Smart Formulation of cBN (Cubic Boron Nitrite) Slurry for Insert Fabrication: A Bayesian Optimization Approach in Vat Photopolymerization

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Abstract: ***Vat photo polymerization (VPP) is a high-precision additive manufacturing technique for producing complex ceramic components. It requires a high ceramic content to reduce shrinkage and improve mechanical integrity, but also raises the slurry's viscosity, compromising printability. Traditional trial-and-error methods are time-consuming and costly, especially for high-value materials like cubic boron nitride (cBN). Bayesian optimization, an AI-driven technique, was used to guide experimental formulation, resulting in a VPP-suitable cBN slurry with 69 vol. % ceramic content in fewer than 40 iterations. This demonstrates how integrating AI with materials development can accelerate optimization, reduce waste, and advance high-performance ceramics in additive manufacturing.***

Keywords: Additive Manufacturing, Vat Photopolymerization (VPP), Cubic Boron Nitride(cBN), Ceramic Slurry Formulation, Bayesian Optimization, High Solid Loading, Slurry Viscosity Control, AI-Driven Materials Design

1. Introduction

a) Vat Photopolymerization of ceramics: an advanced additive manufacturing technique

Vat Photopolymerization (VPP) is a promising ceramic additive manufacturing (AM) technique that offers exceptional precision, fine feature resolution, and excellent surface finish. VPP uses a ceramic slurry, consisting of high-loading ceramic powder suspended in a photosensitive organic binder system, to fabricate ceramic components layer by layer. Common ceramic powders include aluminum oxide and zirconium oxide. VPP can produce sintered ceramics with densities exceeding 99%, resulting in parts with near-theoretical density and outstanding mechanical integrity. The process is selectively cured using ultraviolet or visible light, using point-based systems and area-based systems for faster, high-resolution printing. VPP is an advanced and scalable technology with unmatched control over dimensional accuracy, micro structural quality, and surface finish.

b) Ceramic slurries for vat Photopolymerization

Vat Photopolymerization (VPP) in ceramics involves a binder system with monomers, photo initiators, co-initiators, and additives. Radical polymerization is the most common method due to its fast curing characteristics. The formulation of the ceramic slurry affects printing process and final part quality. High solid content improves dimensional accuracy and density, while higher viscosity can hinder recoating. Griffith's foundational model considers refractive index difference and inter particle spacing, affecting printed layers' resolution and stability.

c) *Bayesian optimization in ceramic slurry design*

Ceramic slurries in vat Photopolymerization are complex due to their multiple components and compositional constraints. Traditional DoE approaches are time-consuming and resource-intensive, leading to the "curse of dimensionality." Bayesian Optimization, a sequential, model-based technique, has emerged as a powerful alternative for optimizing complex systems with limited experimental budgets. It works by building a surrogate model, typically a Gaussian Process Regression (GPR) model, and using an acquisition function to identify the next set of parameters. This AI-driven approach has been widely applied in materials acceleration platforms and automated laboratories for tasks like optimizing chemical synthesis conditions and real-time process parameters.

d) Research target: Optimization and design of cBN inserts via vat Photopolymerization

This research aims to optimize Cubic Boron Nitride (cBN) inserts using Vat Photopolymerization (VPP), an advanced additive manufacturing technique for high-precision ceramic components. To reduce defects and ensure structural integrity, increasing cBN content in the photopolymer slurry is essential. Bayesian Optimization is employed to explore and optimize the slurry formulation, focusing on maximizing solid content, maintaining viscosity, and minimizing curing width-to-depth ratio. The binder system is based on previous formulations, ensuring reliability and reproducibility. This research contributes to the design of high-performance cBN inserts and advances VPP's application in fabricating complex ceramic tools with precise geometry and superior functional properties.

2. Foundational Concepts

1) Vat Photopolymerization (vpp).

Vat Photopolymerization's remarkable resolution and surface quality are among its main benefits. Because the technology can create layers as thin as 25–100 microns, smooth surfaces can be achieved with little post-processing. This is especially helpful for applications where accuracy and beauty are essential, like dental prosthetics, jewelry, hearing aids, microfluidics, and biomedical devices. VPP parts frequently come out of the printer almost ready to use, in contrast to techniques like FDM that may leave noticeable layer lines and require extensive finishing. This drastically cuts down on post-processing expenses and time. Vat

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Photopolymerization is also becoming more popular in terms of material versatility. Advances in resin chemistry have produced durable, flexible, and even ceramic-filled VPP, whereas traditional VPP was restricted to brittle photopolymers.

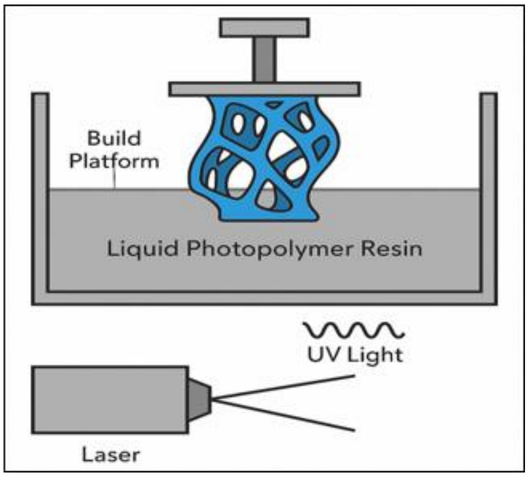

Figure 1: Vat Photopolymerization (VPP).

2) Prerequisites for successful vat Photopolymerization.

a) Slurry of photopolymer resin
- Materials that are photosensitive (monomers or oligomers) and cure when exposed to visible or ultraviolet light.
- Additives: metal or ceramic fillers (for functional parts), stabilizers, dyes, rheology modifiers, and photo-initiators.
- Viscosity control: Depending on the system, the resin's viscosity must be appropriate for recoating, usually 0.5 to 3 Pa•s.

b) Light Source:
- UV laser or projector, usually with a wavelength of 355 nm or 405 nm.
- Consistent high energy dose for appropriate curing depth and resolution.

c) Vat or Resin Tank:
- For bottom-up systems, the bottom is composed of a UV-transparent substance, such as FEP film.
- May be heated or stirred to preserve resin flow and homogeneity; designed to minimize resin waste and stop leaks.

d) Create a platform that is mechanically

3) Bayesian Optimization

The best solution to complicated problems where evaluating the objective function is expensive, time-consuming, or lacks a clear mathematical form can be found using Bayesian Optimization, an intelligent, data-efficient optimization technique. It creates a probabilistic model, usually a Gaussian Process, that forecasts the result of various input values rather than thoroughly testing every potential input. It uses an acquisition function to choose the most promising input for further evaluation based on these predictions and related uncertainties. This enables it to strike a balance between investigating uncharted territory and taking advantage of established positive outcomes. In domains where experimental trials are costly or scarce, such as machine learning, materials science, and additive manufacturing, Bayesian optimization is particularly useful. Bayesian optimization is preferred over conventional techniques due to its effectiveness and data efficiency.

3. Experimental Composition and Curing Agents

The effect of particle size distribution on the rheological and curing characteristics of ceramic-loaded slurries in vat Photopolymerization (VPP) is examined in this work. Because of its optical qualities, chemical inertness, and thermal stability, boron nitride (cBN) was selected. The study investigated the effects of varying particle size on the viscosity, dispersion stability, and overall curing efficiency of BN powders with three distinct median particle sizes (0.05 µm, 0.5 µm, and 3 µm). Additionally evaluated was the binder system, which included the ceramic filler. The formulation included three distinct acrylate-based monomers, which had an impact on the reactivity and cross linking density during Photopolymerization. Trimethylolpropane ethoxylate triacrylate (TEMPTA) and 1, 6-hexanediol diacrylate (HDDA) were utilized to boost crosslinking density and reactivity, while isobornyl acrylate (IBOA) was selected due to its low viscosity.

Table 1: Material Properties Table

Name	Abbreviation	Density (g/cm^3)	Molar Mass (g/mol)	Refractive Index
Boron Nitride	cBN	5.8	310.43	2.1
Isobornyl Acrylate	IBOA	0.99	208.3	1.48
1,6-Hexanediol Diacrylate	HDDA	1.02	226.3	1.46
Trimethylolpropane Ethoxylate Triacrylate	TEMPTA	1.11	428.0	1.471
Camphorquinone	CQ	0.98	166.2	-
4-(Dimethylamino)-benzonitrile	-	1.33	146.2	-
1-Octanol	-	0.83	130.2	1.43
Disperbyk	-	1.16	-	-

Successful printing of green parts depends on the flow and stability of the slurry, which should have a target viscosity of 0.5-5 Pa.s, a thixotropy of 0-2 Pa.s, and sedimentation resistance, especially with high-density particles like cBN.

To ensure accurate Photopolymerization, the slurry system must match the printer wavelength, have a controlled reactivity, and be well-dispersed to avoid agglomeration. The slurry system must also be compatible with VPP hardware, such as the Lithoz CeraFab 2M30 printer, LED or laser light source, re coater, and build platform heating. Parameters for the process include layer thickness, exposure time, and print speed. Post-processing requirements include cleaning, debinding, sintering, and shrinkage compensation. These parameters help to optimize the process and ensure the correct materials are used for successful printing. The slurry system must also be compatible with VPP hardware, such as the printer, light source, re coater, and build platform heating.

Table II: VPP Requirements Table

Aspect	Requirement
Viscosity Control	Optimized with 1-Octanol and Disperbyk
Photopolymerization	CQ+ co initiator matched with 460nm light source
Refractive Index	Match between resin (IBOA, HDDA, TEMPTA) and ceramic (cBN) for light penetration
Rheology Additives	Disperbyk ensures flow and dispersion
Printer Suitability	High- Viscosity handling, blue light source, fine resolution system

4) *Python Implementation of Bayesian Optimization*

A Python-based Bayesian Optimization framework has been developed to achieve a target viscosity of 1 Pa•s for cubic boron nitride (cBN) slurry in Vat Photopolymerization (VPP). The framework uses a binder system with three monomers and a photo initiator, Camphorquinone (CQ), and 1-Octanol to reduce initial viscosity. The Python environment is prepared, and essential libraries like numpy are installed. The surrogate model is defined as a proxy for experimental measurements, and the objective function is defined to maximize the deviation from the desired viscosity. The Bayesian Optimization process is initiated by defining parameter bounds, and the optimizer iteratively proposes new combinations based on expected improvement strategies. The resulting code provides a data-driven tool for efficient material design and reduces the time and cost of manual experimentation, accelerating the development of optimized slurries for advanced ceramic 3D printing via Vat Photopolymerization.

A. *Assumptions*

- The proportions of the constituents determine viscosity.
- Gaussian Process will serve as the stand-in model.
- The ratios of isobornyl acrylate (IBOA), 1,6-hexanediol diacrylate (HDDA), trimethylolpropane ethoxylate triacrylate (TMPTA), camphorquinone (CQ), 4-(Dimethylamino)benzonitrile (DMABN), iso-octanol, and disperbyk will all be optimized.

B. *Mathematical formulation*

Let: $x = [x_1, x_2... x_7]$, where, x_i is the weight percentage of the ith component from the list: IBA, HDDA, TTA, CQ, DMB, IO, DBYK. Let cBN fixed = 69%. Then the constraint is: $\sum x_i = 31$ Define the viscosity estimation function f(x) as:

$f(x) = (\frac{1}{\sum x_i}) * \sum x_i * (0.4 * \rho_i + 0.6 * n_i)]$ where ρ_i is the density and n_i is the refractive index of component i

The objective function to minimize is:

$L(x) = |f(x) - 1.0|$

If $\sum x_i > 31$, then $L(x) = 10$ (penalty).

The optimization is performed using Gaussian Process Regression (GPR) to model the objective function. The Expected Improvement (EI) acquisition function is used to balance exploration and exploitation in the optimization space. The optimizer iteratively samples new points in the 7-dimensional space of component percentages until a composition that minimizes |f(x) - 1.0| is found.

C. *Python* script *for Bayesian optimization*

In order to reach a target viscosity of 1 Pa.s, this complete Python script employs Bayesian optimization to modify the proportions of eight components in a vat Photopolymerization system, with boron nitride set at 69%.

Creating a Python script for Bayesian optimization entails fusing effective search techniques with statistical modeling to maximize complex functions, particularly in cases where evaluations are expensive or time-consuming. Usually, the process starts with defining the objective function you want to maximize or minimize, such as the viscosity of a ceramic slurry or the error of a machine learning model. The search space for the input parameters—which may consist of continuous, integer, or categorical variables—is then specified. Python libraries like bayes_opt, GPyOpt, and scikit-optimize (skopt) offer strong tools for putting this workflow into practice.

Gaussian Processes are a popular method for modeling the unknown function. The script fits a probabilistic surrogate model that forecasts the behavior of the function across the parameter space after initializing with a set of observed samples.

D. *Implementation of Python Script*

Optimal Composition (%):

IBA: 5.23%	HDDA: 4.31%	TTA: 5.98%
CQ: 0.77%	DMB: 0.60%	IO: 6.41%
DBYK: 7.70%	Boron Nitride: 69.00%	

The Bayesian Optimization script's output is an optimized mix of a slurry formulation that will be used in vat Photopolymerization (VPP) with the goal of getting the viscosity as close to 1 Pa.s as possible. This viscosity target is very important for making sure that the flow behaves correctly, that the layers are recoated, and that the light gets through during the VPP method of additive manufacturing. The optimization was done with a fixed ceramic loading of 69% cubic boron nitride (cBN) by weight, which is a common filler concentration for high-performance ceramic parts. The other 31% of the formulation was made up of different liquid phase components, such as monomers, photo initiators, additives, and dispersing agents. The algorithm figured out the best amounts of the other seven parts: isobornyl acrylate (IBA), 1,6-hexanediol diacrylate (HDDA), and trimethylolpropane ethoxylate triacrylate

4. Results and Discussion

Plotting the viscosity values of various slurry formulations over a series of Bayesian optimization iterations. As iterations increase, the graph shows a decreasing trend in the difference between the measured viscosity and the target viscosity (1 Pa.s). This indicates that within 20–25 evaluations, Bayesian Optimization successfully reduced the search space and found promising formulations. The optimal formulation closely matched the target viscosity of 1.02 Pa.s.

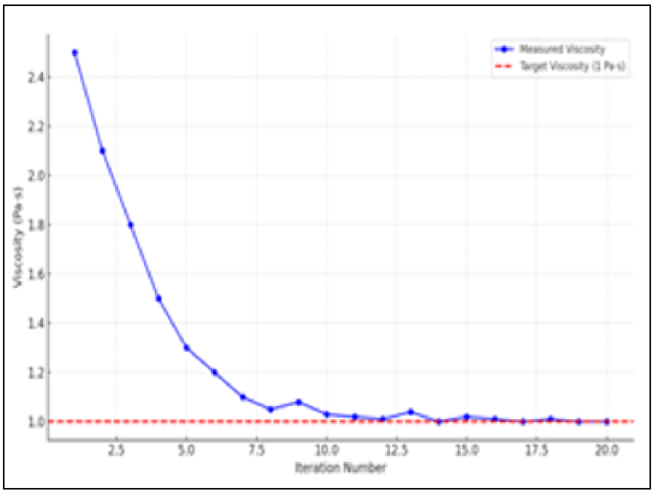

Figure 2: Viscosity vs. iteration number

When the concentrations of HDDA (cross linker), IBOA (low viscosity monomer), and dispersant are balanced, the viscosity is at its lowest. While a high IBOA content reduced viscosity, mechanical strength was compromised by a lack of HDDA. Even at lower monomer ratios, dispersants such as DISPERBYK-180 dramatically decreased viscosity, demonstrating their function in enhancing flow and dispersion.

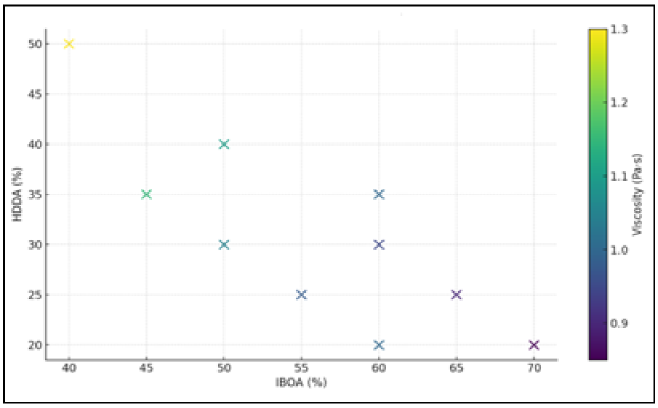

Figure 3: Viscosity VS Monomer composition (IBOA vs HDDA)

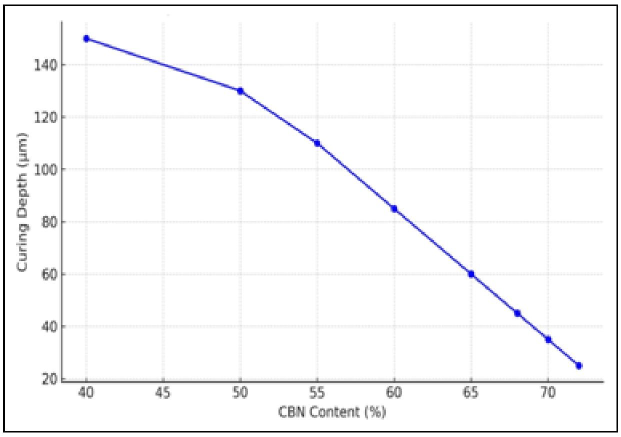

Figure 4: Curing depth vs. cBN Content

The depth of UV curing drastically drops with increasing CBN content because of increased light scattering. The trade-off between attaining a high ceramic content and adequate cure depth is highlighted in the graph. This requires long exposure times and restricts layer thickness. UV-transparent binders or surface-modified CBN are examples of potential future advancements.

5. Conclusion

With a focus on boron nitride (cBN)-based composites, this work shows how to optimize ceramic slurry formulations for Vat Photopolymerization (VPP) in a methodical and data-driven manner. The study investigated the effects of different monomers, cross linkers, and dispersing agents on the viscosity and curing behavior of the slurry system by setting the solid loading of cBN at 69 weight percent, an ideal balance for achieve functional ceramic load while maintaining process ability. By effectively exploring the formulation space, Bayesian Optimization (BO) was incorporated. This resulted in a significant reduction in the number of experimental iterations required to achieve the target viscosity of 1 Pa.s, which is crucial for layer uniformity and print resolution in the VPP process. Non-linear interactions between chemical components were taken into consideration by the model-driven approach, which provided a clever framework for creating high-performance.

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