene clustering (S5 = 0.437, S4 = 0.329, S3 = 0.215). This suggests that low laser power leads to inadequate melting and mixing of the graphene within the Ti-6Al-4V matrix, resulting in graphene clustering. Conversely, Specimens 2 - 1, which were fabricated using laser powers of 350, and 400 W, respectively, have presented the lowest degree of graphene clustering (S2 = 0.082, S1 = 0.029). These findings reinforce the premises presented in the literature which note that higher laser power enhances graphene dispersion by promoting stronger melt pool dynamics and reducing van der Waals-driven agglomeration in the base material. According to the AF hypothesis, minimal AF was achieved in all fabricated specimens since the highest recorded AF value is 0.437 at 200 W, which remains within the acceptable threshold ($x > 0$). This suggests that graphene dispersion is also well-regulated under the experimental process conditions.
Nevertheless, based on the validation results, it was observed that the MMSM did not accurately predict the physical process outcomes. A deviation of 5.71% was observed from the model. This indicates that both the input process parameters and the simulation environment require further optimization to enhance the model's predictive accuracy in real-world applications. Despite the fact that the MMSM replicated a similar trend observed in the experimental data.

5 Conclusion

This study investigated the impact of laser power on graphene dispersion in Ti-6Al-4V + Graphene composites fabricated via SLM. A key focus was the development and application of the AF to quantify graphene clustering to determine the optimal laser power parameters to achieve a uniform dispersion within the base material matrix. The research used a MMSM to determine the optimal laser power parameters prior to validating these findings through experimental fabrication and SEM analysis.
All research objectives were successfully addressed. An Agglomeration Factor (AF) was developed which enabled a quantitative assessment of graphene clustering. Through MMSM, the optimal SLM process parameters were identified. Specimens were fabricated through SLM and graphene dispersion was characterized through SEM. Lastly, a comparison of simulated and experimental data was conducted to validate the reliability of the MSMM.

The results demonstrate an inverse correlation between laser power and graphene dispersion in both simulation and experimentation. Specimens fabricated at lower laser power (200–300 W) presented the highest AF values and prominent clustering, while higher power settings (350–400 W) showed enhanced graphene dispersion. The lowest clustering rate was observed in the specimens SMLed at 400 W, which emphasises that increased energy input enhances melt pool dynamics and reduces van der Waals-driven agglomeration. However, a comparison between simulation and experimental results revealed a deviation of 5.71% from the simulation model, which indicates that while MMSM provides valuable predictive insights, the model and the tool be enhanced to achieve optimal accuracy. As demonstrated in this study, achieving uniform graphene dispersion in SLM-fabricated Ti-6Al-4V composites is highly dependent on laser power regulation. Higher energy input effectively mitigates agglomeration, which enhances material integrity and mechanical performance. This research provides a framework for optimising nanocomposite printing processes and paves the way for advancements in the industry.

5.1 Limitations

Despite the comprehensive nature of this study, certain limitations persist:

a. Microstructural analysis as the sole characterization Method:
   - The study is limited to SEM for microstructure analysis.
   - No mechanical testing, thermal or electrical property evaluations were conducted.

b. No powder characterization before SLM processing:
   - The study does not include pre-SLM powder characterization.
   - It is assumed that graphene dispersion in the starting powder is adequate, although pre-existing agglomeration could affect final results.

c. Absence of large-scale experimentation
   - Due to cost limitations, only 5 specimens were fabricated for the experimental phase.

5.2 Future Studies

While this study has provided critical insights into the interaction between laser power and graphene dispersion in Ti-6Al-4V + Graphene composites in SLM process, several areas of this study may require further investigations to enhance the accuracy, applicability, and industrial relevance of these findings. Future research should focus on the following areas:

a. Expanding process parameter optimization
   - This study focused primarily on laser power; however, other SLM parameters such as scan speed, hatch spacing, powder bed temperature, and layer thickness significantly influence graphene dispersion.
   - Future studies should investigate the combined effects of multiple parameters to establish a more comprehensive process-property relationship for optimizing additive manufacturing conditions.

b. Mechanical and functional property evaluation
   - While microstructural analysis provided insights into graphene dispersion; mechanical properties and functional properties were not directly assessed.
   - Future work should incorporate tensile, fatigue, and wear testing to quantify how dispersion quality affects material performance in real-world applications.

c. Refinement of the MMSM
   - The simulation results deviated from experimental findings with a RMSE of 5.71%, indicating room for improvement for the model and tool.

d. Investigation of powder characteristics and Pre-mixing effects
   - This study assumed a homogeneous graphene distribution in the initial powder mixture
   - Future work should explore powder characterization techniques to assess their influence on final composite properties.

e. Alternative Graphene Integration Techniques
   - Current SLM methods rely on graphene reinforcement within the powder mixture, but alternative integration strategies such as in-situ graphene deposition, functionalized graphene coatings, or hybrid reinforcement may offer better dispersion control.
   - Future studies should explore novel approaches for incorporating graphene into the Ti-6Al-4V matrix to minimize clustering and maximize mechanical enhancements.

f. Industry-level scalability and cost-benefit analysis
   - Future studies should address economic considerations, including production costs, material availability, and process efficiency, to assess whether this technology can be commercially viable for widespread industrial adoption.

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