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# Knowledge-informed graph attention networks enable defect-free alloy design for laser additive manufacturing

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Machine learning offers a promising approach to design high-performance alloys for laser additive manufacturing, by bypassing convoluted physical models and identifying correlations among composition, processing, microcracks/porosity and properties. However, conventional machine learning methods face limitations, e.g., overfitting or unreasonable design results, due to reliance on large, high-quality datasets. Here, we introduce a generic framework operable with smaller experimental datasets, by integrating knowledge-informed graph modeling alongside data uncertainty quantification. The generic physical-metallurgy knowledge and the stochasticity of experimental defect distributions from produced material are rationally balanced. To validate the approach, we detail the development of a new defect-free Ni superalloy possessing excellent laser printability, thermal stability, and high mechanical strength. Mechanism mining revealed a possible origin for this performance, which was confirmed by atom probe tomography. Subsequently, we developed a new laser-printable aluminum alloy through the same approach, highlighting the framework's potential to accelerate next-generation alloy design for additive manufacturing.

Laser-based additive manufacturing (AM), such as laser powder bed fusion (L-PBF) and laser directed energy deposition (L-DED), enables the fabrication of metallic parts with complex geometries and tailored microstructures, once thought to be unattainable<sup>1,2</sup>. However, the use of powders with compositions developed for traditional processes such as casting, rolling, forging, and sintering, in laser-assisted additive manufacturing often leads to poor results due to high levels of internal microcracks and porosity, and formation of intermetallic compounds and oxides, leading to poor mechanical behavior or even spontaneous failure. The main bottleneck in designing new laser-printable alloys lies in the necessity of considering the effects and non-linear interactions

of both material chemistry and processing conditions toward the final material and product properties<sup>3,4</sup>. Previous alloy design studies for laser-assisted additive manufacturing either used laboriously demanding trial-and-error approaches<sup>5–8</sup>; or adopted empirical equations<sup>9,10</sup> and thermodynamic models<sup>11–14</sup> which largely neglect the kinetic aspect of cyclic rapid solidification of a microstructure formed originally from molten feedstock particles, thus rendering the outcomes machine specific and mostly non-transferable.

The development of high-performance engineering alloys specifically tailored for laser additive manufacturing remains a formidable challenge, primarily due to their limited printability. This issue is

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particularly acute for safety-critical applications, where defect-free fabrication is essential<sup>3,4</sup>. For instance, Ni-based superalloys with high  $\gamma'$  volume fractions exhibit complex solidification behavior and a pronounced susceptibility to cracking, a consequence of their intricate multi-component compositions<sup>15</sup>. Although certain compositional modifications have been proposed to reduce cracking, these adjustments seldom account for the synergistic effects with AM process parameters<sup>16</sup>. Conversely, high-strength aluminum alloys, while possessing simpler chemistries and operating at lower temperatures, still require precise control over eutectic solidification or heterogeneous nucleation to mitigate cracking<sup>17</sup>. For both alloy families, a fundamental trade-off persists between printability and mechanical performance, which is a direct result of the complex interplay among composition, process, microstructure, and properties. Consequently, the creation of robust, AM-suitable alloys that maintain high performance across varying processing conditions represents a critical unsolved problem, necessitating integrated design strategies that simultaneously optimize both printability and target properties.

Machine learning (ML) has expanded rapidly in materials research over the past decade as advances in computing, algorithms and digitized data have enabled the identification of complex nonlinear relationships and increasingly supported data-driven alloy design<sup>18–22</sup>. However, significant challenges remain in this data-driven approach. Under the general constraints of limited sample datasets (as often the case in materials science), exclusively data-driven approaches, which are devoid of integration with physical metallurgical mechanisms, are susceptible to overfitting<sup>23</sup>. This phenomenon may lead to the generation of less insightful solutions during inverse design processes, thereby undermining design effectiveness and reliability<sup>23,24</sup>. To address these challenges, recent advances in machine learning-driven alloy design have prioritized the integration of domain-specific knowledge, such as established physics-based composition-microstructure-processing-property relationships<sup>25–29</sup>. While such approaches (e.g., cast in the form of neural networks and ensemble learning frameworks) excel at processing numerical data<sup>30,31</sup>, they face great difficulties managing qualitative information (e.g., logical frameworks or empirical guidelines). These limitations are critical in materials science, where material behavior and its interdependencies with composition, processing, and microstructure are often governed by highly nonlinear, partially empirical principles. This challenge is amplified in additive manufacturing, where domain knowledge frequently exists as semi-quantitative or qualitative models that resist straightforward encoding into numerical machine learning frameworks. Consequently, current machine learning applications in additive manufacturing remain largely confined to optimizing processing parameters or geometric design, neglecting the complex coupling between materials and processes, and therefore fall short of enabling breakthroughs in novel material systems and multifunctional capabilities<sup>32,33</sup>. Moreover, defects such as porosity and microcracks, which are persistent challenges in AM material development, exhibit heterogeneous spatial distributions within components<sup>9,34–36</sup>. Their stochastic occurrence and localized variability introduce significant complexity for traditional machine learning models, which are fundamentally reliant on deterministic input-output relationships inherent to conventional data-driven approaches. These dual challenges, namely the inability to resolve causal mechanisms in complex material interactions and the inherent variability of stochastic defect, hinder the application of machine learning in designing high-performance alloys for additive manufacturing. To address these gaps, a transformative machine learning framework is needed, capable of (1) assembling heterogeneous data (numerical, qualitative, empirical) to mitigate data scarcity and embed domain knowledge, and (2) reconciling statistical uncertainty (e.g., defect stochasticity) and model uncertainty (e.g., mean-field approximations) to ensure effective predictions under real-world AM process variability.

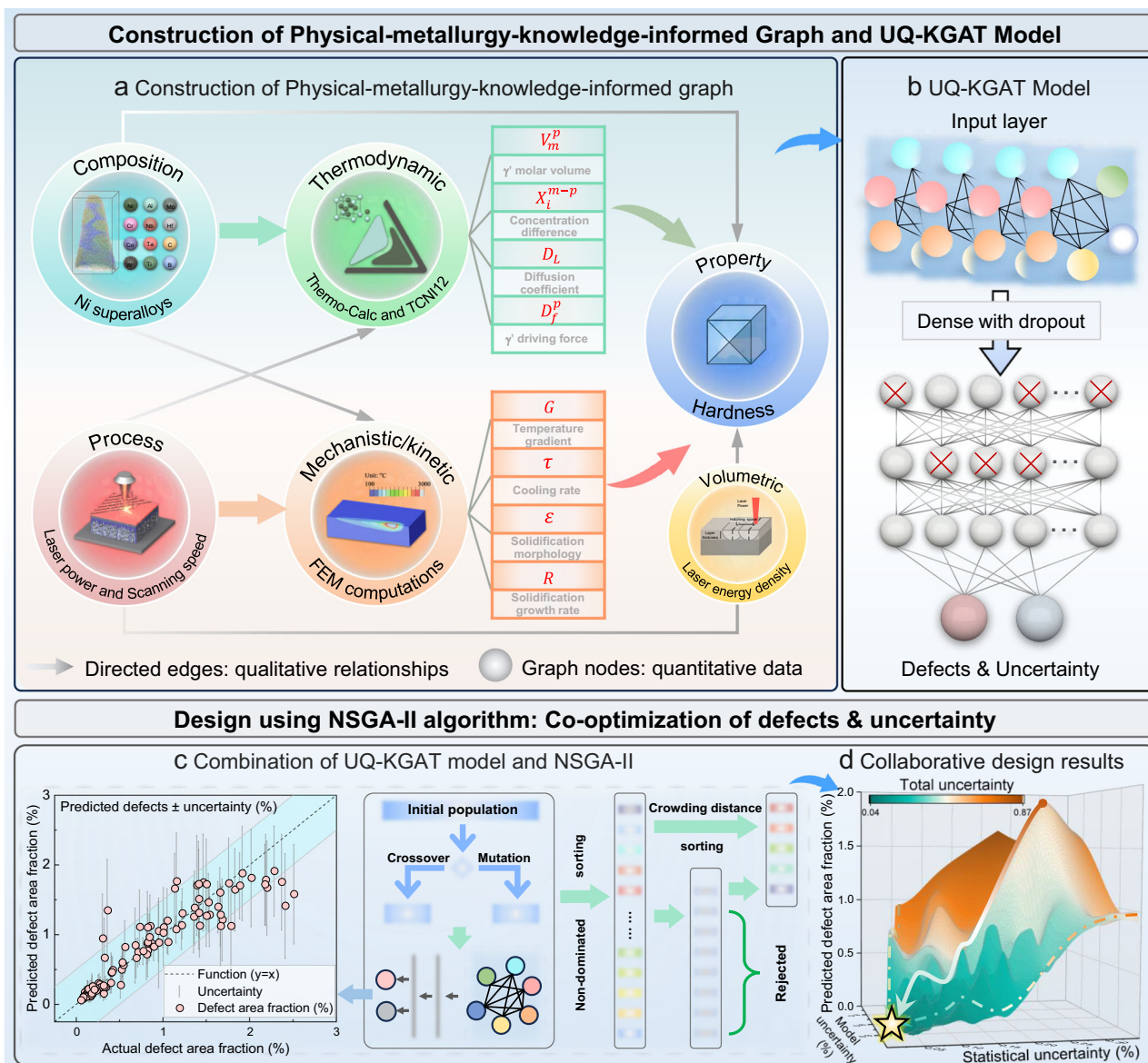
This study introduces a machine learning-driven alloy design framework that integrates Graph Neural Networks<sup>37,38</sup> (GNNs) with Knowledge Graph (KG) architectures. The framework aims to address the previously mentioned two critical challenges in adopting machine learning for additive manufacturing: embedding non-quantitative metallurgical knowledge and managing stochastic process-induced data uncertainties. By employing a hierarchical knowledge graph that explicitly encodes causal relationships across alloy chemistry, processing parameters, microstructural variables, and mechanical properties, the approach enables GNNs to prioritize physically meaningful feature interactions through domain-informed attention mechanisms. To address stochasticity in additive manufacturing (e.g., porosity and microcrack variability), observational noise modeling techniques<sup>39–41</sup> are used to disentangle measurement errors from inherent material variations. Concurrently, variational inference algorithms<sup>39,40</sup> are applied to quantify model uncertainties in model predictions, facilitating probabilistic data interpretations and strengthening resilience against sparse, noisy, or conflicting datasets.

Through this approach, two alloys have been successfully developed across multidimensional composition-process spaces, i.e., a defect-free Ni-based superalloy with exceptional printability (crack-free with a pore area fraction <0.1% across a wide processing range<sup>42,43</sup>), thermal stability (>900 °C), and mechanical strength (Ultimate tensile strength >1.2 GPa); and a novel high-performance Al alloy exhibiting exceptional printability. By unifying knowledge-guided constraints with probabilistic uncertainty quantification, the framework establishes a generalized paradigm for elucidating multiscale composition-process-property interdependencies, advancing the computationally rational design of next-generation printable alloys that harmonize performance optimization with manufacturing reliability.

## Results and discussion

### Design framework for defect-free Ni superalloys

The workflow of the current study to design a defect-free Ni superalloy for additive manufacturing is shown in Fig. 1. The approach includes two main stages: (i) the construction of a knowledge-informed graph based on physical metallurgical principles (i.e., composition-microstructure-processing-property relationships) and a Graph Attention Network (i.e., an attention-enhanced Graph Neural Network<sup>37,38</sup>, which can effectively capture empirical relationships and quantitative data structured within a knowledge graph) embedded with uncertainty quantification techniques (i.e., heteroscedastic regression<sup>39–41</sup> and Monte-Carlo Dropout<sup>39,40</sup>), which is referred to here as the UQ-KGAT model in this study, and (ii) the inverse design using Non-dominated Sorting Genetic Algorithm II (NSGA-II), owing to its widespread adoption in alloy design tasks<sup>12,23,44</sup>. For demonstrating the concept on a highly demanding model system, we next picked first a dataset of Ni superalloys fabricated by the laser directed energy deposition (L-DED) technology collected through in-house experiments. The final dataset contains 142 samples, each with 15 features (data distribution in Supplementary Table 1). These samples originate from five distinct Ni-based superalloys containing 12 elements (Al, Co, Cr, Mo, Ta, Ti, W, C, B, Nb, Hf, with Ni as the base element; see Supplementary Table 2). This constitutes a classic small-sample problem with inherent out-of-domain challenges. Across all samples, only the laser power (600–1600 W) and scanning speed (4–14 mm s<sup>−1</sup>) were varied over wide ranges (Supplementary Fig. 1). The area fractions of defects (i.e., both porosity and microcracks) in each sample were quantified via optical microscopy (OM) image analysis and served as the output labels for the model. The indentation hardness, a key screening mechanical property linked to alloy composition, microstructure and segregation profiles resulting from the L-DED process, was measured across all conditions.



**Fig. 1 | Workflow of additive manufacturable Ni superalloy design using UQ-KGAT (Uncertainty-Quantified Knowledge-informed Graph Attention network) and NSGA-II (Non-dominated Sorting Genetic Algorithm II).**

**a** Construction of a physical-metallurgy-knowledge-informed graph, where nodes represent the quantitative information such as composition, process, physical-metallurgy parameters and mechanical property respectively, while directed edges encode hierarchical qualitative relationships (e.g., composition → physical-

metallurgy parameters). **b** The UQ-KGAT model is constructed using knowledge-informed graph and uncertainty method to predict the defect level and its uncertainty per sample. **c** Coupling of the UQ-KGAT model with the NSGA-II algorithm for inverse composition-process design. Error bars indicate predicted total uncertainty. **d** Collaborative design results showing the predicted defect area fraction and uncertainty across the design space.

On top of these primary inputs (i.e., chemical composition and processing conditions), secondary inputs derived from them using finite element computations of temperature fields and solidification characteristics, and thermodynamic/kinetic calculations based on alloy compositions, along with the laser volumetric energy density levels were also used as model inputs, due to their non-negligible impact on defect formation<sup>7,45,46</sup>. Kinetic factors (refer to Supplementary Fig. 2a–d) governing the solidification characteristics (e.g., thermal gradient and cooling rate) were evaluated through calculating a heat transfer and fluid flow model using a finite element solver. Key parameters such as solidification growth rate  $R$ , maximal temperature gradient  $G$ , cooling rate  $\tau$ , and solidification morphology  $\varepsilon$  were obtained. Thermodynamic variables serve as critical quantitative descriptors governing the intrinsic stability and phase behavior of multicomponent chemical systems. The parameters were calculated

using Thermo-Calc software based on TCNI12 and MOBNI6 database (refer to Supplementary Fig. 2e–h), including the diffusion coefficients  $D_L$ , the concentration difference between the  $\gamma$  matrix and  $\gamma'$  phase  $X_i^{m-p}$ , the molar volume of the  $\gamma'$  phase  $V_m^p$  and the driving force of  $\gamma'$  phase  $D_f^p$ . Subsequently, input features from different sources were normalized using the z-score method to eliminate scale and unit differences<sup>23,44,47</sup>. Following this, a knowledge-informed graph was constructed based on physical metallurgical principles (Fig. 1a), where nodes represent quantitative information (e.g., composition, process, physical metallurgical parameters and mechanical property), and directed edges represent hierarchical qualitative relationships in materials science mechanisms, such as the connection from composition to physical metallurgical parameters, represented as (1,0) in the adjacency matrix (see Supplementary Fig. 4). A knowledge-informed graph was constructed based on the hierarchical relationships among

compositions, thermodynamic variables, processing parameters, mechanistic variables, volumetric energy density and hardness, as illustrated in Fig. 1a. Then, the Graph Attention Network model was trained using the physical-metallurgy-knowledge-informed graph, as detailed in Fig. 1b. During the modeling process, heteroscedastic regression (i.e., a method that accounts for unequal variance in residuals), was employed to model observation noise. Unlike traditional regression which assumes constant noise, this approach captures how data uncertainty varies with input variables (e.g., composition or processing parameters), reflecting real-world scenarios where measurement errors or inherent variability may depend on experimental conditions<sup>39</sup>. To address model uncertainty (i.e., limitations in model architecture or parameterization), Monte Carlo Dropout was integrated into the framework. By retaining dropout layers during inference, this technique simulates Bayesian behavior, generating probabilistic predictions that quantify the model's confidence in its outputs<sup>39,41</sup>. Together, these methods enable simultaneous evaluation of statistical uncertainty (stemming from stochastic defect distributions in AM-ed samples) and model uncertainty, providing a comprehensive error estimate for predictions of defect area fraction. Predictions are generated across a broad parameter space (see Supplementary Table 1), linking composition and processing variables to defect formation trends while transparently reporting the associated uncertainties.

In the inverse design process, secondary inputs (e.g., thermodynamic parameters, solidification mechanistic variables and volumetric energy density) and hardness values were first derived from primary data (alloy compositions and processing conditions) via machine learning models for real-time integration within the design loop (as detailed in Supplementary Note 3). This step greatly reduced the computational costs and provided critical material insights, such as hardness, which are challenging to predict accurately with conventional methods. The hierarchical relationships were encoded into a physical-metallurgy-knowledge-informed graph to serve as the model input. Building on this framework, the UQ-KGAT model, which serves as the objective function to predict defect level and uncertainty, was integrated with the dual-objective genetic algorithm NSGA-II (Fig. 1c) for the simultaneous optimization of chemical compositions and process conditions, as shown in Fig. 1d. The strategy enabled coupled composition-process design, efficiently exploring the vast composition-process space to identify novel alloy compositions and laser processing parameters that minimize defects and uncertainty. Finally, newly designed alloys were fabricated via L-DED using the optimized parameters, and their defect levels and hardness were experimentally validated, with physical mechanisms analyzed to interpret the outcomes.

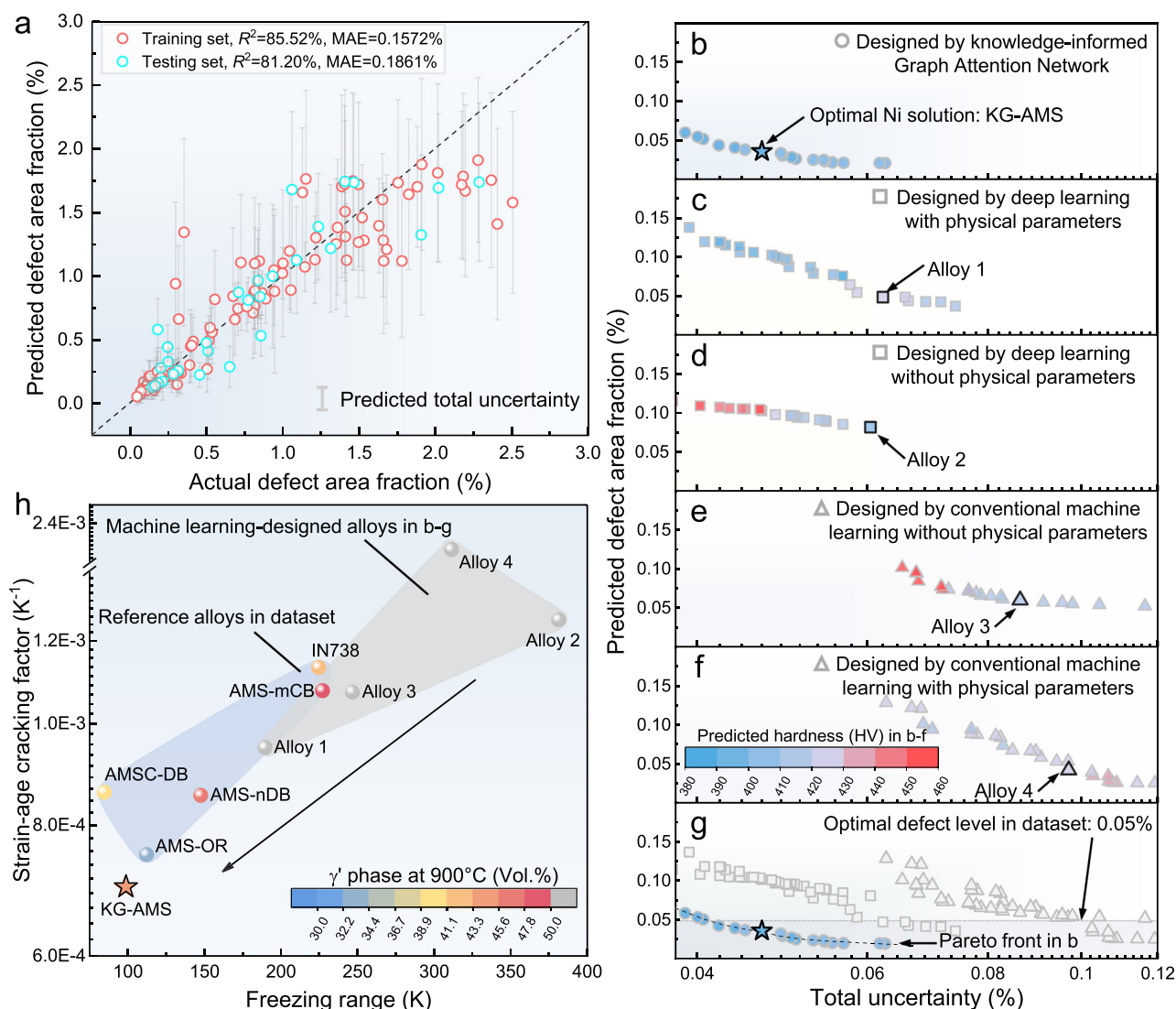
### Benchmarking UQ-KGAT against ML and thermodynamic models

The effectiveness of this framework was validated by benchmarking its defect prediction and composition design performance against conventional machine learning and thermodynamic models, as shown in Fig. 2. For defect prediction, different machine learning algorithms, e.g., Gaussian Process Regression (GPR) and Uncertainty-Quantified Convolutional Neural Network (UQ-CNN), were evaluated. Their  $R^2$  and MAE values are directly compared in Supplementary Fig. 5. Current machine learning models face great challenges in accurately predicting the defect area fractions, with even the proposed Uncertainty-Quantified Knowledge-informed Graph Attention Network (UQ-KGAT) achieving only an average squared correlation coefficient ( $R^2$ ) of 76.7%, and a mean absolute error (MAE) of 0.238% (20 random splits). This limitation stems largely from the stochastic spatial distribution of defects in AM-ed samples, which makes it difficult to capture bulk defect levels reliably via localized two-dimensional optical microscopy (OM) analysis. However, the UQ-KGAT model explicitly incorporates

both statistical uncertainty (inherent to AM sample variability) and model uncertainty (model structure limitations) during training, achieving effective prediction of defect area fraction with quantified uncertainty, as shown in Fig. 2a. Supplementary Fig. 6a and b further reveal that statistical uncertainty dominates over model uncertainty, confirming that stochastic defect distribution—not model architecture—is the primary barrier to accurate predictions in conventional machine learning approaches.

To identify optimal alloy compositions, initial trials employed KGAT models incorporating distinct uncertainty types (Supplementary Fig. 6c and d) to assess their impact on design accuracy. Results demonstrate that a dual-objective optimization strategy to simultaneously minimize total uncertainty (statistical + model) and defect area fraction, is critical for identifying alloys with combined low defects and low uncertainty. The roles of the physical-metallurgy-knowledge-informed graph convolutions were further investigated by comparing the design results of different machine learning models, as shown in Fig. 2b–g. The UQ-KGAT model, leveraging domain knowledge via graph-based learning, identified the novel alloy denoted KG-AMS (Knowledge Graph-based Additive Manufacturable Superalloy), which exhibits markedly reduced defect levels and uncertainties, as shown in Fig. 2b. In contrast, the Pareto front solution sets generated by deep learning model UQ-CNN (Convolutional Neural Network embedded with uncertainty quantification techniques, see Fig. 2c, d) and conventional machine learning model UQ-ANN (Artificial Neural Network embedded with uncertainty quantification techniques, in Fig. 2e, f), generally exhibit higher defects and uncertainties, as further summarized in Fig. 2g. Notably, designs obtained with no physical metallurgical information involved generally shift to an inferior domain with higher levels of uncertainty or defect fraction. Moreover, reducing the training data size had only a minor impact on the design performance of the proposed UQ-KGAT model (as detailed in Supplementary Fig. 7), which further demonstrates that knowledge-graph integration can enhance the extrapolation ability of AI models<sup>48</sup>. The superior performance of UQ-KGAT underscores the necessity of integrating quantitative physical models and non-quantifiable domain knowledge (e.g., microstructure-property relationships, solidification mechanics) into machine learning frameworks for inverse design tasks in materials science.

Although the proposed framework aims at minimizing the overall defect level, cracking represents the most critical and detrimental defect in additive manufacturing, and is a primary focus in studies of additively manufactured Ni superalloys<sup>9,12,42</sup>. Therefore, the crack susceptibility of alloys designed by machine learning models was further analyzed through appropriate thermodynamic criteria, with the distinct mechanisms underlying different defect types set as a key focus for future investigation. Specifically, as shown in Fig. 2h, two thermodynamic cracking criteria that are commonly employed to assess the likelihood of cracking in additive manufacturing, i.e., the freezing range (FR) factor and the strain-age cracking (SAC) factor, were selected and calculated for the newly designed alloys, and the results were compared with several existing Ni superalloys (as detailed in Supplementary Note 7). Thermodynamically, the newly designed alloy KG-AMS exhibits optimal printability with the lowest susceptibility to both hot cracking (FR) and cold cracking (SAC), well outperforming the alloys designed using conventional machine learning models and deep learning models, as well as the existing commercial Ni superalloys. Unexpectedly, the results in Fig. 2h indicate that, compared to the existing printable and hard-to-print alloys in the dataset, the preferred KG-AMS alloy has a relatively high fraction of  $\gamma'$  phase at the target service temperature. Computational validation confirms that the proposed machine learning framework, which combines a physics-informed graph neural network rooted in metallurgical principles with Bayesian uncertainty quantification, achieves physically consistent and computationally



**Fig. 2 | Design results of additive manufacturable Ni superalloys and computational validation.** **a** Prediction of defect area fractions using UQ-KGAT model for the Ni-superalloy dataset containing  $n = 142$  samples. Data were evaluated using 20 random 4:1 training/testing splits. Error bars indicate predicted total uncertainty. **b–g** Comparison of design results using different machine learning methods: **b** UQ-KGAT developed in this work, yielding designed alloy KG-AMS, **c** deep learning model—Uncertainty-Quantified Convolutional Neural Network (UQ-CNN) trained with physical parameters, yielding designed Alloy 1 and **d** trained without physical parameters, yielding designed Alloy 2, **e** conventional machine learning model—

Uncertainty-Quantified Artificial Neural Network (UQ-ANN) trained with physical parameters, yielding designed Alloy 3 and **f** trained without physical parameters, yielding designed Alloy 4, **g** overall comparison of Pareto fronts obtained from different models. **h** Thermodynamic validation showing  $\gamma'$  phase content at 900 °C versus cracking criteria (freezing range and strain-age crack factor). The arrow in **c** denotes the compositional trend toward alloys with reduced crack susceptibility. Colors in **b–g** indicate predicted hardness. Colors in **h** indicate  $\gamma'$  phase content at 900 °C. No frequentist inferential statistical tests were performed. Source data are provided as a Source Data file.

efficient alloy design, surpassing conventional methods in predictive accuracy and scalability. By harmonizing domain knowledge with probabilistic modeling, the framework accelerates discovery cycles while rigorously adhering to metallurgical constraints.

### Experimental validation of defect levels and model performance

To substantiate the practicality of the design approach, the newly designed KG-AMS alloy was prepared according to the chemical composition listed in Table 1. A diverse range of printing parameters around the optimal processing condition (1500 W and 10 mm s<sup>-1</sup>) was employed to validate the processing parameter design results, as well as to explore the processing window of the KG-AMS alloy to achieve crack-free bulk samples. The defect area fractions of the as-printed specimens were quantified using stereological assessment of digitized optical micrographs, with the raw data displayed in Supplementary Fig. 9.

Figure 3a compares the defect-hardness correlation of the KG-AMS alloy samples in the as-printed condition (yellow stars) with 142 reference alloy samples from the dataset, covering a wide range of LDED processing parameters. Specifically, the as-printed KG-AMS alloy exhibits ultralow defect area fractions (0.037%–0.133%, corresponding to 1/defect area fraction% = 27.03–7.51) and concurrently higher hardness values of 391–417 HV, surpassing printable alloys in the dataset (blue dots) while avoiding the cracking propensity of high-hardness alloys (red dots), as further detailed in Supplementary Fig. 10. Thus, the newly designed alloy KG-AMS achieves a superior balance between printability and mechanical properties, reaching the upper limit of hardness within the printable range.

The prediction accuracy of the UQ-KGAT model was further validated by comparing the experimentally measured defect area fractions of the KG-AMS alloy with the model predictions, as presented in Fig. 3b. The actual defect area fraction of the alloy is closely

**Table 1 | The alloy composition of new alloy KG-AMS (in wt.%)**

| Alloy    | Al   | Co    | Cr   | Mo   | Ta   | Ti   | W    | C    | B    | Nb   | Hf    | Ni   |
|----------|------|-------|------|------|------|------|------|------|------|------|-------|------|
| Designed | 6.31 | 14.59 | 5.06 | 0.25 | 1.56 | 0.14 | 2.25 | 0.21 | 0.01 | 2.1  | 0.006 | Bal. |
| Actual   | 6.33 | 14.24 | 5.12 | 0.31 | 1.54 | 0.08 | 2.38 | 0.2  | 0.01 | 2.14 | 0.011 | Bal. |

in line with the predicted trend of the model, exhibiting an MAE of 0.0188%. Optical microscopy analysis (Fig. 3c–f) reveals parameter-robust manufacturability. The optimized parameter set (Fig. 3d) yields an ultralow defect area fraction of 0.037%, which is consistent with the porosity determined by X-ray computed tomography (an average porosity of 0.038%, as detailed in Supplementary Fig. 11). Even the worst-case specimen (a defect area fraction of 0.13% in Fig. 3e) shows only sparse porosity compared to reference alloy samples in the dataset. The good integrity of the printed bulk samples, combined with their low sensitivity to processing parameter fluctuations, reaffirms the excellent printing performance of the designed alloy KG-AMS.

Figure 3g demonstrates that the model-predicted hardness values align with experimental measurements across 18 distinct printing parameter sets (MAE = 4.65 HV), further underscoring the predictive capability of the alloy design framework. Microstructural evolution governed by energy input is revealed in Fig. 3h–k, showing an increase in  $\gamma'$  phase size with laser power. To investigate the reason for the enhanced hardness of the KG-AMS alloy compared to reference printable alloys in the dataset, the strengthening mechanisms including the precipitation strengthening effects and the solid solution strengthening effects were considered. To this aim, the content and the mean size of the  $\gamma'$  phase of different alloys in the dataset were characterized under various AM processing parameters. The designed alloy has a higher  $\gamma'$  phase content ( $47.74 \pm 2.1\%$  vs.  $40.74 \pm 3.5\%$  in reference printable alloys) while maintaining thermal-history-resistant architecture ( $\gamma'$  size =  $87.38 \pm 14.72$  nm vs.  $51.19 \pm 9.3$  nm; see the following section for a detailed discussion). This trend holds true for specimens produced using lower volumetric energy density as well, as quantified in Supplementary Fig. 12. Following such analysis, the strengthening contributions of AM-built alloys were further clarified based on the empirical formulas, as detailed in Supplementary Note 9. The results indicate that the designed alloy KG-AMS exhibits higher solid solution strengthening and precipitation strengthening effects (e.g., a total yield strength ranging from 520–612 MPa vs. 500–563 MPa in reference printable alloys), thus resulting in its relatively higher hardness level (391–417 HV vs. 367–401 HV).

Benefiting from the advantages of the UQ-KGAT model, the underlying mechanism for the newly designed alloy's optimal combination of printability and strength can be unveiled by the mechanism mining method, such as the Integrated Gradients (IGs) method, which is a sensitivity analysis technique that quantifies input feature contributions through path-integrated gradients<sup>49</sup>, as detailed in Supplementary Note 10. The results reveal that those elements that promote formation of  $\gamma'$  phase, such as Nb, and the thermodynamic variables, i.e., the driving force for  $\gamma'$  phase precipitation and molar volume of  $\gamma'$  phase, have the greatest significance. The thermodynamic and kinetic features of the  $\gamma'$  phase, predicted to be the dominating factors determining the excellent properties of KG-AMS alloy, were experimentally studied in more detail and the results are reported in the following section.

#### $\gamma/\gamma'$ elemental partitioning and lattice misfit in KG-AMS

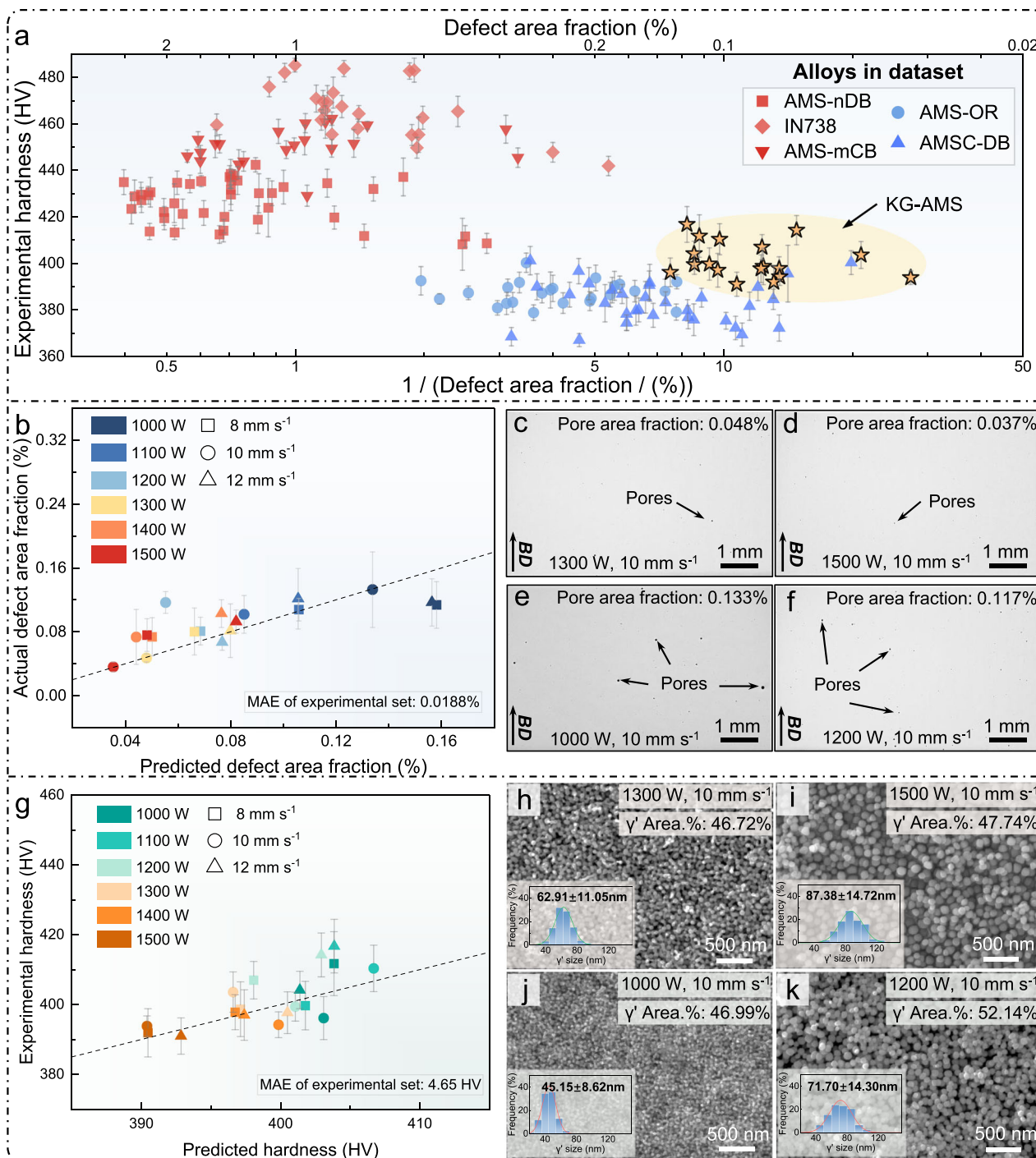
Analysis of the mechanism mining results revealed that the superior printability of the newly designed KG-AMS alloy stems from the controlled precipitation thermodynamics and kinetics of the  $\gamma'$  phase. Characterization of the  $\gamma'$  phase across laser processing parameters and sample heights (Fig. 4a–d and Supplementary Fig. 15a–f)

demonstrated a uniform particle size distribution in KG-AMS, with minimal sensitivity to laser processing conditions. In stark contrast, the crack-prone reference alloy AMS-mCB exhibited pronounced  $\gamma'$  size heterogeneity ( $44.75 \pm 8.2$  nm to  $128.98 \pm 29.8$  nm; Supplementary Fig. 15g–l) alongside heightened susceptibility to laser parameter fluctuations, as further confirmed in Supplementary Fig. 16. This variability, particularly evident across sample heights, highlights the critical role of  $\gamma'$  stability in mitigating process-induced defects and ensuring consistent AM performance.

To further validate the key factors identified by the UQ-KGAT model, atom probe tomography (APT) was used to probe the elemental partitioning between  $\gamma$  and  $\gamma'$  phases in KG-AMS at different sample heights: the substrate-adjacent region (2.5 mm from substrate, rapid cooling) and the bulk region (7.5 mm from the substrate, cyclic thermal exposure). Despite exposure to divergent thermal conditions, both regions exhibited nearly identical elemental distributions (Fig. 4e–k). Nb and Ta showed strong  $\gamma'$  phase partitioning, with  $\gamma/\gamma'$  partition coefficients  $k_{\gamma/\gamma'} \approx 10$ , while Cr and Co preferentially segregated to the  $\gamma$  matrix. This behavior aligns with STEM-based elemental mapping (Supplementary Fig. 18), confirming that the alloy's compositionally stabilized  $\gamma/\gamma'$  architecture resists thermal-gradient-induced microstructural destabilization—a key factor enabling uniform  $\gamma'$  distributions independent of AM process fluctuations.

Figure 4l, m present the neutron diffraction analysis of the KG-AMS alloy at different spatial locations, revealing uniform and minimal lattice misfit (0.05% for the bulk region vs. 0.07% for the substrate-adjacent region of the as-built sample). In contrast, the neutron diffraction results for the cracked alloy AMS-mCB, presented in Supplementary Fig. 19, demonstrate a higher lattice misfit level across different locations, with the bulk region exhibiting greater misfit (0.12%) than the substrate-adjacent region (0.08%), implying substantial tensile residual stresses near the substrate-adjacent regions<sup>50</sup>. It becomes apparent that the unique and robust elemental distribution between the  $\gamma$  and  $\gamma'$  phases of the KG-AMS alloy contributes to its slow precipitation and coarsening kinetics of the  $\gamma'$  phase, consistent with the mechanism uncovered by the UQ-KGAT model. This feature greatly enhances the thermal stability and minimizes the lattice misfit despite the repeated precipitation and dissolution events induced by laser cyclic heating inherent to AM processes. Thus, these findings further underscore the considerable value of integrating both quantitative and qualitative physical mechanisms into machine learning frameworks, accelerating alloy design and mechanism discovery in materials science.

For 3D-printed alloys, a balanced combination of tensile strength and ductility is crucial for ensuring the structural integrity of complex components<sup>15</sup>, especially for Ni-based superalloys, where severe strength degradation commonly occurs during high-temperature service<sup>12,51</sup>. Therefore, the primary design focus was placed on defect level and room-temperature hardness, as these are directly supported by the current dataset, while the direct optimization of tensile and creep properties remains a promising direction for future work. Nevertheless, the tensile properties and creep performance of the KG-AMS alloy were also evaluated, as detailed in Supplementary Fig. 20. The KG-AMS alloy exhibits ultimate tensile strength and elongation of 1307 MPa and 22.2% at room temperature (see Supplementary Fig. 20a and b), and 655 MPa and 7.5% at high temperature (900 °C), outperforming the crack-free alloy AMSC-DB from the input database (see Supplementary Fig. 20c and d).

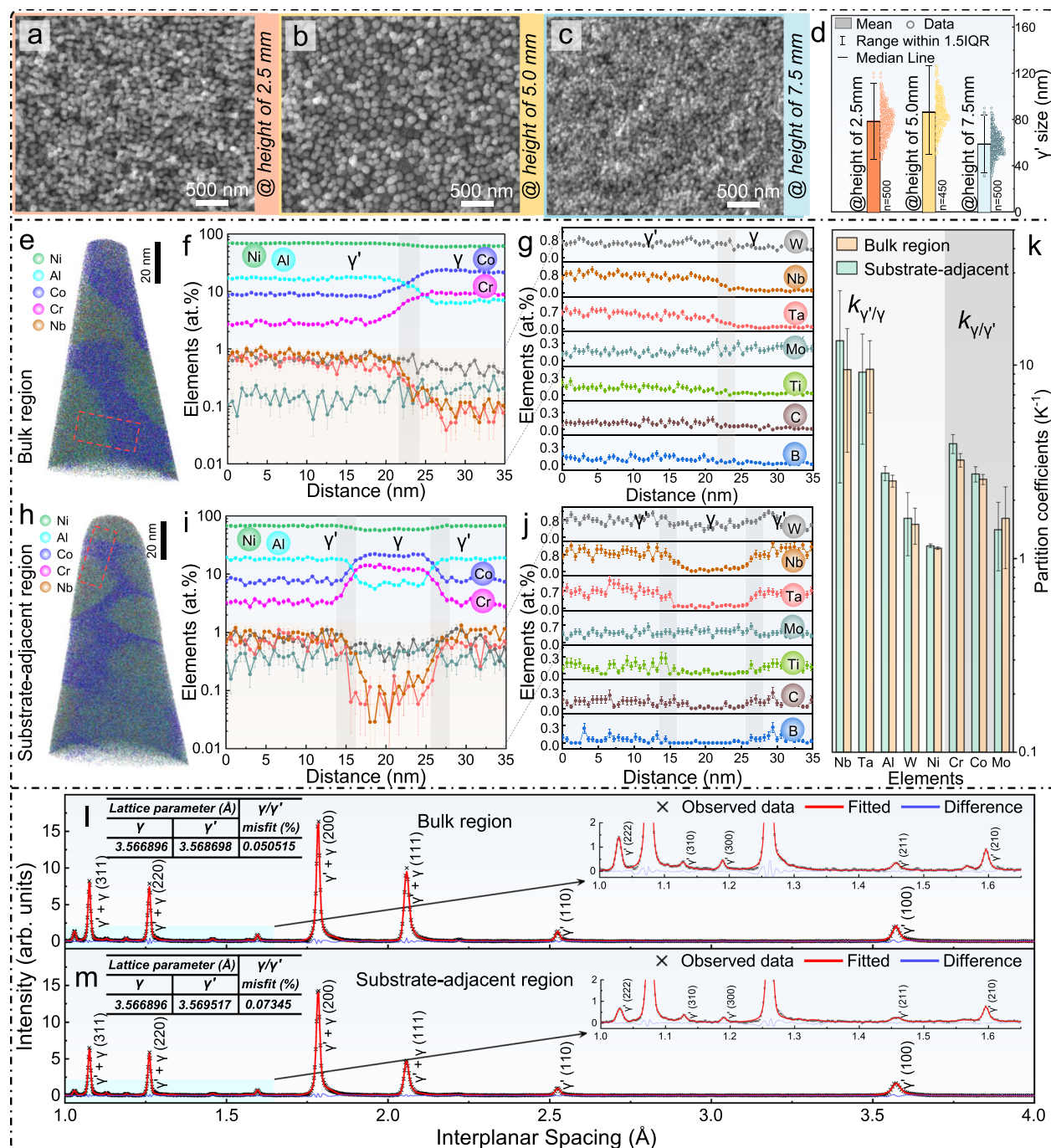


**Fig. 3 | Experimental validation of designed alloy KG-AMS and comparison with existing materials. a** Hardness-defect correlation map comparing KG-AMS with 142 reference alloy-processing samples in the Ni-superalloy dataset. Yellow stars denote KG-AMS samples, red markers denote crack-prone reference samples and blue markers denote printable crack-free reference samples. Error bars indicate SD from  $n=14$  hardness indents per sample. **b** Comparison between model-predicted and experimentally measured defect area fractions for  $n=18$  KG-AMS printing parameter sets. Experimental defect area fractions were obtained from  $n=5$  optical-microscopy image fields per sample; error bars indicate SD. **c–f** Representative optical micrographs of KG-AMS alloy

samples under different laser processing parameters. **g** Comparison between model-predicted and experimentally measured hardness values for  $n=18$  KG-AMS printing parameter sets. Experimental hardness values were obtained from  $n=14$  Vickers indents per sample; error bars indicate SD. **h–k** Representative SEM images of  $\gamma'$  precipitates in KG-AMS under different laser processing parameters, with a scanning speed of 10 mm s<sup>-1</sup> and laser power of **h** 1300 W, **i** 1500 W, **j** 1000 W, and **k** 1200 W. Insets show gamma-prime size distributions, with  $n=501$ , 450, 502 and 630  $\gamma'$  precipitates for (**h–k**), respectively; values are mean  $\pm$  SD. No frequentist inferential statistical tests were performed. Source data are provided as a Source Data file.

Moreover, when tested under conditions of 900 °C/200 MPa and 800 °C/400 MPa, the heat-treated KG-AMS alloy demonstrated a creep rupture life of 97.8 h and 70.7 h, respectively, outperforming other existing printable Ni superalloys (see Supplementary Fig. 20e

and f). We postulate that the excellent tensile and creep properties primarily stem from the uniform distribution of the  $\gamma'$  precipitate and the minimized  $\gamma/\gamma'$  lattice misfit. However, as with conventional superalloys<sup>52,53</sup>, there is likely to be a considerable potential for high-



**Fig. 4 | Spatial distribution results of the  $\gamma'$  precipitates, elemental distribution in  $\gamma/\gamma'$ , and lattice misfit in KG-AMS.** **a–c** SEM images of the  $\gamma'$  precipitates in the KG-AMS bulk sample printed at 1500 W and 10 mm s<sup>-1</sup>, measured at heights of **a** 2.5 mm, **b** 5.0 mm and **c** 7.5 mm from the substrate. **d**  $\gamma'$  size distributions at the three heights. Dots represent individual  $\gamma'$  precipitates. Box plots show median center lines, interquartile-range box limits and whiskers extending to 1.5 times the interquartile range; squares indicate means. The sample sizes are  $n = 500$  precipitates at 2.5 mm,  $n = 450$  precipitates at 5.0 mm and  $n = 500$  precipitates at

7.5 mm. **e–j** Atom probe tomography results of elemental partitioning behavior in  $\gamma/\gamma'$ : **e–g** the bulk region of the as-built sample, and **h–j** the substrate-adjacent region of the bulk sample. Colors denote the labelled elements shown in each panel. **k** Elemental partition coefficients between  $\gamma$  and  $\gamma'$  phases in the bulk and substrate-adjacent regions. **l, m** Neutron diffraction (ND) patterns and fitted  $\gamma/\gamma'$  lattice parameters for **l** the bulk region and **m** the substrate-adjacent region of KG-AMS bulk sample. No frequentist inferential statistical tests were performed. Source data are provided as a Source Data file.

temperature properties enhancement through post-fabrication heat treatment optimization. It is also noteworthy that, while the current results confirm the alloy's intrinsic resistance to cracking under standard testing conditions, further validation on larger components (such as vertical builds exceeding 100 mm), would be valuable to fully assess the influence of residual stress accumulation, particularly if transferring to other AM processes.

Having validated the framework for printable superalloys, we demonstrate its versatility by applying it to design a high-strength printable aluminum alloy, detailed in the following section.

#### Extension of the UQ-KGAT design framework to Al alloys

To further validate the generality of the UQ-KGAT model, a new printable aluminum alloy was designed using literature-derived

data<sup>54–65</sup>. Detailed modeling procedures are provided in Supplementary Note 14. The optimal UQ-KGAT model demonstrated high predictive accuracy on the testing set ( $R^2 = 95.21\%$ ,  $\text{MAE} = 0.3501\%$ ), with predicted uncertainty showing an inverse correlation with the density of AM-processed samples, consistent with established defect prediction trends (Fig. 5a). Pareto optimization was employed to identify alloy compositions that successfully balance printing quality with mechanical performance (Fig. 5b). The resulting Pareto-optimized candidates were predicted to exhibit exceptional printability, with relative densities between 99.9–100% and low uncertainties of 0.04–0.08%, alongside enhanced mechanical performance (hardness: 113–123 HV).

From this Pareto front, the alloy designated KG-AMAA (Knowledge Graph-based Additive Manufacturable Al Alloy) was selected for its superior predicted properties: a relative density of 99.99% (exceeding the dataset benchmark of 99.98%) and a low uncertainty of 0.063% (composition provided in Table 2). Thermodynamic analysis revealed favorable non-equilibrium solidification characteristics for this alloy. The formation of primary  $\text{Al}_3\text{Sc}$  phases during initial solidification provides potent heterogeneous nucleation sites, refining the  $\alpha\text{-Al}$  matrix to mitigate epitaxial grain growth, residual stress, and cracking risks<sup>4,57,66</sup>, as shown in Supplementary Fig. 23a. Furthermore, the alloy exhibits a narrow critical solidification interval (38.4 K), indicating low hot-cracking susceptibility. Equilibrium calculations also predict ~10 vol.% of various precipitates at lower temperatures (shown in Supplementary Fig. 23b), suggesting a strong potential for precipitation strengthening and excellent mechanical properties.

The designed KG-AMAA alloy was experimentally validated using laser powder bed fusion (L-PBF). As shown in Fig. 5c–e, the alloy demonstrated superior printability across a wide range of processing parameters (detailed in Supplementary Fig. 24), achieving crack-free fabrication with defect levels predominantly below 0.1%. The optimal processing parameters were identified at a laser power of 350 W and a scanning speed of  $1100 \text{ mm s}^{-1}$  (volumetric energy density of  $106.1 \text{ J mm}^{-3}$ ), minimizing the defect level to 0.03% (Fig. 5d). Microstructural analysis via EBSD revealed a fine-grained microstructure, with melt pool boundaries consisting of cellular grains ( $3.9 \pm 1.3 \mu\text{m}$ ) and melt pool interiors exhibiting a mixture of columnar and cellular grains ( $12.7 \pm 3.3 \mu\text{m}$ ) (Fig. 5f, g); this heterogeneity can be attributed to the extreme thermal conditions inherent to L-PBF and the associated solidification pathway, driving the synergistic precipitation of multiple phases in the KG-AMAA alloy (see Supplementary Fig. 23).

The experimentally measured properties of the KG-AMAA alloy were benchmarked against 163 reference alloys from the dataset (Fig. 5h). The fabricated alloy achieved a superior combination of high hardness ( $128.3 \pm 3.99 \text{ HV}$ ) and exceptional relative density ( $99.96 \pm 0.019\%$ ), outperforming all reference alloys and confirming the model's success in guiding the design of an aluminum alloy that optimally balances printability and mechanical performance.

The successful design and experimental validation of a high-performance aluminum alloy, following a similar achievement in the nickel-based superalloy system, robustly demonstrates the generalizability and power of the UQ-KGAT framework. Its ability to accurately navigate complex composition-property-process relationships across distinct material systems proves its potential as a versatile and transformative tool. This work establishes a robust, data-driven pathway that can significantly accelerate the creation of next-generation, high-performance alloys specifically tailored for the unique demands of additive manufacturing.

In summary, we developed a generally applicable machine learning framework for alloy design that simultaneously optimizes chemical compositions and processing conditions. Central to this framework is the Knowledge-informed Graph Attention Network embedded with uncertainty quantification techniques (UQ-KGAT), which integrates the hierarchical physical-metallurgy relationships spanning alloy

compositions, AM processing conditions, solidification mechanistic variables, thermodynamic variables, and hardness property—to effectively predict defect levels and uncertainties in AM-fabricated alloys. The main challenge in developing this general approach was to integrate, on the one hand, precise thermodynamic data, and on the other hand, empirical and often imprecise knowledge such as process conditions into a unified framework. Applied to Ni superalloys, probably the most complex alloy family used in industry, the approach successfully developed KG-AMS, an AM optimized alloy exhibiting exceptional printability and mechanical strength. Its underlying defect-mitigation mechanisms were revealed through data-driven mechanism mining and experimental validation. Demonstrating broader utility, the framework also engineered a high-strength printable Al alloy KG-AMAA, achieving simultaneous optimization of printability and mechanical properties. This newly constructed machine learning framework provides a highly flexible alloy design paradigm which can integrate qualitative domain knowledge, quantitative physical models, and machine learning strategies, allowing for elucidating multiscale composition-process-property interdependencies. Beyond single alloy systems, the framework exemplifies the Artificial Intelligence for Science (AI4Sci) paradigm, offering a transferable methodology for accelerating the discovery of AM-adapted materials across diverse alloy families.

## Methods

### Data preprocessing

All numerical input features were standardized independently using the z-score transformation<sup>23,44,47</sup> to place features with different units and numerical ranges on a comparable scale. For sample  $i$  and feature  $j$ , the standardized value was calculated as:

$$z_{ij} = \frac{x_{ij} - \mu_j}{\sigma_j} \quad (1)$$

where  $x_{ij}$  is the original value, and  $\mu_j$  and  $\sigma_j$  are the mean and standard deviation of feature  $j$ , respectively.

The UQ-KGAT model and the conventional machine learning algorithms were implemented in Python using PyTorch and scikit-learn. The data were randomly divided into training and testing sets following a ratio of 4:1. To assess the sensitivity of model performance to random partitioning, this procedure was repeated 20 times. Model performance was evaluated using the squared correlation coefficient ( $R^2$ ) and mean absolute error (MAE). The formulas for these metrics are given below:

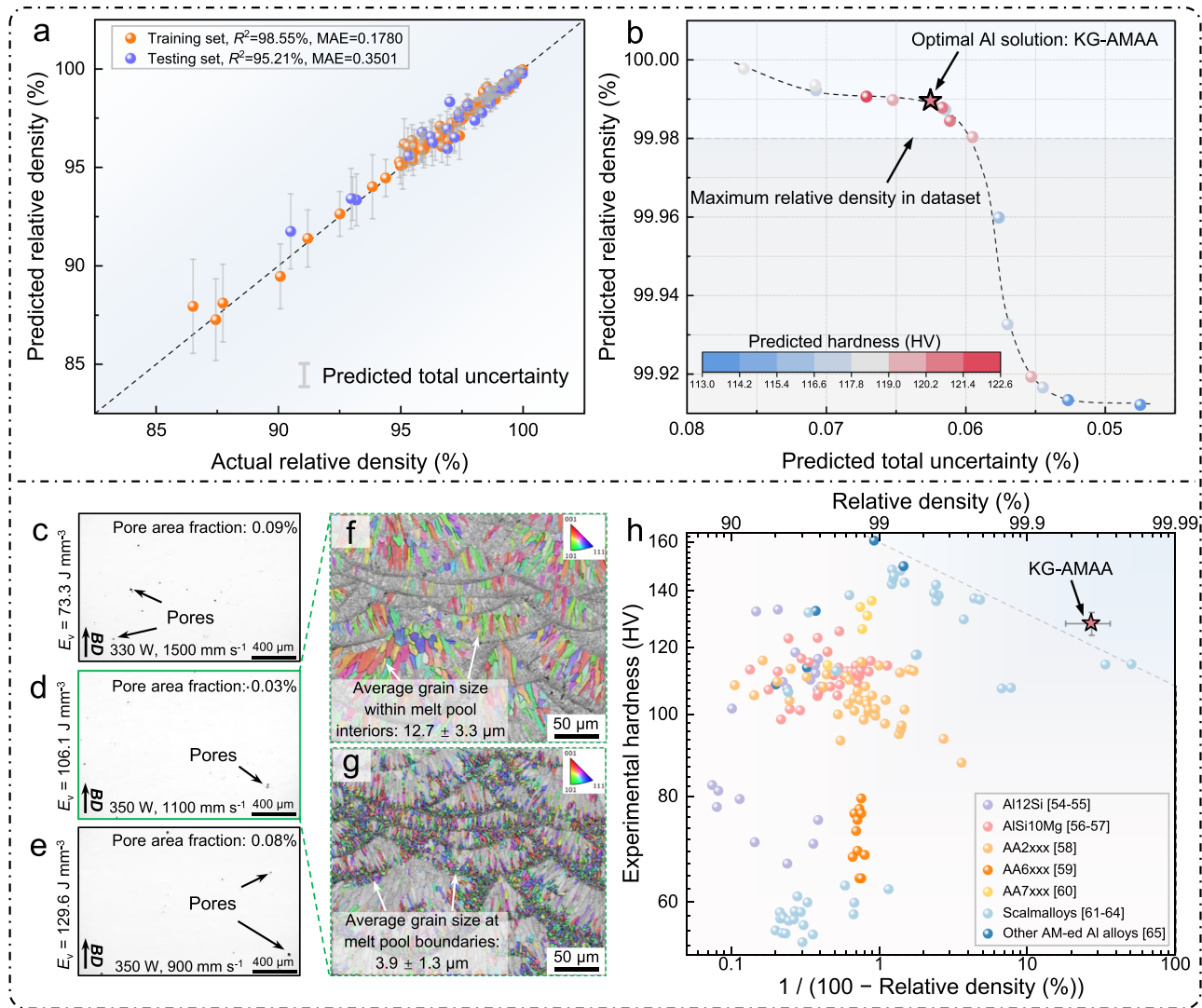
$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |f(x_i) - y_i| \quad (2)$$

$$R^2 = \frac{(n \sum_{i=1}^n f(x_i) y_i - \sum_{i=1}^n f(x_i) \sum_{i=1}^n y_i)^2}{(n \sum_{i=1}^n f(x_i)^2 - (\sum_{i=1}^n f(x_i))^2) (n \sum_{i=1}^n y_i^2 - (\sum_{i=1}^n y_i)^2)} \quad (3)$$

where  $n$  is the number of samples,  $f(x_i)$  denotes the model prediction for the  $i$ -th sample (with input features  $x_i$ ), and  $y_i$  is the corresponding experimentally measured value.

### Construction of the KGAT model

Graph attention networks (GATs) were applied due to the high efficiency in learning and mining of graph data structures<sup>37,38</sup>, while the combination of graph attention mechanisms and physical-metallurgy-knowledge-informed graphs can further enhance the model's prediction accuracy, interpretability, and generalization capabilities, even with limited data<sup>48</sup>. First, a knowledge-informed graph is used to convolve the input features, which include material compositions, processing parameters, thermodynamic variables, solidification



**Fig. 5 | Extension results of the UQ-KGAT framework to high-strength Al alloys.** **a** Prediction of relative density using the UQ-KGAT model for the Al-alloy dataset containing  $n = 163$  literature-derived samples. Error bars indicate predicted total uncertainty. **b** Design results of AM-ed Al alloys, showing predicted relative density, total uncertainty and hardness. **c–e** Representative optical micrographs of KG-AMAA alloy samples produced by laser powder bed fusion at different volumetric energy densities, with pore area fractions labelled in each panel. **f, g** EBSD inverse pole figure (IPF)

results of **d** (sample produced at 350 W and 1100 mm s<sup>-1</sup>), showing **f** mixed columnar and cellular grains within melt pool interiors and **g** fine cellular grains at melt pool boundaries. Grain-size values are reported as mean  $\pm$  SD. **h** Comparison of experimental hardness and relative density for KG-AMAA with  $n = 163$  reference AM-ed Al alloys from the Al-alloy dataset, including Al12Si<sup>54,55</sup>, AlSi10Mg<sup>56,57</sup>, AA2xxx<sup>58</sup>, AA6xxx<sup>59</sup>, AA7xxx<sup>60</sup>, Scalpallloys<sup>61–64</sup> and other AM-ed Al alloys<sup>65</sup>. No frequentist inferential statistical tests were performed. Source data are provided as a Source Data file.

**Table 2 | The compositions for the newly designed aluminum alloy KG-AMAA (in wt.%)**

| Alloy    | Al   | Si   | Fe   | Cu   | Mg   | Sc   | Zr    | Mn   | Zn   | Ni   |
|----------|------|------|------|------|------|------|-------|------|------|------|
| Designed | Bal. | 4.41 | 0.2  | 2.63 | 0.11 | 1.08 | 0.001 | 0.47 | 0.4  | 0.25 |
| Actual   | Bal. | 4.62 | 0.21 | 2.59 | 0.17 | 0.99 | 0.01  | 0.52 | 0.54 | 0.25 |

variables, and property variables. The knowledge-informed graph is defined as  $G = (V, E)$ , where  $V$  is the set of nodes representing the distinct physical variables and  $E \subseteq V \times V$  is the set of directed edges encoding known physical relationships between them. An edge  $(j, i) \in E$  indicates that node  $j$  influences node  $i$ . The initial representation of each node  $i$  is  $\mathbf{h}_i^{(0)} \in \mathbb{R}^{d_0}$ , which captures the raw feature value of the corresponding physical variable. In the input layer, all neighboring nodes are initially assumed to be equally important<sup>38</sup>. The layer takes the node representations  $\{\mathbf{h}_i | i \in V\}$  and the edge set  $E$  and updates each node representation  $\mathbf{h}_i'$  using the general neighborhood

aggregation framework (Eq. 4):

$$\mathbf{h}_i' = f_{\theta}(\mathbf{h}_i, \text{AGGREGATE}(\{\mathbf{h}_j | j \in \mathcal{N}_i\})) \quad (4)$$

where  $\mathcal{N}_i$  denotes the set of neighboring nodes of node  $i$ , and the aggregation operation is taken as summation. In the attention layer, a score function (Eq. 5) computes the importance of each edge  $(j, i)$ :

$$e_{ij} = \text{LeakyReLU}(\mathbf{a}^T [\mathbf{W}_i \parallel \mathbf{W}_j]) \quad (5)$$

Here,  $\mathbf{W}$  is a learnable weight matrix that linearly transforms the node features,  $\parallel$  denotes vector concatenation, and  $\mathbf{a}$  is a learnable weight vector of the attention mechanism. The attention coefficients are then normalized across all neighbors using the SoftMax function (Eq. 6):

$$\alpha_{ij} = \text{softmax}_j(e_{ij}) = \frac{\exp(e_{ij})}{\sum_{k \in \mathcal{V}_i} \exp(e_{ik})} \quad (6)$$

The updated representation of node  $i$  is obtained by a weighted average of the transformed neighbor features, followed by a non-linearity  $\sigma$  (Eq. 7):

$$\mathbf{h}'_i = \sigma \left( \sum_{j \in \mathcal{V}_i} \alpha_{ij} \mathbf{W} \mathbf{h}_j \right) \quad (7)$$

Finally, a multi-head attention mechanism is used to enhance the stability of the model. The results of  $K$  independent attention heads are averaged by Eq. (8) to obtain the final output feature representation, which is then passed through a fully connected layer to obtain the defect prediction results<sup>37</sup>. For details of the model parameters, please refer to the Supplementary Information.

$$\mathbf{h}'_i = \sigma \left( \frac{1}{K} \sum_{k=1}^K \sum_{j \in \mathcal{V}_i} \alpha_{ij}^k \mathbf{W}^k \mathbf{h}_j \right) \quad (8)$$

**The introduction of uncertainty.** In machine learning, predictive uncertainty originates from two main sources: model uncertainty (epistemic uncertainty) and statistical uncertainty (aleatoric uncertainty). Model uncertainty reflects the inherent limitations of the model, primarily arising from uncertainty in the model parameters and architecture; it can be reduced, to some extent, by increasing the amount of training data. Statistical uncertainty, on the other hand, stems from noise inherent in the observations themselves (lower data uncertainty indicates higher sample quality) and cannot be reduced by acquiring more observations. In our study, model uncertainty is estimated through Monte Carlo dropout and is quantified for each sample by the variance of the predictions across stochastic forward passes (Eq. 9):

$$\text{Model uncertainty}_i = \frac{1}{N} \sum_{n=1}^N \left( \hat{y}_i^{(n)} - \bar{y}_i \right)^2 \quad (9)$$

where  $N$  is the number of stochastic forward passes,  $\hat{y}_i^{(n)}$  is the prediction in the  $n$ -th pass, and  $\bar{y}_i$  is the mean prediction over all passes. Statistical uncertainty  $\hat{\sigma}_i$  is learned directly from the data by treating it as a loss attenuation factor<sup>39</sup>, making the training process more robust to noisy labels (Eq. 10):

$$\mathcal{L}_{\text{NN}}(\theta) = \frac{1}{D} \sum_i \frac{1}{2\hat{\sigma}_i^2} \|y_i - \hat{y}_i\|^2 + \frac{1}{2} \log(\hat{\sigma}_i^2) \quad (10)$$

Here,  $D$  is the number of training samples,  $\hat{y}_i$  is the predicted mean,  $y_i$  is the experimental observation, and  $\hat{\sigma}_i^2$  is the predicted variance capturing the statistical uncertainty for that sample. Minimizing this loss encourages the model to predict higher uncertainty for noisy data points, automatically down-weighting their influence.

### Sample fabrication

Pre-alloyed KG-AMS and KG-AMAA powder were produced by vacuum induction melting followed by argon gas atomization. The major-

element compositions were quantified using inductively coupled plasma optical emission spectrometry (ICP-OES) and are reported in Tables 1 and 2. The measured impurity concentrations in KG-AMS were 100 ppm O, 20 ppm N, and <10 ppm S. Its particle-size distribution was characterized by D10, D50, and D90 values of 45.87, 78.13, and 134.7  $\mu\text{m}$ , respectively. The corresponding impurity concentrations in KG-AMAA were 301.59 ppm O, 11.08 ppm N, and 1.49 ppm S. Its D10, D50, and D90 values were 16.85, 35.0, and 55.4  $\mu\text{m}$ , respectively.

Ni-based bulk specimens were fabricated using a custom-built laser directed energy deposition (L-DED) system assembled at the Institute of Metal Research, Chinese Academy of Sciences. The system was equipped with a ytterbium fiber laser and a coaxial powder-delivery nozzle. Processing was conducted under argon shielding, with the residual oxygen concentration maintained below 1000 ppm. A pulsed laser with a beam diameter of ~3.0 mm was used, and the powder feed rate was fixed at 7 g min<sup>-1</sup>. A comprehensive matrix of processing parameters was designed to establish the dataset, encompassing laser power from 600 to 1600 W, scanning speeds from 4 to 14 mm s<sup>-1</sup>, hatching space from 1.2 to 2.0 mm, and layer thickness from 0.6 to 0.7 mm. A 90° interlayer rotation scanning strategy was adopted, wherein the scanning direction was rotated by 90° after each layer, and the powder-feeding head was elevated by one layer thickness.

Laser powder bed fusion (L-PBF) was performed using an AmPro SP-160 (AmPro Innovation) with an 80  $\mu\text{m}$  laser spot. Processing was conducted under flowing argon, with the residual oxygen concentration maintained below 1000 ppm. Before printing, the powder was vacuum-dried at 120 °C for 2 h. During fabrication, an interlayer rotation angle of 67° was applied. A systematic parameter screening varied laser power from 250 to 390 W and scanning speed from 700 to 1700 mm s<sup>-1</sup>. The hatching space and layer thickness were fixed at 0.10 mm and 30  $\mu\text{m}$ , respectively.

### Microstructure observations

Cubic samples (10 × 10 × 10 mm<sup>3</sup>) were wire-cut parallel to the building direction at 1/2 of the sample width, traversing from the edge to the center. The resulting longitudinal sections were ground, polished and finally vibration-polished with 50 nm colloidal silica. Metallographic examination was conducted using a Leica DM6 Optical Microscopy (OM). For chemical etching, a solution of 5 g CuCl<sub>2</sub>, 100 ml HCl and 100 ml C<sub>2</sub>H<sub>5</sub>OH was applied for 20 seconds; alternatively, electrolytic etching was performed in 30% phosphoric acid at 8 V direct current for 5 seconds, to preferentially reveal the  $\gamma'$  phase or  $\gamma$  matrix. Defect area fractions were quantified from binarized OM images using ImageJ Pro software to ensure statistical representativeness and precision. Subsequently, the average defect area fraction and its statistical error for each sample were derived from five measurements taken at different locations. The microstructure was further examined using a JSM-7800 F field emission scanning electron microscope (SEM) operated at an accelerating voltage of 20 kV. The area fraction of the  $\gamma'$  phase was approximated by the object-to-total area ratio (Obj./Total). Crystallographic features were characterized by electron backscatter diffraction (EBSD) on an Oxford Instruments system with a step size of 0.35  $\mu\text{m}$ , and the data were processed using Aztec Crystal 2.0 software. Specimens for transmission electron microscopy (TEM) were extracted from regions 5 mm away from the stress rupture fracture surface on the gauge section, and then were mechanically ground to ~50  $\mu\text{m}$  thickness and thinned using a twin-jet polisher at -30 °C and 20 V in a solution of 10% perchloric acid and in methanol (Vol.%). TEM analyses were carried out using an FEI-Talos F200X microscope operated at 200 kV and equipped with a Super-X™ EDS detector. The three-dimensional distribution of micropores in the as-fabricated specimens was characterized using X-ray computed tomography (XCT; XRADIA 620 VERSA system). Cuboidal samples (1 × 1 × 5 mm<sup>3</sup>) were extracted from the center of the deposited bulk with the long axis parallel to the building direction. Tomography was performed at an accelerating

voltage of -160 kV, acquiring 995 projections to reconstruct a volume with a voxel size of  $\sim 2\ \mu\text{m}$  and a field of view of  $1 \times 1 \times 2\ \text{mm}^3$ . All 3D reconstruction, processing, and visualization were conducted using Dragonfly software.

### Mechanical property measurements

Vickers hardness was measured using a ZD-HVZHT-10 microhardness tester equipped with a diamond Vickers indenter. A 0.5 kg load was applied, and 16 measurements were taken on cross-sections parallel to the building direction (BD). Specimens for mechanical testing were fabricated as  $16 \times 16 \times 60\ \text{mm}^3$  cuboids and extracted parallel to the building direction from the deposited bulks. Cylindrical tensile bars were machined to the dimensions of  $M6 \times \phi 3$ , with a gauge length of 20 mm, diameter of 3 mm, thread segment diameter of 6 mm, and total length of 45 mm. To minimize edge effects, all tensile samples were extracted from the center of printed material. Surfaces were ground and polished to a 1200-grit finish. Uniaxial tensile tests were conducted at room temperature and a strain rate of  $10^{-3}\ \text{s}^{-1}$  for both as-printed and heat-treated conditions. Stress rupture tests were performed on an F-25 creep testing machine at 800 °C/400 MPa and 900 °C/200 MPa until fracture to assess high-temperature mechanical performance.

### Atom probe tomography

APT analysis was employed to characterize the elemental partitioning behavior between  $\gamma'$  phase and  $\gamma$  matrix in the different parts of the designed alloy KG-AMS. APT specimens were prepared from  $10 \times 10 \times 10\ \text{mm}^3$  blocks and analyzed using a CAMECA LEAP 6000XR instrument. Measurements were conducted under ultra-high vacuum conditions ( $\sim 4.9 \times 10^{-11}$  Torr) and at a base temperature of  $\sim 50\ \text{K}$ . The experiment utilized ultraviolet laser pulsing at a frequency of 200 kHz and energy of 25 pJ, with a target evaporation rate of 1%. Data reconstruction and subsequent analysis were performed using the IVAS<sup>TM</sup> 3.6.8 software package (CAMECA Instruments Inc.) to achieve nanoscale spatial resolution and quantify three-dimensional compositional distributions.

**Neutron diffraction.** ND experiments were conducted using the ERNI time-of-flight (TOF) engineering diffractometer at the China Spallation Neutron Source (CSNS). Diffraction patterns were acquired simultaneously in two distinct orientations: perpendicular to the building direction, and at  $45^\circ$  to it, utilizing two detector banks positioned at  $+90^\circ$ , and  $+45^\circ$  relative to the incident beam. A defined scattering gauge volume was established through an incident slit configuration of  $8\ \text{mm} \times 6\ \text{mm}$  and a 5 mm radial collimator, ensuring sufficient sampling statistics for the analysis of macroscopic parameters evolution. Data acquisition was segmented into consecutive 20-minute intervals using the VDRIVE software. The average lattice parameters of  $\gamma'$  and  $\gamma$  phase in the as-built state were fitted by the Rietveld method using GSAS software. The Pseudo-Voigt function was employed to fit the  $\gamma'$ - $\gamma$  composite diffraction peak of (111), (200) and (220) to obtain their integrated intensities<sup>67,68</sup>.

**Statistics and reproducibility.** No statistical method was used to predetermine sample size. No data were excluded from the analyses. The experiments were not randomized. The investigators were not blinded to allocation during experiments and outcome assessment. For machine-learning model evaluation, the Ni-superalloy dataset contained  $n=142$  samples and was evaluated using 20 random 4:1 training/testing splits. The Al-alloy dataset contained  $n=163$  literature-derived samples. Defect area fractions were obtained from  $n=5$  optical-microscopy image fields per sample. Vickers hardness values were obtained from  $n=14$  indents per sample. Unless otherwise stated, quantitative experimental values are reported as mean  $\pm$  SD. Individual image fields, indents and precipitates are technical measurements; the

independently fabricated sample or alloy-processing condition is the experimental unit. No frequentist inferential statistical tests were performed for the comparisons shown in the main figures; therefore, no  $p$  values, confidence intervals or frequentist effect-size statistics are reported.

### Data availability

The data generated and analyzed during this study are included in this article, the Supplementary Information and the Source Data file. The dataset generated in this study has been deposited in Figshare<sup>69</sup>. Source data are provided with this paper.

### Code availability

The code used for model training, uncertainty quantification, inverse design and plotting is available at (<https://github.com/Fujiabo-NEU/ML-AM-alloy-design.git>).

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## Author contributions

J.F. and H.Y. contributed equally to this work. J.F., H.Y. and C.W. conceived the project. J.F. and H.Y. developed the alloy design framework and performed the experiments. J.F. and H.Y. wrote the manuscript with guidance from C.W., Z.S. and W.X. L.W., J.L., S.Z. and D.R. provided feedback on the manuscript. All authors participated in discussing the results and provided comments and suggestions on the various sections of the manuscript. C.W. and W.X. supervised and directed the overall project. All authors reviewed the final manuscript.

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## Competing interests

The authors declare no competing interests.

## Additional information

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