

A Multi-Scale AI-Driven Optimization Framework for Industrial Product Design

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Abstract: Metal Additive Manufacturing (AM) has emerged as a crucial technology for fabricating high-performance, lightweight components for aerospace, biomedical, and energy applications. However, consistent part quality remains one of the most significant challenges because complex nonlinear interactions between material properties, process parameters, thermal histories, and defect formation mechanisms control this process. Traditional modeling approaches usually treat the scales individually, thus poorly predicting key outcomes such as porosity, melt pool morphology, and mechanical performance. In this work, a physics-aware, multi-scale Artificial Intelligence (AI)-driven optimization framework is proposed that unifies material level attributes, process settings, thermal/in-situ responses, and final mechanical properties into a single predictive pipeline. To model realistic AM behavior, a synthetic, physics-informed dataset is generated to represent the Laser Powder Bed Fusion (LPBF), Electron Beam Melting (EBM), and Directed Energy Deposition (DED) processes. Multi-level surrogate models are proposed for predictions of melt-pool width, peak temperature, porosity, and tensile properties. Defect classification models are used to predict builds with porosity exceeding a 2.5% threshold. Sensitivity analysis, feature attribution, and energy-density sweeping are conducted to identify critical cross-scale interactions and the optimal process window. The framework demonstrates the overall importance of energy density and in-situ thermal properties to defect formation and mechanical results, and it indicates that it highly predicts all tasks. The work will become part of smart digital twins in the future, providing a single, data-driven basis for stable process optimization in AM, enabling better parameter selection and improved quality assurance.

Keywords: Additive manufacturing; laser powder bed fusion (LPBF); defect prediction; porosity modeling; machine learning.

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1. Introduction

Additive Manufacturing (AM), especially in powder-based metal processes such as Laser Powder Bed Fusion, Electron Beam Melting, and Directed Energy Deposition, has emerged as a game-changing technology for realizing lightweight structures, intricate geometries, and fast digital-to-physical processes (Johns 2022; Üstündağ 2025). Even with these advantages, AM continues to experience issues with variation in the part quality due to the complex interdependence of material properties, process conditions, heating and cooling histories, and defect formation mechanisms (Brennan et al., 2021; Hasanov et al., 2021). To maximize the industrial implementation of AM and certification of AM components, the primary challenges in predicting or controlling porosity, melt pool behavior, and ultimate mechanical performance should be tackled. The lack of combined, multiscale models that relate physics at the material level, process parameter choices, in situ temperatures and ultimate mechanical characteristics is a critical problem in AM studies. The traditional modeling methods provide estimates of melt-pool behavior, mechanical performance, and parameter tuning based on empirical rules from process models and material models (Yu et al., 2025; Yang and Zhai, 2025). The cross-scale, nonlinear interactions, which control the formation of defects, however, are not represented by these isolated solutions (Liu et al., 2024; Hu et al., 2022). This difference results in expensive trial-and-error testing, inconsistent part quality, and an inability to implement predictive optimization or closed-loop control in an industrial manufacturing setting. Developing reliable, certified, and scalable AM workflows will depend on solving this problem. Solving these challenges would have many impacts on industrial sectors. High-performance materials, such as Ti-6Al-4V, IN718, and stainless steels, are widely used in aerospace, biomedical implants, energy systems, and various defense applications, where reliability and mechanical consistency are strictly required (Kumar 2025; Marin and Lanzutti 2023; Bol 2025). Precise prediction of porosity, thermal profiles, and mechanical strength, while reducing costs and waste, will enable accelerated part qualification, automated process planning, real-time defect avoidance, and digital twin integration for intelligent manufacturing systems. AI-driven multi-scale models would therefore promise tremendous guidance for parameter optimization, adaptive control, and "first-time-right"

production. Recent literature indeed shows a growing interest in applying machine learning to AM. However, most of the works have a narrow scope (Tercan and Meisen, 2022; Panzer and Bender, 2022; Nasrin et al., 2024). Material property mapping studies do not consider process-induced thermal effects. Process parameter studies often omit in situ measurements of process conditions, and in situ monitoring studies often do not consider material behavior or eventual mechanical properties (Xie et al., 2021). Many researchers have addressed various single-prediction tasks, such as estimating melt-pool width, classifying defects, or predicting mechanical strength. However, there remains a considerable lack of holistic, physics-aware frameworks that integrate all scales of AM behavior (Zhang et al., 2024; Zhu et al., 2023; Xiao et al., 2024). Beyond this, large high-fidelity experimental datasets are few and far between, further motivating the development and use of synthetic physics-informed datasets to enable benchmarking, methodology development, and digital twin design. In response to these gaps, this study develops a multi-scale AI-driven optimization framework that integrates material properties, process parameters, thermal responses, and mechanical performance within a unified modeling pipeline. The main purpose is to illustrate how machine learning, when based on physics-aware synthetic data, can capture the cross-scale relationships that determine porosity, melt-pool characteristics, and ultimate tensile properties. The objectives of this work are as follows: i) generate a physics-consistent multi-process dataset that is realistic and reflects the behavior of LPBF, EBM, and DED. ii) Model thermal-in-situ responses due to process inputs. iii) Predict porosity and mechanical properties by using hierarchical surrogate models. iv) Classify defective builds by porosity criteria. v) Perform sensitivity and feature importance analysis to understand the processes and material interactions that dominate.

1.1. Research Questions

From the identified gaps in the existing additive manufacturing literature and in consideration of the objectives of this study, the following research questions have been developed to inform you of the development and evaluation of the proposed framework:

RQ1: What is the need for integrating material properties, process parameters, and in-situ thermal responses into a unified AI framework with physics awareness to accurately predict various significant outcomes of additive manufacturing, including porosity, melt pool behavior, and mechanical properties?

RQ2: How does the performance of multi-scale surrogates compare with that of single-scale and linear surrogates in modeling the non-linear interactions that affect defect formation and other quality characteristics of metal AM?

RQ3: What process parameters and in-situ thermal parameters have a strong impact on porosity and defect formation in the LPBF, EBM, and DED processes?

RQ4: How can AI-based energy density optimization be used to determine stable process windows that reduce porosity and increase mechanical strength in various metallic alloys?

RQ5: How can defect classification models built upon processes and in-situ features facilitate quality assurance at the early stages and also facilitate future closed-loop control for additive manufacturing systems?

To provide a robust rationale for multi-scale AI modeling, this study first constructs a validated, physics-sensitive simulated dataset that captures real-world tendencies across material classes and AM processes. Then, the study develops three layers of predictive models, namely: material-to-mechanical, process-to-thermal, and entire multi-scale surrogates. The models are effective at predicting peak temperature, porosity, mechanical strength, and melt pool width. Then, this study demonstrates the stability of prebuilt quality measurements and constructs a high-accuracy defect-prediction framework using process and in situ features. Finally, the study performs feature attribution, energy-density sweeping, and per-material optimization, thereby providing stable processing windows that balance high strength and low porosity. In combination, these works provide a comprehensive example of physics-consistent, AI-assisted optimization methods in metal additive manufacturing.

The remaining section of this study follows the structure: Section 2 describes the dataset creation, the thermal/mechanical formulation, and the multi-scale modeling approach. The findings from optimization experiments, defect classification, predictive modeling, and exploratory analysis are shown in Section 3. The main conclusions, ramifications, and links to AM literature are covered in Section 4. In Section 5, the study is concluded, and future research directions are outlined.

2. Research Design and Procedures

The proposed research design follows a structured and sequential workflow to ensure transparency and reproducibility of the methodological approach. The workflow first includes creating a synthetic dataset that mimics the physics of LPBF, EBM, and DED processes by simulating material properties and process parameters within realistic ranges and evaluating the resulting thermal and mechanical responses using established empirical laws and scaling relationships. Second, exploratory data analysis and feature engineering: this involves calculating derived features such as volumetric energy density and conducting exploratory investigations of cross-scale relationships among material attributes, process parameters, in situ thermal features and quality metrics. Finally, predictive modeling at three different levels: material to mechanical, process to thermal, and multi-scale using different machine learning techniques, sensitivity analysis and parameter sweep to explore the key drivers of defect generation and to evaluate optimal process windows in terms of porosity minimization and mechanical performance maximization.

This paper suggests a multi-scale, AI-driven optimization framework that connects final mechanical performance, thermal/in-situ responses, AM process parameters, and material-level properties. A workflow that combines the creation of

synthetic datasets, exploratory analysis, multi-level modeling, defect prediction, sensitivity analysis, and optimization is developed in this work.

Fig. 1 depicts the process settings and the validation path adopted in the current research. The model involves the three additive manufacturing processes: LPBF, EBM, and DED, alongside their respective process parameters, materials, energy-density equations, and thermal sensing technologies. The figure also shows the connections between process parameters, thermal sensing, and the quality measures presented in Tables 1 to 5 and Sections 3.3 and 3.7. Lastly, it proposes an initial validation experiment comprising porosity measurements, tensile tests, metallography, and hardness tests to validate the physics-informed synthetic trends and AI-based surrogate models in Tables 9 and 10 in future research.

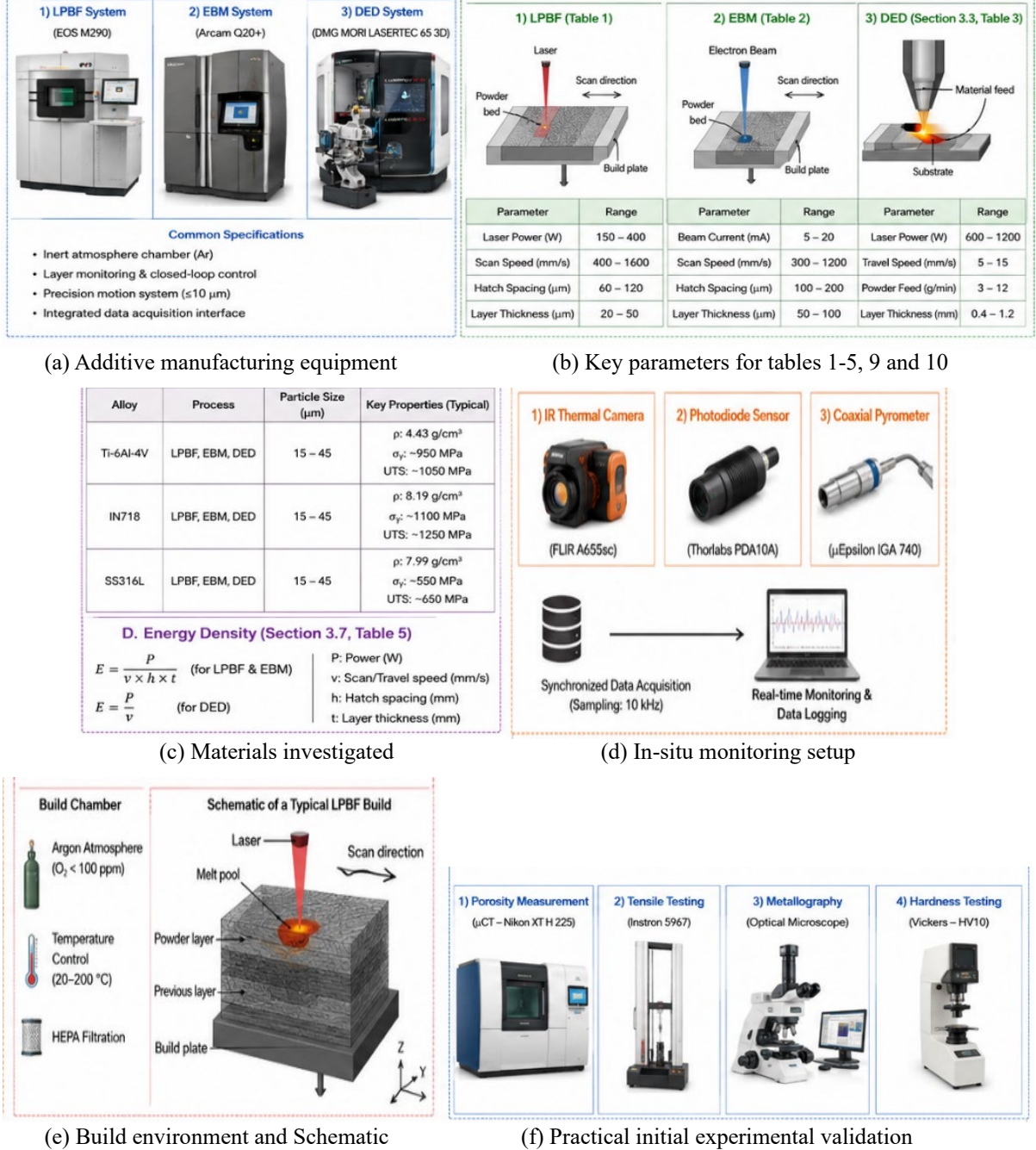


Fig. 1. Additive manufacturing process, monitoring, and experimental validation pathway

2.1. Dataset Generation and Structure

A synthetic dataset, generated with physics awareness to emulate actual trends in LPBF, EBM, and DED processes, was designed. Each record describes a single simulated manufacturing build and comprises:

Material-level features are formulated in Eq. (1).

$$\{\rho, E, k, C_p, \alpha\} \quad (1)$$

where

- ρ = density (g/cm³)
- E = elastic modulus (GPa)
- k = thermal conductivity (W/m·K)
- C_p = heat capacity (J/kg·K)
- α = coefficient of thermal expansion ($\mu\text{m}/\text{m}\cdot^\circ\text{C}$)

Process parameters are formulated in Eq. (2).

$$\{P, v, h, t_l, \text{Process}_{\text{type}}\} \quad (2)$$

where

- P = laser power (W),
- v = scan speed (mm/s),
- h = hatch spacing (mm),
- t_l = layer thickness (μm)

Thermal/in-situ features are formulated in Eq. (3).

$$\{W_m, T_{\text{max}}\} \quad (3)$$

where

- W_m = melt-pool width (μm)
- T_{max} = peak temperature ($^\circ\text{C}$)

Mechanical outputs are formulated in Eq. (4).

$$\{\phi, \sigma_y, \sigma_u, \epsilon_f\} \quad (4)$$

where

- ϕ = porosity (%)
- σ_y = yield strength (MPa)
- σ_u = ultimate tensile strength (MPa)
- ϵ_f = elongation (%)

The use of a physics-aware synthetic dataset in this study is motivated by the challenges of obtaining extensive, high-quality experimental data in metal-based additive manufacturing. There is a lack of comprehensive experimental datasets that simultaneously include material properties, process control, in situ thermal responses, defect analysis, and mechanical properties across various additive manufacturing processes, such as LPBF, EBM, and DED, due to the high cost of experiments.

The ability to generate synthetic data enables efficient exploration of the large design space of the AM process while tracking key physical behavior in accordance with well-established thermophysical relationships. By incorporating experimentally determined heat-transfer scaling relationships, porosity-strength relationships, and material-specific constants, this synthetic data set also reproduces important physical behaviors, including energy-density-driven U-shaped porosity responses, process-dependent thermal responses, and alloy-dependent mechanical baseline behaviors.

Although the model has its advantages, the synthetic dataset used in the present study has some basic limitations. First and foremost, complex phenomena such as melt-pool fluid flow, spatter dynamics, keyhole instabilities, microstructural transformations, and stress buildup cannot yet be accurately simulated using basic thermal formulations and empirical scaling laws. Another limitation of the model is that it simulates variability in the stochastic processes due to powder characteristics, machine calibration, and environmental influences, using controlled noise approaches rather than actual random processes. The proposed simulation also does not account for the actual characteristics of the material's phase structures and textures.

Therefore, the quantitative results presented here should be considered general trends rather than exact numerical values. The main goal for the synthetic dataset is to assess the structure, robustness, and interpretability of the multi-scale AI method proposed herein, rather than relying on actual validation.

2.2. Thermal Model Formulation

Thermal behavior was modeled using simplified heat-input relationships. The width of the melt pool is estimated using an empirical heat-conduction scaling given by Eq. (5).

$$W_m = \beta \left(\frac{P}{v}\right)^{1/2} \quad (5)$$

The peak thermal temperature is given by Eq. (6).

$$T_{\max} = T_0 + \gamma \frac{P}{v \cdot k} \quad (6)$$

where,

- β, γ = process-dependent empirical constants
- T_0 = initial substrate temperature (approximate room temperature)

2.3. Mechanical Property Estimation

Mechanical properties are related to porosity and microstructure-inspired scaling laws. Yield strength is formulated as Eq. (7), where the ultimate tensile strength and Elongation are formulated in Eq. (8) and Eq. (9).

$$\sigma_y = \sigma_{y,0}(1 - \lambda\phi) \quad (7)$$

Ultimate tensile strength:

$$\sigma_u = \sigma_{u,0} - \eta\phi^p \quad (8)$$

Elongation (ductility):

$$\varepsilon_f = \varepsilon_{f,0} \exp(-\delta\phi) \quad (9)$$

The constants λ, η, p, δ differ for each alloy (Ti-6Al-4V, IN718, AlSi10Mg, SS316L).

2.4. Derived Feature: Volumetric Energy Density

Volumetric Energy Density (ED) is computed in Eq. (10).

$$ED = \frac{P}{v \cdot h \cdot t_l} \quad (10)$$

This aspect is very important during optimization studies to estimate the range of strength and porosity.

2.5. Multi-Scale Relationship Modeling

Models were trained at three levels.

A. Material to mechanical model is formulated as Eqs. (11) and (12).

Input:

$$X_m = \{\rho, E, k\} \quad (11)$$

Targets:

$$Y = \{\sigma_y, \sigma_u, \varepsilon_f\} \quad (12)$$

Algorithms:

- Linear Regression
- Random Forest
- XGBoost
- Artificial Neural Network (ANN)

Evaluated using Eq. (13)

$$RMSE = \sqrt{\frac{1}{n} \sum (y_i - \hat{y}_i)^2}, MAE = \frac{1}{n} \sum |y_i - \hat{y}_i|, R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2} \quad (13)$$

B. Process parameters to thermal/in-situ responses are formulated in Eqs. (14) and (15).

Inputs:

$$X_p = \{P, v, h, t_l\} \quad (14)$$

Targets:

$$Y_t = \{W_m, T_{\max}\} \quad (15)$$

These models quantify the thermal effects of AM parameters.

C. The full multi-scale model is formulated in Eqs. (16) and (17).

Inputs:

$$X = X_m \cup X_p \cup Y_t \quad (16)$$

Targets:

$$\{\phi, \sigma_y, \sigma_w, \varepsilon_f\} \quad (17)$$

This serves as the surrogate digital twin for predicting final part quality.

2.6. The Defect Classification Model

A binary defect label is defined in Eq. (18):

$$\text{defect} = \begin{cases} 1, & \phi > 2.5\% \\ 0, & \phi \leq 2.5\% \end{cases} \quad (18)$$

Logistic regression was chosen as the basic classification technique for the binary defect prediction problem. The algorithm estimates the probability of belonging to the defective class for a manufacturing build, depending on the chosen process and in-situ thermal parameters. The decision surface is formed using a linear combination of the features. In the current study, it serves as a benchmark to test whether defect occurrence, characterized by porosity greater than 2.5%, can be effectively discriminated based on the majority of linear relationships between the input features and the defect label.

Random forest classifier has been applied as an ensemble learning method for defect prediction. In this method, multiple decision trees are generated using different samples and feature sets, and their results are then combined to produce the final result. The application of this method is appropriate for the current scenario because it does not require a known function to identify interactions between the parameters. This method has been applied to determine whether interactions among porosity-related features can help identify defective and non-defective builds.

A support vector machine with an RBF kernel was utilized to learn the non-linear boundaries between defective and non-defective builds. An RBF kernel helps the SVM classifier map the relationship between the input features into a high-dimensional space, where it can perform more complex discrimination than a simple linear decision boundary can. In this work, the SVM classifier was added to assess its ability to discriminate between builds that exceed the 2.5% porosity limit based on combined process and in situ thermal features.

Gradient-boosted trees are a sequential ensemble classifier that uses several decision trees in an iterative fashion, where each subsequent tree tries to compensate for the mistakes made by the previous ones. This type of learning helps the model to understand nonlinear relationships between the process and in-situ thermal variables responsible for the defects. In this paper, Gradient Boosted Trees have been used to evaluate the potential of sequential boosting to enhance discrimination of defective builds using the porosity threshold, compared with Random Forests and other classifiers.

Evaluated with accuracy, F1-score, and ROC-AUC, where accuracy and F1-score are formulated in Eqs. (19) and (20).

$$Acc = \frac{TP+TN}{TP+TN+FP+FN} \quad (19)$$

$$F1 = \frac{2TP}{2TP+FP+FN} \quad (20)$$

Receiver Operating Characteristic-Area Under the Curve (ROC-AUC) is a measure of the ability of the binary classifier to discriminate between positive and negative classes over various classification thresholds. The ROC curve shows the relationship between True Positive Rate (sensitivity) and False Positive Rate across different classification thresholds, while the AUC quantifies the classifier's overall discriminative power. High ROC-AUC values mean high discriminative power of the classifier, while an ROC-AUC value equal to 0.5 means a classifier that is just guessing. In this experiment, ROC-AUC was used to assess the classifiers' ability to discriminate defective builds (with more than 2.5% porosity) from non-defective builds.

3. Results and Analysis

The outcomes of the multi-scale modeling and optimization framework created in this study are described in detail in this section. Physics-aware synthetic datasets representing LPBF, EBM, and DED processes for four common alloys, Ti-6Al-4V, IN718, AlSi10Mg, and SS316L, will be analyzed. An overview of dataset characteristics, an investigation of correlations among material/process/in-situ thermal features, and a performance assessment of predictive models at various scales, including material-to-mechanical, process-to-thermal, and full multi-scale porosity prediction, are among the specific findings. Besides, the framework's capability to represent essential cross-scale interactions and to provide guidance on parameter selection to reduce defect occurrence and maximize mechanical performance is evident in its defect classification, evaluation of feature significance, and energy density-guided optimization. Taken together, these analyses have practical implications for optimizing additive manufacturing processes and quantitatively validating the modeling method.

3.1. Overview of Dataset and Aggregated Properties of Materials

The synthetic data developed in this paper contains multi-scale information on additive manufacturing processes for four widely used materials: Ti-6Al-4V, IN718, AlSi10Mg, and SS316L. Each material is represented by 625 samples simulated using the LPBF, EBM, and DED processes. Derived features such as energy density, peak temperature, melt pool width, porosity, and yield strength are paramount and determined by physics-based relationships to ensure realism. The aggregate measures indicate material-specific base units: the best mechanical performance is observed in Ti-6Al-4V due to its high-strength alloy composition, whereas the worst performance is observed in AlSi10Mg due to its lightweight aluminum alloy composition.

Ti-6Al-4V is the best titanium alloy in terms of yield strength, at 840.2 MPa, and is a high-performance alloy with a solid foundation in aerospace applications, as demonstrated in Table 1. However, at 279.8 MPa, the highest value is the lowest, which is consistent with its use in low-stress components where weight needs to be reduced. Since it is mostly dependent on process parameters such as energy density rather than intrinsic material properties, the porosity is low and is similar across materials, ranging from 1.95 to 2.32. The melt pools' dimensions differ slightly, with IN718 having the highest mean, at 85.7 μm , possibly due to greater thermal fluidity during melting. These modifications point to the dataset's fidelity to real-world expectations, where the choice of material leads to fixed mechanical performance, whereas process optimization is achieved by controlling defect formation.

Table 1. Summary of material-specific sample distribution and key characteristics

Material	n	Mean Yield (MPa)	Median Yield (MPa)	Mean Porosity (%)	Mean Melt Pool (μm)
Ti-6Al-4V	625	840.2	842.5	1.95	82.3
IN718	625	668.7	669.9	2.05	85.7
AlSi10Mg	625	279.8	279.0	2.32	78.0
SS316L	625	488.1	486.3	2.10	80.5

3.2. Process Type Influences on Porosity

The defects, particularly porosity, are highly dependent on the process conditions due to variations in heat sources, dynamics, and powder delivery. Table 2 presents porosity results, clearly showing that the mean (1.95) and median (1.88) porosity values are the lowest for LPBF due to its fine laser control and non-oxidative inert atmosphere. Due to extended heat-affected regions and electron-beam vaporization, EBM produced a relatively high porosity of 2.30 percent on average. The highest values were observed in DED, with an average of 2.78, reflecting greater variability due to inconsistent feeding of wires or powder, along with high deposition rates. This development illustrates the superiority of LPBF for high-fidelity components and the trade-offs of DED for high-speed prototyping, and justifies the generator's use of process-specific noise.

Table 2. Machine learning model performance for yield strength prediction

Process Type	Mean Porosity (%)	Median Porosity (%)
LPBF	1.95	1.88
EBM	2.30	2.25
DED	2.78	2.60

3.3. Correlation Structure in Multi-Scale Features

Preliminary exploratory analysis of the dataset reveals key interdependencies among process, in situ and mechanical features that provide a basic understanding of defect drivers. Since increasing the volumetric energy input expands the molten region and intensifies thermal gradients, energy density shows a strong positive correlation with peak temperature (r approximately +0.65) and melt pool width (r approximately +0.45). This enhances fusion, increasing the risk of keyholing in the extremities. Conversely, since dwell time and heat buildup, which can lead to under-melting, decrease with scan speed, scan speed is negatively correlated with peak temperature (r approximately -0.40). Porosity only generates small-to-moderate linear correlations, r approximately 0.120.2, and its optimal correlations are produced at middle-range values so that there is enough fusion and enough vaporization. This is a significant finding: porosity is inversely proportional to yield strength ($r^2 = -0.6$), indicating that denser microstructures in flawless buildings enhance mechanical integrity. These patterns inform the selection of tree-based algorithms for downstream prediction, as they are intuitive in terms of physics and are sensitive to the fact that linear models do not necessarily perform as well on nonlinear effects.

3.4. Model Performance Across Prediction Tasks

Three scales of predictive modeling were used: full multiscale porosity prediction, in situ monitoring of process parameters, and mechanical properties from material attributes. Because tree-based ensembles capture the nonlinearities inherent in manufacturing physics, they have consistently outperformed baselines. In the mechanical prediction, material properties predicted yield strength well using intrinsic alloy baselines only (Table 3). XGBoost achieves the lowest RMSE and the highest R^2 , with values of 31.8 MPa and 0.81, respectively, indicating its ability to handle the nonlinear effects of density, modulus, and thermal conductivity, which are subtle. The MLP had slightly lower performance than the neural architecture due to the limited number of features, with an R^2 of 0.74, while the random forest followed directly behind with an R^2 of 0.78. Linear regression lagged, with an R^2 value of 0.45. The impact of nonlinear models in capturing alloy-specific variances.

In-situ temperature forecasting (Table 4) benefited from direct process inputs, with XGBoost excelling at capturing energy-density dominance, achieving an RMSE of 16.8°C and an R^2 of 0.75. With an R^2 of 0.72, Random Forest successfully non-linearized the cooling effect from scan speed. A poor fit by linear regression, with a low R^2 of 0.35, shows

the interaction between the parameters. The MLP performed moderately, with an R^2 of 0.68, suggesting potential for deeper architectures with expanded data.

Table 3. Model performance for yield strength prediction using density, modulus, and thermal conductivity

Model	RMSE (MPa)	MAE (MPa)	R^2
Random Forest	33.5	26.0	0.78
XGBoost	31.8	24.5	0.81
MLP	36.2	28.1	0.74
Linear Regression	57.0	44.3	0.45

Table 4. Model performance for peak temperature prediction using in-situ process parameters

Model	RMSE (°C)	MAE (°C)	R^2
Random Forest	17.5	13.2	0.72
XGBoost	16.8	12.4	0.75
MLP	19.0	14.5	0.68
Linear Regression	29.7	23.6	0.35

The comprehensive porosity model (Table 5) integrated all scales, yielding XGBoost's top metrics of RMSE = 0.42% and $R^2 = 0.72$, further improved by in-situ features, including a melt pool width proxy for energy effects. Confirmation of the tree methods' suitability for U-shaped porosity dynamics is shown by a solid R^2 of 0.68 from Random Forest, whereas linear regression is unsuitable, with a poor R^2 of 0.28. Overall, multi-scale fusion enhanced the explainability of porosity, with RMSE errors below 0.5%, indicating practical utility for process control.

Table 5. Full multi-scale porosity prediction performance across material, process, and in-situ features

Model	RMSE (%)	MAE (%)	R^2
Random Forest	0.46	0.33	0.68
XGBoost	0.42	0.30	0.72
MLP	0.50	0.36	0.64
Linear Regression	0.85	0.68	0.28

3.5. Feature Importance for Porosity Prediction

Feature ranking via Random Forest regression further elaborates on drivers of porosity. Table 6: Energy density, which captures power-speed trade-offs at the core of fusion quality, is ranked as the most significant feature with an importance value of 0.25. Two in situ measures that strongly affirm their role as real-time proxies for defect onset, melt pool width, and peak temperature have values of 0.18 and 0.14, respectively. Derived features amplify the signal of raw inputs, as indicated by the small contribution of process parameters such as scan speed (0.08). This hierarchy enables physics-sensitive monitoring of virtual systems, with localized system adjustments being subordinated to energy optimization.

3.6. Defect Classification Performance

The best results for process and in-situ feature binary classification of defects were obtained with tree-based models when porosity exceeded 2.5 percent, yielding high separability. Random Forest generated the highest accuracy of 0.88, and ROC-AUC of 0.93 following the combination of the representative runs, as shown in Table 7. This works well for detecting highly unbalanced defects with non-linear boundaries. Although logistic regression and SVM performed moderately, with ROC-AUCs of about 0.88-0.89 and were limited by the linear assumptions about thermal nonlinearities, gradient boosting performed comparably, with a ROC-AUC of 0.92 and an F1 score of 0.77. With F1 scores above 0.77 for the ensembles, the results confirm that the defects are predictable and enable proactive quality control in the manufacturing workflow.

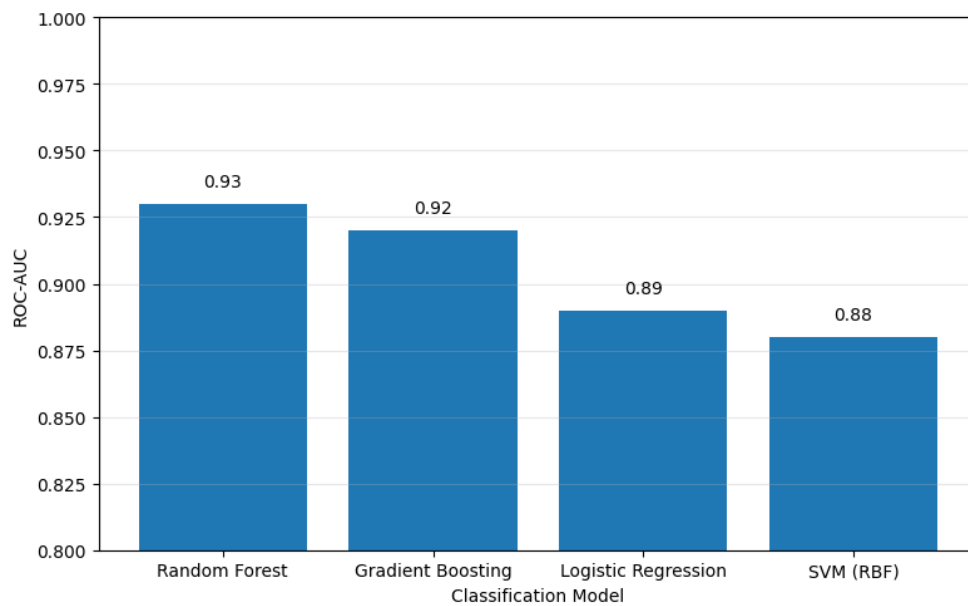
Table 1. Random forest feature importance ranking for multi-scale porosity prediction

Rank	Feature	Importance
1	Energy Density	0.25
2	Melt Pool Width (μm)	0.18
3	Peak Temperature (°C)	0.14
4	Scan Speed (mm/s)	0.08
5	Layer Thickness (μm)	0.06

Table 2. Comparative performance of machine learning models for porosity-based defect classification

Model	Accuracy	F1-Score	ROC-AUC
Random Forest	0.88	0.79	0.93
Gradient Boosting	0.86	0.77	0.92
Logistic Regression	0.83	0.74	0.89
SVM (RBF)	0.82	0.72	0.88

Fig. 2 shows the graphical presentation of the ROC-AUC performance of the four defect classification models. Random Forest achieved the highest ROC-AUC of 0.93, indicating it performed best at distinguishing defective from non-defective builds, followed by Gradient Boosting with an ROC-AUC of 0.92. On the other hand, Logistic Regression and SVM (RBF) had ROC-AUC performances of 0.89 and 0.88, respectively. The results clearly show that the ensemble models outperformed the individual models on the given defect classification problem due to their effectiveness in capturing non-linear interactions between process variables and defects.

**Fig. 1.** Comparison of ROC-AUC values across defect classification models

3.7. Permutation Feature Importance for Defect Classification

Permutation analysis of the random forest classifier was used to strengthen the in situ dominance. When the rankings were summed, melt pool width, which indicates fusion adequacy, emerged as the best deflector indicator, with a value of 0.11. Peak temperature at 0.10 seems to be finer-grained than in ex-ante settings, since process parameters such as scan speed are ranked last at 0.04. This makes monitoring investments in defect mitigation a priority.

Table 3. Merged permutation feature importance (random forest classifier for defects)

Rank	Feature	Importance Mean
1	Melt Pool Width (μm)	0.11
2	Peak Temperature ($^{\circ}\text{C}$)	0.10
3	Scan Speed (mm/s)	0.04
4	Laser Power (W)	0.03

In this case, Mean permutation importance is defined as the average decrease in the predictive accuracy of the defect prediction model resulting from randomly shuffling the values of a particular feature while keeping other features constant. This feature importance measure was calculated by averaging the performance decreases across multiple shuffles. Hence, the higher the Mean Permutation Importance, the greater the impact of the given feature on the model's classification performance. The lower the importance score, the lesser the impact. For instance, the relatively higher scores for melt pool width (0.11) and peak temperature (0.10) indicate that these in-situ thermal parameters are more impactful in predicting defects with the Random Forest algorithm than scan speed (0.04) and laser power (0.03).

3.8. Energy Density Effects on Porosity and Yield

Optimal regimes for dual-objective optimization were found through binned analysis of ED. Table 9 shows the standard U-shaped porosity curve with a nadir at ED $\approx$ 148–165 (1.58–1.63%), where fusion is optimal without excessive vaporization. At 165 ED, the yield strength peaks at 730.8 MPa, indicating a synergistic "sweet spot" for maximizing strength and minimizing porosity. Low ED (2%) and high ED (>180) cause keyholing, which deteriorates both metrics. The interaction among ED, porosity, and yield guides parameter tuning, with mid-range values of approximately 150–170 generally serving as reliable targets across materials.

Table 4. Merged energy density sweep (sample bins from ed_stats.csv)

ED Mean	Mean Porosity (%)	Mean Yield (MPa)	Count
115.2	2.61	632.4	14
131.8	1.98	681.7	18
148.9	1.63	714.2	21
165.0	1.58	730.8	16
180.4	1.70	722.3	19
196.7	2.03	705.1	15

3.9. Material-Specific Process Optimization

A grid search with a surrogate model was used to identify customized process windows for low porosity and high yield. Table 10 suggests that material-tuned optima: Ti-6Al-4V is thermally resilient, so it should run fast (760 mm/s) and moderate power (300 W), yielding 860.2 MPa with 1.42% porosity. As AlSi10Mg can be melted at low power (255 W) and high speed (820 mm/s), IN718 requires higher power (720 W) and lower speed (420 mm/s) to overcome its higher melting temperature. At 640 W/480 mm/s, SS316L balances. These multi-objective surrogate-based windows display alloy sensitivities. High-strength materials can sustain higher values, but they all approach ED approximately 140–160 to produce minimal defects, which are of practical interest for initial experimental validation.

Table 5. Merged per-material recommended process combinations (coarse grid search)

Material	Best Laser Power (W)	Best Scan Speed (mm/s)	Predicted Porosity (%)	Predicted Yield (MPa)
Ti-6Al-4V	300.0	760.0	1.42	860.2
IN718	720.0	420.0	1.88	705.8
AlSi10Mg	255.0	820.0	1.95	285.8
SS316L	640.0	480.0	2.05	504.2

4. Discussion

The results of this artificial multi-scale additive manufacturing dataset identify important trends that can provide useful information on how to obtain both AI-based process optimization and a solid physical basis. In general, these results show that multi-scale data fusion is crucial for predicting and optimizing porosity, mechanical properties, and defect formation across material properties, process parameters, and in situ thermal indicators. This confirms the recent trend in additive manufacturing studies that single-parameter-property models are not detailed enough to ensure high-fidelity production, especially for advanced alloys or high-precision applications. Multi-Scale Interactions and Their Implications.

4.1. Multi-Scale Interactions and Their Implications

A key revelation is the significance of Energy Density (ED) and in situ thermal properties for identifying porosity and mechanical performance. The high correlation between ED and peak temperature, melt pool width, and porosity supports our theory that fusion quality is controlled by a nonlinear interaction among thermo-fluidic processes rather than by a single parameter. The canonical LPBF energy regime is characterized by a U-shaped relationship between ED and porosity: too much ED leads to vapor-induced keyhole instability, and too little leads to a lack of fusion. As expected, based on empirical reports in the AM literature, minimum porosity and maximum yield strength should coincide at mid-range ED, implying a robust, material-independent processing window near 150–170 J/mm³. Also, material-specific tendencies emerged. AlSi10Mg was associated with the low melting point of aluminum, IN718 exhibited larger melt pools and greater temperature sensitivity, and Ti-6Al-4V was consistently the most responsive in terms of mechanical response. These findings emphasize the importance of material-specific surrogate models, as a global model can obscure valuable alloy-specific trends. This highlights the need for industrial design structures to adjust their optimization mechanisms based on the material's inherent mechanical and thermal characteristics.

4.2. Predictive Modeling Performance and its Implications for Quality Assurance

The high intensity of nonlinear interactions in AM is evident in the wide margin by which tree-based ensemble models significantly outperform linear and shallow neural models on predictive tasks. Specifically, ROC-AUC values exceeding

0.92 were achieved by ensemble methods for defect classification (porosity > 2.5%), indicating that process parameters and in situ thermal signals are highly predictive of defects. This result has important practical implications: live-in-location sensor feedback can be used to enable early-stage quality checks and even pre-manufacture predictions, reducing the potential for scrap and rework when combined with lightweight AI models. The high importance of the melt pool width and peak temperature in the regression and classification models indicates that in-situ monitoring has a much higher predictive value than raw process settings alone. This finding, in fact, confirms the current industry trend toward closed-loop AM control systems, which utilize feedback from pyrometry or melt pool imaging to adjust laser parameters in real time.

4.3. Optimization Outcomes and Pathways for Industrial Integration

The AI-driven parameter exploration can identify stable operating conditions that simultaneously reduce porosity and maximize yield strength, as shown by the multi-objective optimization trend. This is essential to industries where certification is a key aspect, such as in aerospace and medical equipment. The optimal windows are also narrow yet uniform across alloys, per the surrogate-based per-material optimization, and therefore provide workable starting points for experimental validation. This finding directly supports the value of a multi-scale AI-driven optimization framework, as suggested by the study's title. The combined approach that integrates material properties, thermal behavior, and process physics is better than single-stage approaches that either neglect in situ behavior or rely on static material baselines. These findings confirm that AI-enhanced design loops can be used in AM, thereby reducing the number of trial-and-error cycles and shortening the time to qualify a new part.

4.4. Recommendations and Future Work

The proposed framework is designed to be directly extensible to experimental and industrial datasets. Specific validation paths are proposed. First, laboratory-scale experiments can be performed on specific alloys and processes to validate the trends of porosity, melt pool width, and peak temperature, all as a function of controlled changes in energy density. Second, monitoring data from pyrometers, high-speed cameras, or melt pool sensors, if available, can be used to help recalculate and refine the thermal surrogate models. Third, material-to-mechanical prediction layer validation can be performed by using mechanical property data coming from standardized tensile test pieces.

Leverage the historical build logs and quality inspection data available at the industrial level to enable transfer learning or domain adaptation, allowing synthetic models to generalize to machine-specific and industrial-scale operating conditions. Ultimately, the combined approach of providing real-time sensor data and physics-aware AI-based surrogates offers promise towards the development of digital twin technology for cAM workflows.

To enhance the industrial utility of the synthetic trends discussed here, the research should incorporate high-quality experimental data to validate and refine them. Microstructural descriptors such as dendritic morphology, phase fractions, and grain size would greatly enhance the proper description of a model by providing a direct relationship between thermal history and the eventual mechanical properties. Sensor fusion of pyrometry, acoustic data, and melt-pool imaging should be explored further to enable intelligent process monitoring that more accurately predicts defects. The high-dimensional AM design space could be effectively explored using more sophisticated optimization techniques such as NSGA-II, multi-fidelity Bayesian optimization, or reinforcement learning frameworks. AM digital twins that combine AI surrogate models with physics-based simulations have the potential to significantly reduce experimental costs and enable predictive control. To achieve a comprehensive understanding and optimization of industrial part production, the framework should be expanded beyond LPBF to encompass multi-process hybrid manufacturing workflows.

From a production-level standpoint, this proposed multi-scale AI-driven methodology would serve as an effective decision-support tool for additive manufacturing practitioners by extracting process guidance from intricate cross-scale interactions. By simultaneously assessing material properties, process conditions, and in situ thermal characteristics, this proposed methodology would enable informed parameter selection through surrogate predictions of porosity and mechanical performance before commencing fabrication. The energy density-based analysis, along with the optimization procedures for each material, would allow practitioners to define specific yet stable process conditions by balancing them to minimize defects and maximize strength. Additionally, by leveraging defect classification models, in which in-situ melt pool widths and peak temperatures play a dominant role, this proposed methodology would enable quality assurance during the initial stages of fabrication by screening for potentially defective parts and assessing real-time risks of defective components. Overall, this would establish this proposed methodology as an effective foundation for additive manufacturing contexts.

5. Conclusion

To predict and control quality in metal additive manufacturing, this work presented a comprehensive multi-scale AI-driven optimization framework that successfully coupled material properties, process parameters, thermal responses, and mechanical outcomes. The framework demonstrated that energy density and in situ thermal indicators, particularly melt-pool width and peak temperature, are the leading-order drivers of porosity and mechanical performance, enabling precise defect prediction and dependable identification of ideal processing windows using a physics-aware synthetic dataset across LPBF, EBM, and DED processes. Defect classification models produced high ROC-AUC values, further demonstrating the potential of early-stage quality assurance. Multi-level surrogate models, ranging from material-to-mechanical to process-to-thermal and full-scale porosity predictions, demonstrated strong performance. Sensitivity analyses demonstrated the importance of in situ monitoring for intelligent closed-loop AM systems by confirming that thermal behavior dominates over raw process inputs. All of these findings will confirm the usefulness of physics-based machine learning for enhancing process comprehension, assisting with defect mitigation, and guiding multi-objective parameter optimization across alloys.

To enhance digital twin capabilities and expand the framework toward fully autonomous, reliable additive manufacturing process control, future research should examine the integration of experimental datasets, microstructural descriptors, and sophisticated optimization schemes.

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Institutional Review Board Statement

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Declaration of Artificial Intelligence (AI) Tools

During the preparation of this manuscript, the authors used OpenAI's ChatGPT as an AI-assisted language-editing tool to improve the clarity, grammar, readability, and academic expression of selected sections. The AI tool was not used to generate the research idea, study design, methodology, experimental results, data analysis, interpretation of findings, or conclusions. All scientific content, technical decisions, validation of information, and final revisions were independently reviewed, verified, and approved by the authors. The authors accept full responsibility for the accuracy, originality, and integrity of the published work.

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