

Supplementary Information

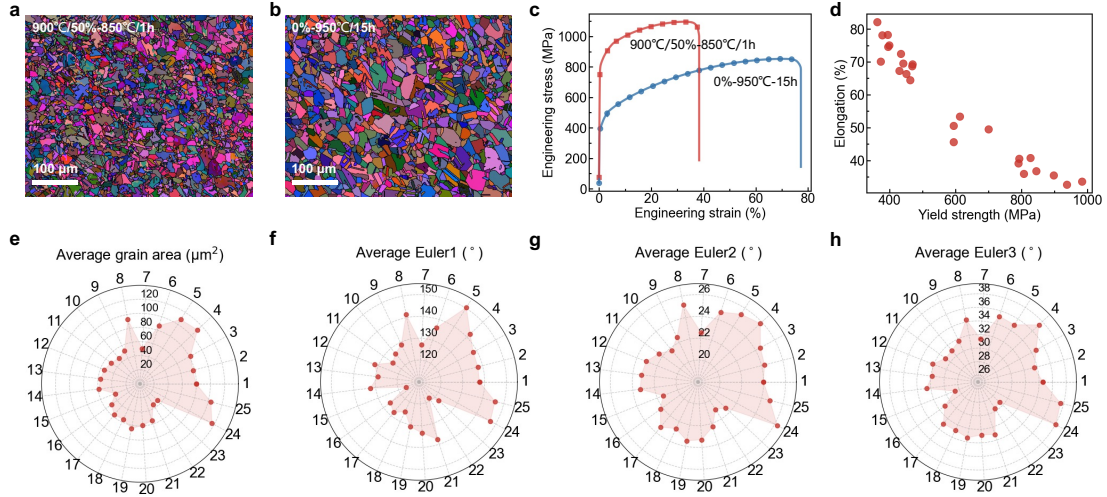
Generative design of high-fidelity microstructures using physics-aware machine learning

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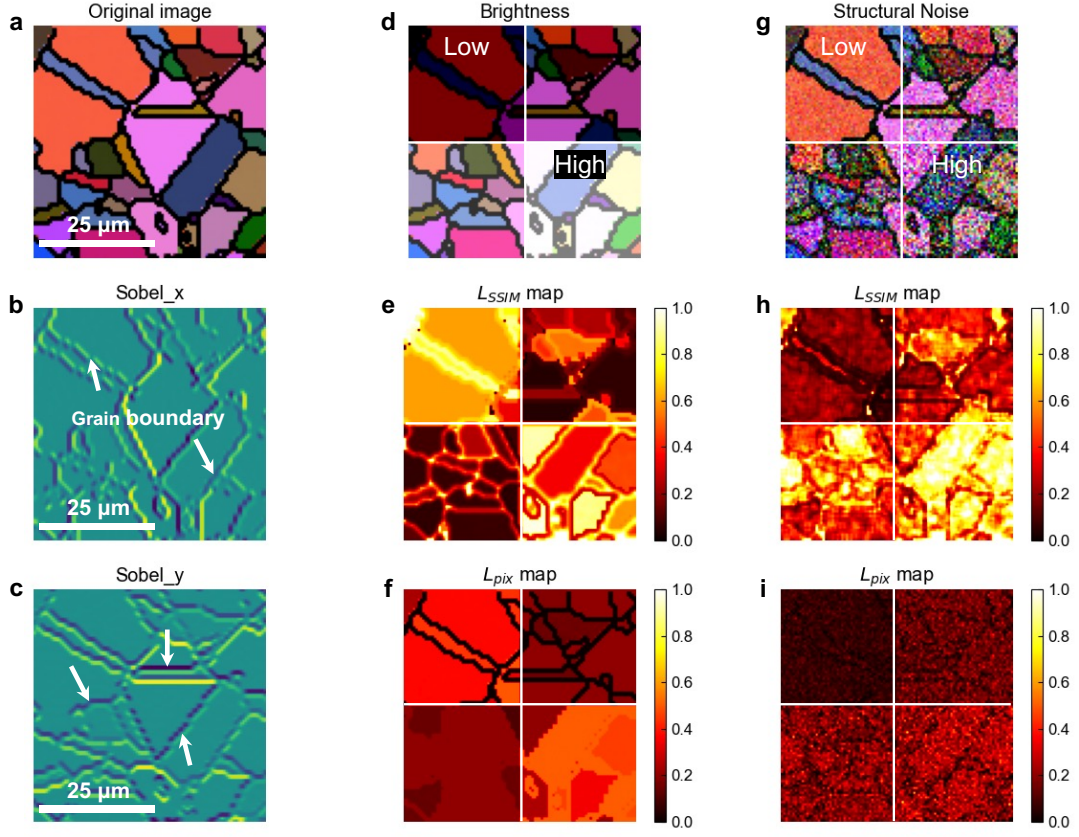
Supplementary Figure 1: Overview of the constructed dataset including microstructures and tensile properties. **a** and **b**, Representative EBSD microstructures of two selected alloys from the dataset, illustrating microstructural variability induced by different thermo-mechanical processing conditions. As an example, 900°C/50%-850°C/1h indicate 50% hot rolling at 900°C followed by heat treatment at 850°C for 1h. **c**, Room-temperature tensile stress-strain curves corresponding to the alloys shown in **a** and **b**. **d**, Pareto front illustrating the trade-off between yield strength and elongation across the 25 investigated alloys. **e-h** Radar plots summarizing the distributions of average grain area and mean crystallographic orientations (Euler1, Euler2, and Euler3) for all alloys in the dataset.

Supplementary Note 1: Physical information analysis in loss function

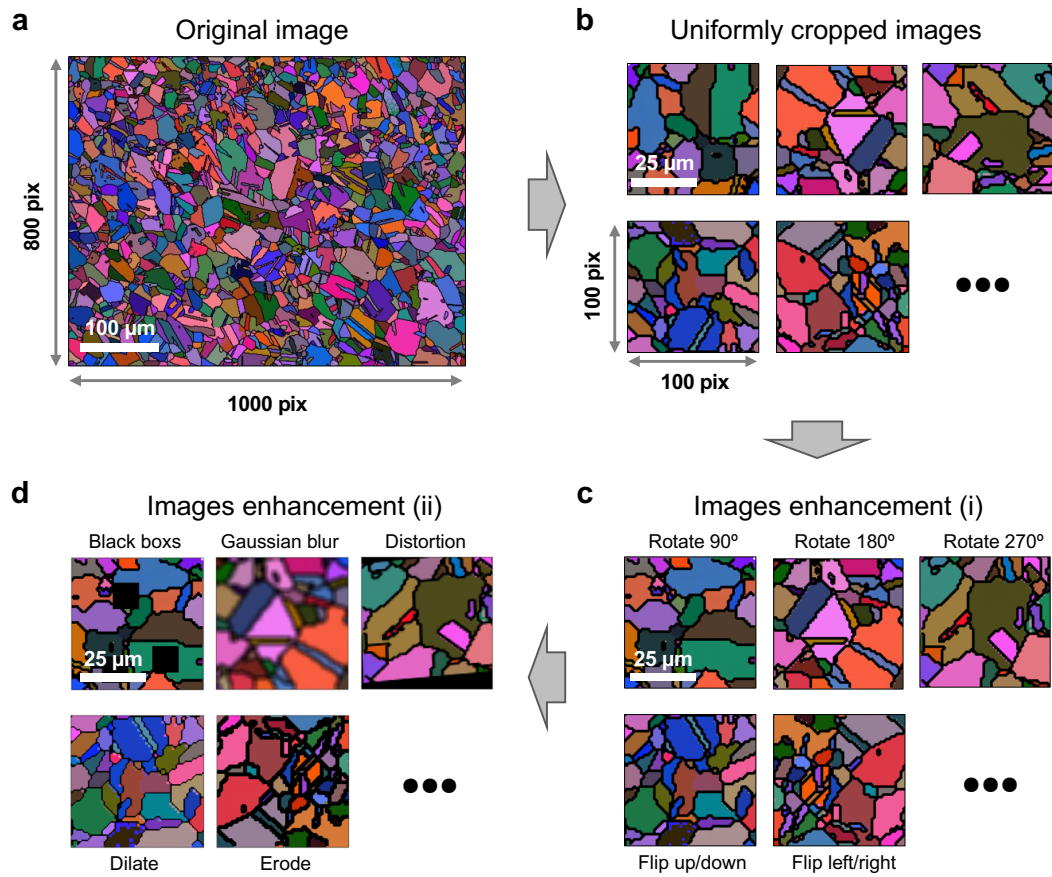
To elucidate the physical information embedded in the loss function, we conduct a visual analysis of the structural regions activated by different loss components. As shown in Supplementary Figure 2a, a representative microstructure image is randomly selected as the reference. For the edge-based loss term L_{edge} , the Sobel operator is applied to the original image to extract intensity gradients in the horizontal and vertical directions (Supplementary Figure 2b and c). These gradients correspond to grain boundaries or interfacial regions in the microstructure and thus explicitly encode interfacial information, enabling the loss function to emphasize physically meaningful structural features during model training.

To further interpret the role of the structural similarity loss L_{SSIM} , we introduce controlled image perturbations to the original microstructure to mimic different types of structural variations and examine the corresponding activated regions. Specifically, we independently apply systematic brightness modulation and structural noise to the original image. As shown in Supplementary Figure 2d, the four quadrants exhibit progressively varying brightness from dark to light, representing global decreases and increases in pixel (or orientation) values. The resulting loss maps between Supplementary Figure 2a and Supplementary Figure 2d are shown in Supplementary Figure 2e and f for L_{SSIM} and L_{pix} , respectively. Notably, L_{SSIM} produces pronounced responses not only in regions with extreme brightness differences but also along the interfaces separating regions of distinct brightness levels. These interfacial activations indicate that L_{SSIM} is sensitive to spatial transitions in local statistics and effectively highlights crystallographic discontinuities across grain boundaries or intergranular regions. In contrast, L_{pix} primarily captures absolute numerical differences and shows limited sensitivity to structural features, particularly in low-intensity regions.

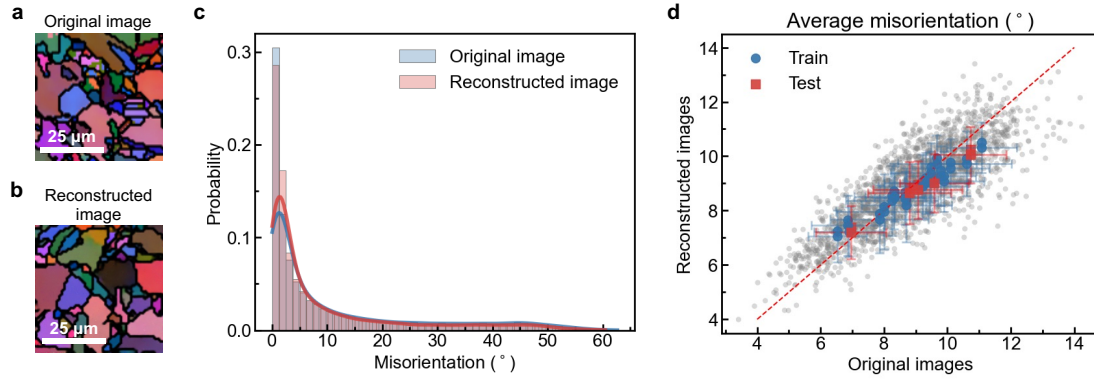
We further examine the response of the loss functions to intragranular orientation inconsistency by adding different levels of noise to the original microstructure (Supplementary Figure 2g), corresponding to increasing degrees of orientation fluctuation within grains. The associated loss maps for L_{SSIM} and L_{pix} are shown in Supplementary Figure 2h and i, respectively. For low noise levels, both loss functions exhibit relatively weak activation, indicating minor deviations from the original structure. As the noise intensity increases, L_{pix} mainly responds to localized pixel-wise variations, resulting in scattered activations that lack grain-level coherence. By contrast, L_{SSIM} shows a markedly different behavior: regions with high noise levels activate entire grains rather than isolated pixels. This collective activation reflects the sensitivity of L_{SSIM} to the loss of intragranular orientation consistency, emphasizing deviations from coherent crystallographic patterns within grains. Such behavior highlights the ability of L_{SSIM} to capture physically meaningful grain-scale structural integrity, which is not accessible through purely pixel-based loss terms.



Supplementary Figure 2: Microstructural information captured by physics-informed loss terms. **a**, A representative microstructure image randomly selected from the dataset. **b** and **c**, Grain boundary features extracted from the image **a** using horizontal and vertical Sobel operators, respectively, which are employed to compute the L_{edge} . **d**, Region-wise brightness modulation applied to the original image, with pixel (or orientation) values progressively increasing from the top-left to the bottom-right. **e** and **f**, Loss maps of L_{SSIM} and L_{pix} computed between **a** and **d**, respectively. **g**, Microstructure image with systematically increasing noise levels added to the original image, where noise intensity increases from the top-left to the bottom-right region. **h** and **i**, Loss maps of L_{SSIM} and L_{pix} computed between **a** and **g**, respectively.



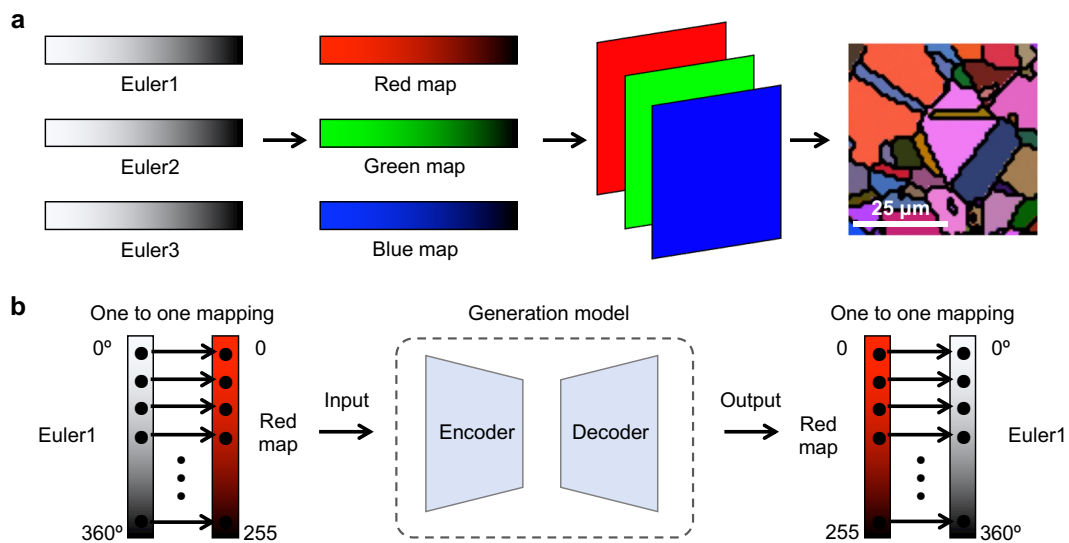
Supplementary Figure 3: Illustration of the dataset expansion strategy. **a**, Original large-scale microstructure image with a resolution of 1000 × 800 pixels. **b**, Representative 100 × 100 pixel patches obtained by uniform cropping of the original image. **c**, Augmented images generated by rotation and flipping at different angles. **d**, Further augmented images produced by applying black-block occlusion, blurring, distortion, dilation, and expansion operations.



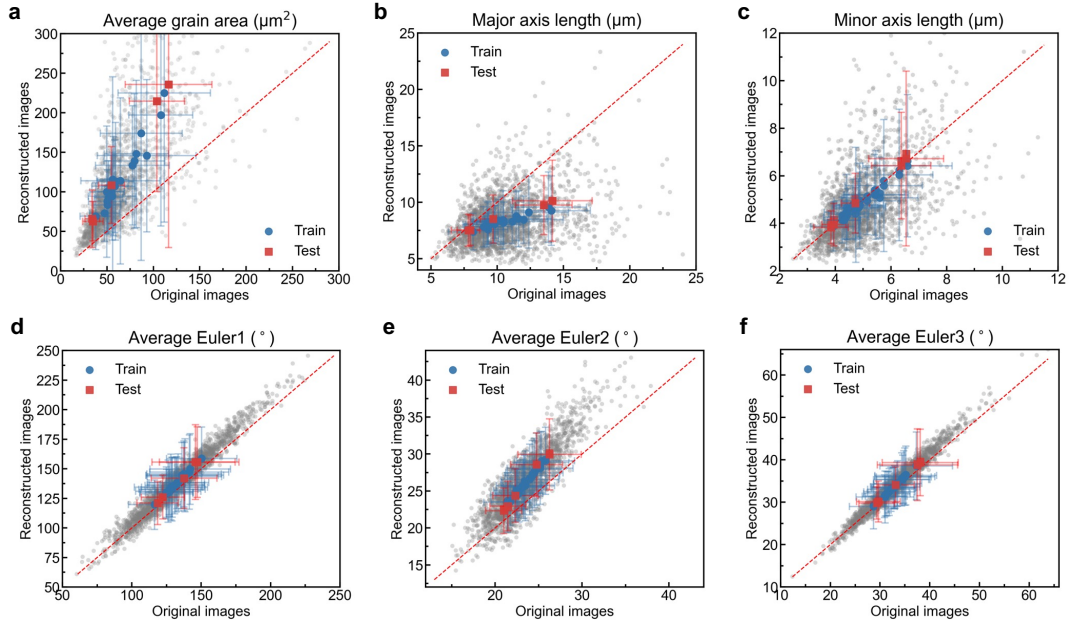
Supplementary Figure 4: The analysis of orientation difference distributions between original and reconstructed images. **a**, The original image. **b**, The reconstructed image. **c**, The misorientation distributions of the original and reconstructed images closely align. **d**, Comparison of average misorientation for all original and reconstructed images. The grey points represent the cropped patches. The blue and red points with error bars indicate the mean and standard deviation of the physical features for the original large images in the training and test sets, respectively.

Supplementary Note 2: One-to-one mapping from Euler angle to image pixel

The Euler-angle data and the image pixel values have a one-to-one reversible mapping relationship. Therefore, pixel-based loss calculation, including SSIM loss, does not cause information loss. Supplementary Figure 5 illustrates how the Euler angles are mapped to the pixel values for training image generation models, from which the output image pixels are mapped back to Euler angles for misorientation calculations. Supplementary Figure 5a shows that three Euler angles are mapped to the red, green, and blue channels, respectively, which constitute an image. Taking Euler1 as an example (Supplementary Figure 5b), each angle is first transformed to a pixel value using $\text{Pixel values} = \text{Euler1 values} / 360 \times 255$. These pixel values are used to train a model to generate pixels for a certain image. Then the pixels of the generated images are transformed back to Euler1 angles using the same method. That is, such a one-to-one mapping allows us to reserve the original information in the Euler angles and the SSIM based on pixel values will not cause information loss.



Supplementary Figure 5: One-to-one mapping from Euler angle to image pixel. **a**, Schematic illustration of the conversion from three Euler angles to the RGB image, where Euler1, Euler2, and Euler3 are mapped to the red, green, and blue channels, respectively. **b**, One-to-one mapping from each value in Euler1 to each pixel in the red channel before model training, and the reverse transformation after image generation.



Supplementary Figure 6: Fidelity analysis of reconstructed microstructures using the generation framework trained without L_{edge} and L_{SSIM} . Grey points denote individual cropped image patches. Blue and red points with error bars represent the mean values and standard deviations of the six physical features extracted from the original large-scale microstructures in the training and test sets, respectively.

Supplementary Note 3: Comparative analysis of other image generation models

We have extended the benchmarking study by including three additional baseline models: a Wasserstein GAN (WGAN), a standard VAE, and a standard DDPM. The results show that the proposed framework outperforms all three models. The WGAN is selected because it is a representative GANs variant with improved training stability and reduced mode collapse. The WGAN employ a critic network C to estimate the Wasserstein distance between the true distribution P_r and the generated distribution P_g , expressed as Equation (S1) ,

$$WD(P_r, P_g) = \max_{\|C\|_L \leq 1} \mathbb{E}_{x \sim P_r}[C(x)] - \mathbb{E}_{z \sim P_z}[C(G(z))] \quad (\text{S1})$$

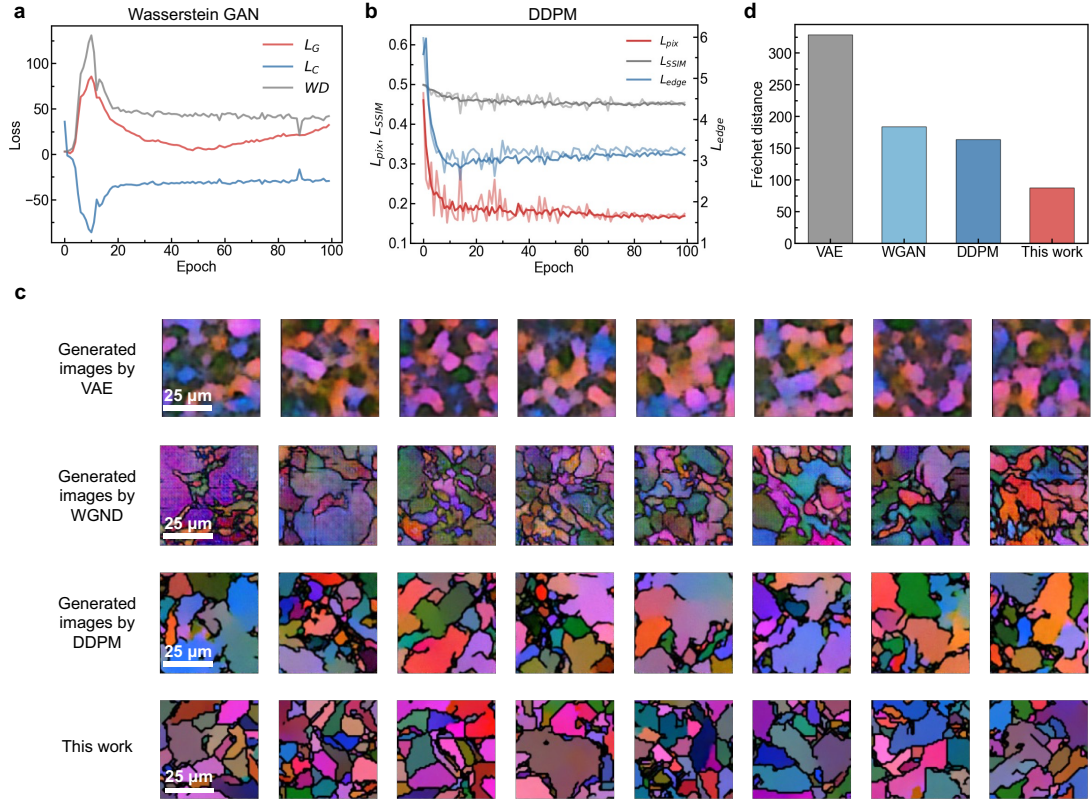
where G denotes the generator and the critic C satisfies the 1-Lipschitz constraint. Accordingly, the optimization objectives for the critic and the generator are defined as $L_C = -\mathbb{E}_{x \sim P_r}[C(x)] + \mathbb{E}_{z \sim P_z}[C(G(z))]$, and $L_G = -\mathbb{E}_{z \sim P_z}[C(G(z))]$, respectively. By alternately optimizing these objectives, the generator is gradually brought closer to the true data distribution, thereby achieving a more stable adversarial training process with good gradient properties. The detailed architecture of the WGAN is listed in Supplementary Table 7.

We also test the standard VAE model which has the same parameters to that used in the main text. In addition, the standard DDPM model uses the same architecture to that in the main text except for employing the VAE output as condition layer. Supplementary Figure 7a and b show the loss as a function of epoch for WGAN and DDPM. The losses for WGAN fluctuate in the first ~ 20 epochs because of adversarial optimization and then gradually become stable. The losses for DDPM gradually become stable after ~ 40 epochs. Supplementary Figure 7c compares the generated images by different models, those from our model is also included as comparison. The VAE generates the blurriest microstructures than the others, while WGAN and DDPM generated microstructures exhibit substantial noise and hallucination in crystallographic orientations and interfaces.

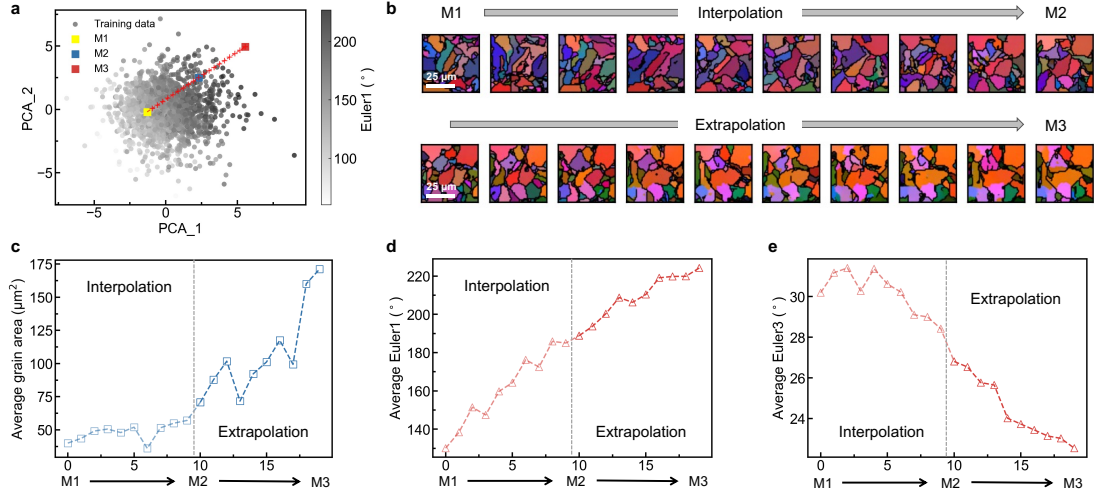
We further quantitatively compare the generations from the four models, in total 2,000 microstructures (the same number to the cropped original images) are generated by each model. The Fréchet Distance (FD) is used as the metric to assess the similarity between generated and original images, which is a widely used metric for evaluating generative model performance at the distribution level. Specifically, the generated and original images are first input into an Inception-v3 network to extract the feature representations. Then the FD between the two feature representations of generated images ($N(\mu_1, \Sigma_1)$) and original images ($N(\mu_2, \Sigma_2)$) by Equation (S2),

$$FD = \|\mu_1 - \mu_2\|^2 + \text{Tr}(\Sigma_1 + \Sigma_2 - 2(\Sigma_1 \Sigma_2)^{1/2}) \quad (\text{S2})$$

where μ_1 and μ_2 are the mean vectors of the two distributions, and Σ_1 and Σ_2 are the covariance matrices, and Tr denotes the matrix trace. A lower FD indicates a better image fidelity of generated microstructures with original ones. Supplementary Figure 7d compares FD of the four models and indicates that the images generated by our model has the highest fidelity.



Supplementary Figure 7: The comparison of generative model performance. **a**, The loss functions of the discriminator and generator in WGANs. **b**, The loss functions evolution for standard DDPMs. **c**, Randomly generated microstructures from the standard VAE (first row), WGAN (second row), standard DDPM (third row), and this work (fourth row). **d**, The Fréchet distance (FD) evaluation results for different generative models.



Supplementary Figure 8: Latent-space exploration and generation of out-of-distribution microstructures using the framework. **a**, Low-dimensional latent space learned by the VAE, where grey points correspond to training images and color intensity indicates the average Euler1 value of the microstructures. Yellow and blue markers denote the locations of images M1 and M2, respectively. The red dashed line and cross symbols indicate interpolation and extrapolation trajectories between M1 and M2. **b**, Generated microstructures corresponding to the interpolation and extrapolation points shown in **a**. **c-e**, Evolution of average grain area, Euler1, and Euler3 values for the generated microstructures along the sampling trajectory.

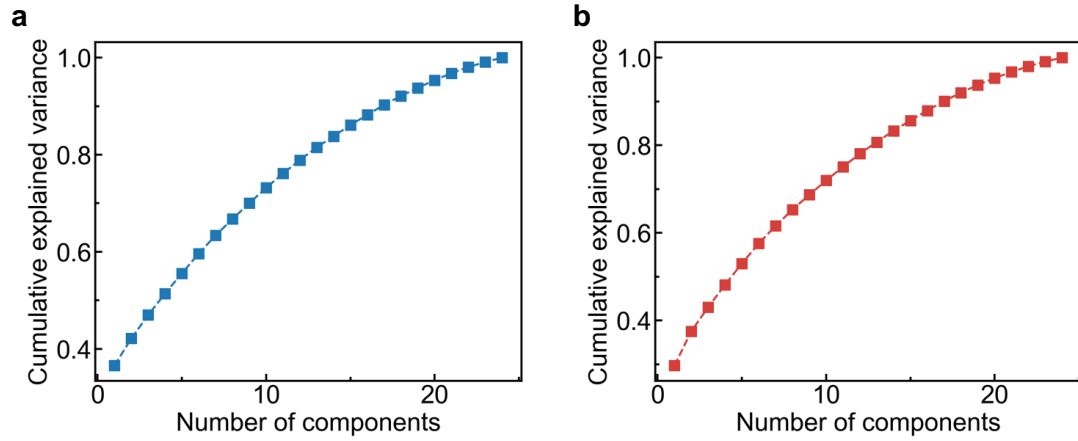
Supplementary Note 4: The impact of PCA on the fidelity of reconstruction images

We have analyzed both the cumulative retained variance and the reconstruction fidelity as functions of the number of principal components (PCs). The PCA used in the optimization stage is not applied directly to the latent variable of a single image. Instead, it is applied separately to the mean and variance vectors of the latent space constructed from 80 cropped patches originating from the same initial large microstructure image. As shown in Supplementary Figure 9, the first principal component (PC) of both vectors explains more than 35% of the variance, while the cumulative retained variance exceeds 90% after approximately 20 PCs. However, the following analysis suggests that using more PCs is not necessarily to improve the microstructure fidelity. This is due to the fact that PCA only guarantees optimality for second-order statistics, and PCs ranked lower may introduce redundant information or noise that have no influence on image fidelity.

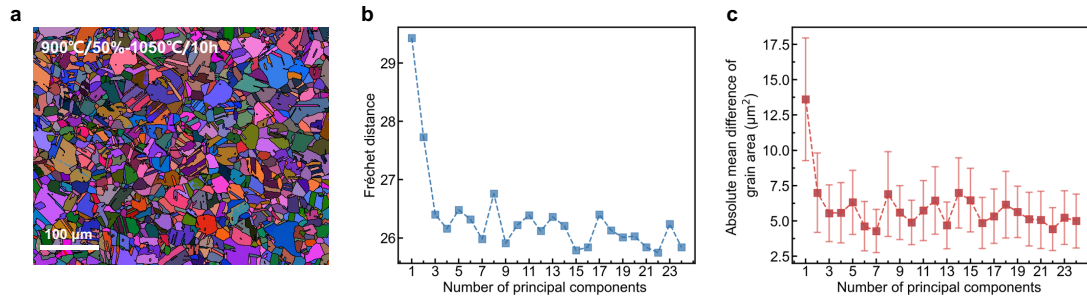
We next systematically evaluate the effect of the number of PCs on the representation of original microstructure and the fidelity of the generated microstructure. Specifically, we randomly select an initial large image from the test data to examine the effect, as shown in Supplementary Figure 10a. Following the same image cropping method in the main text, the initial large image is cropped into 80 smaller images which are encoded by the trained VAE, resulting in a 128×80 latent variable matrix. We applied PCA to the mean (μ) and standard deviation (σ) vectors of the 128×80 latent variable matrix with different numbers of retained PCs. Then different number of PCs are mapped back to new μ and σ vectors, from which 80 latent variables are sampled into a 128×80 matrix and decoded to produce the corresponding microstructures.

We use a quantitative metric to measure the similarity, which is based on the encoded latent variables of original and generated images. The metric, Fréchet distance (FD) is given by Equation (S2), simplified as $FD = FD(P, Q)$, where P and Q represent the 128×80 latent variable matrix for the original and generated images, respectively. A lower FD means a higher similarity.

Supplementary Figure 10b shows that the FD decreases monotonically with increasing PCs. Note that after the third one, the FD becomes almost stable. This suggests that adding more PCs has little positive effect on the fidelity of the generated microstructures. To obtain a simple model that can benefit the inverse optimization process, we thus select 3 PCs for each μ and σ vector. The fidelity is further confirmed by examining the grain area of generated microstructures with varying PCs, as shown in Supplementary Figure 10c. The tendency is similar to that in Supplementary Figure 10b, that is, the deviation in grain area between original and generated microstructures becomes close when 3 or more PCs are used.



Supplementary Figure 9: The cumulative retained variance plot for the μ and σ obtained via Principal component analysis (PCA). a, PCA applied to the μ vector. b, PCA applied to the σ vector.



Supplementary Figure 10: The fidelity analysis between original and generated images as the number of principal components (PCs) increases. a, A randomly selected initial microstructure from the test set. **b,** The Fréchet distance (FD) between the overall latent-variable distributions of 80 original images and 80 generated images as a function of the number of PCs. **c,** The absolute mean difference in grain area between 80 generated images and the original image **a**, with error bars indicating the standard deviation.

Supplementary Note 5: Crystal plasticity finite element (CPFE) simulation

The CPFE constitutive model employed in this work incorporates twelve $\{111\}\langle 110 \rangle$ octahedral slip systems, with the conventional power-law shear strain rate relation modified to account for damage effects:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^{1/m} \text{sign}(\tau^\alpha) \quad (\text{S3})$$

where α denotes the slip-system index, $\dot{\gamma}_0$ is the reference shear strain rate, m is the rate sensitivity exponent, τ^α and g^α represent the resolved shear stress and the slip resistance of the α -th slip system, respectively.

The slip resistance is described by a Taylor-type multi-slip hardening equation:

$$g^\alpha = g_0 + \alpha_0 G b \sqrt{\sum_{\beta=1}^{N_{slip}} A^{\alpha\beta} \rho^\beta} + g_{HP}(d) \quad (\text{S4})$$

where g_0 is the initial slip resistance, α_0 is a material constant, G is the shear modulus, b is the magnitude of the Burgers vector, and N_{slip} denotes the number of slip systems, which is 12 in the present study. A is the interaction matrix, and ρ^β represents the dislocation density. The term $g_{HP}(d)$ accounts for the grain-boundary-affected zone (GBAZ). According to prior work^[1], its normal distribution provides an accurate description of the grain-boundary strengthening effect in the Inconel 625 alloy, and it can be expressed as:

$$g_{HP}(d) = A \cdot \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left[-\frac{(d-\mu)^2}{2\sigma^2}\right] + g_0 \quad (\text{S5})$$

where d denotes the distance from the integration point to the grain boundary. The parameters A and σ^2 are adjustable parameters that control the strength distribution within the GBAZ. The mean value μ is set to zero, implying that the center of the strength field coincides with the grain boundary.

The evolution of dislocation density in Equation (S4) follows the Kocks-Mecking formulation^[2, 3]:

$$\dot{\rho}^\alpha = \frac{1}{b} \left(\frac{\sqrt{\sum_{\beta=1}^{N_{slip}} H^{\alpha\beta} \rho^\beta}}{K} - k_b \rho^\alpha \right) |\dot{\gamma}^\alpha| \quad (\text{S6})$$

where $H^{\alpha\beta}$ characterizes the mutual immobilization between dislocations on different slip systems and has the same functional form as $A^{\alpha\beta}$. K is a similitude coefficient, and k_b represents the coefficient governing dynamic recovery of dislocations.

Given that ductile fracture is governed by the nucleation, growth, and coalescence of microvoids^[4, 5], which are closely related to dislocation interactions and pile-up processes^[6], the accumulated plastic work density W_p is employed in this work as the fundamental damage history variable, and its increment can be expressed as:

$$\Delta W_p = \sum_{\alpha=1}^{N_{slip}} \bar{\tau}^\alpha |\Delta \gamma^\alpha| \quad (\text{S7})$$

where $\bar{\tau}^\alpha$ is give as follows:

$$\bar{\tau}^\alpha = \frac{\tau_n^\alpha + \tau_{n+1}^\alpha}{2} \quad (\text{S8})$$

where n denotes the increment step number.

Therefore, the W_p is given by:

$$W_p^{n+1} = W_p^n + \Delta W_p \quad (\text{S9})$$

In addition, microvoid growth is highly dependent on the local stress state of the material,

which is commonly characterized by the dimensionless stress triaxiality^[7, 8]. Therefore, the effect of stress triaxiality η is also incorporated into the present damage model, and the increment of damage history variable $\Delta\kappa_d$ is defined as:

$$\Delta\kappa_d = (1 + c\eta_+^d)\Delta W_p \quad (\text{S10})$$

where η_+ can be expressed as:

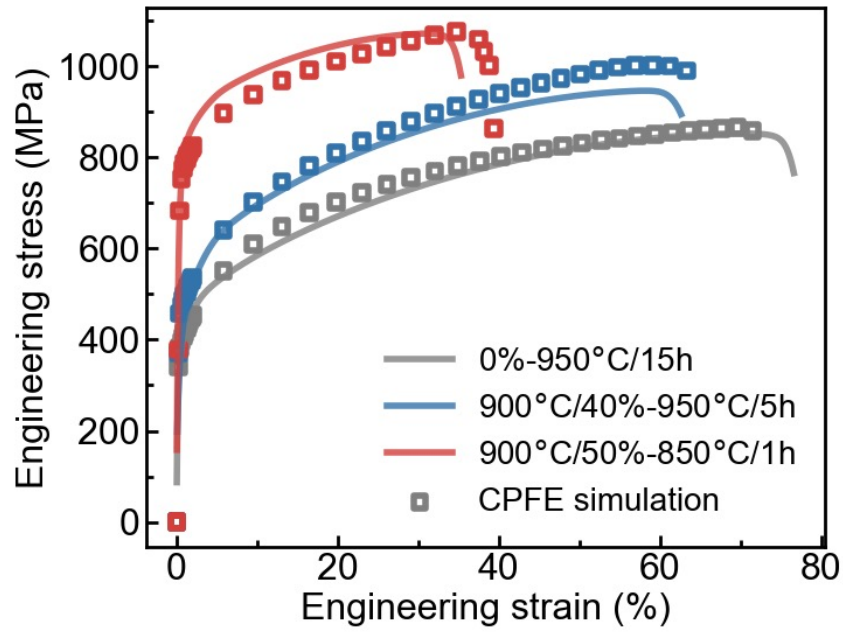
$$\eta_+ = \max(\eta, 0) \quad (\text{S11})$$

Referring to the damage formulation proposed by Kim^[9], and further accounting for the combined effects of plastic work density and stress triaxiality, the damage variable is modified as follows:

$$D = \begin{cases} 0, & \kappa_d \leq \kappa_{ini} \\ D_{max} \left(\frac{\kappa_d - \kappa_{ini}}{\kappa_{max} - \kappa_{ini}} \right)^q, & \kappa_{ini} < \kappa_d < \kappa_{max} \\ D_{max} & \kappa_d \geq \kappa_{max} \end{cases} \quad (\text{S12})$$

where κ_{ini} and κ_{max} are the damage initiation and saturation thresholds, respectively, and q is a constant governing the damage evolution rate.

Based on the aforementioned microstructure model and constitutive framework, tensile simulations were conducted for Inconel 625 alloy under a strain rate of 0.002 s^{-1} , consistent with the experimental conditions. By performing accurate fitting on the raw data (Supplementary Figure 11), specific parameters relevant to the CPFE simulations are obtained. The crystal plasticity constitutive parameters and damage model parameters are provided in Supplementary Table 2, Supplementary Table 3 and Supplementary Table 4.



Supplementary Figure 11: CPFE-simulated tensile responses of initial microstructures. Calibration of the CPFE model using experimental stress-strain curves from representative processed alloys. The solid lines represent the experimental curves, and the square points represent the CPFE simulation results.

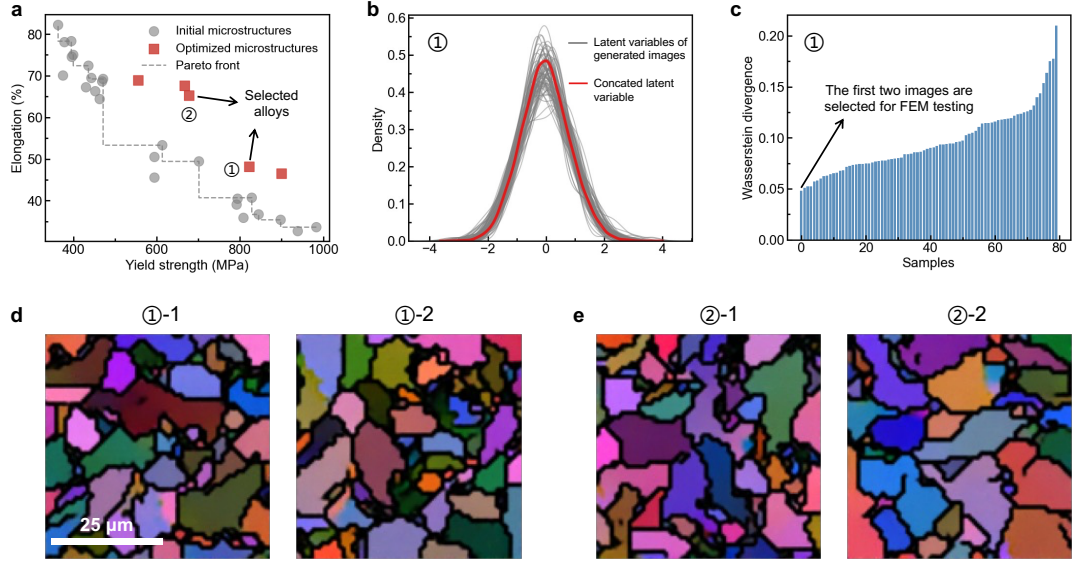
Supplementary Note 6: Selection of candidate microstructures

For each optimized solution obtained from the inverse design process, 80 corresponding microstructural images are generated. To identify representative microstructures suitable for subsequent crystal plasticity finite element (CPFE) simulations, we develop a selection strategy based on latent-space similarity analysis. As illustrated in Supplementary Figure 12a, two optimized solutions (points ① and ②) are first selected as candidate alloys.

Taking point ① as an example, the latent variables z_i ($i=1, 2, \dots, 80$) corresponding to its 80 generated microstructures are extracted, as shown by the grey curves in Supplementary Figure 12b. The overall latent distribution z_L is then constructed by concatenating these 80 latent vectors, represented by the red curve in Supplementary Figure 12b. This concatenated distribution serves as a statistical descriptor of the collective microstructural characteristics associated with the optimized point.

To quantify the similarity between individual microstructures and the overall latent distribution, the Wasserstein distance between each z_i and z_L is calculated according to Eq. (S1). A smaller Wasserstein distance indicates a closer correspondence between the probability distributions of the two latent variables, implying that the associated microstructure is more representative of the overall structural characteristics of the optimized solution.

Based on this criterion, the two microstructures exhibiting the smallest Wasserstein distances are selected as candidates for CPFE simulations, as shown in Supplementary Figure 12c. The final selected microstructures corresponding to optimized points ① and ② are presented in Supplementary Figure 12d and e, respectively.



Supplementary Figure 12: Selection of candidate microstructures and data preprocessing for CPFE simulations. **a**, The candidate samples selected for subsequent validation. **b**, Distribution of latent variables for the generated image patches (grey) and the concatenated latent descriptors (red). **c**, Wasserstein distance between latent variables of individual patches and the corresponding concatenated descriptors. **d** and **e**, Representative microstructures selected for validation at points ① and ②.

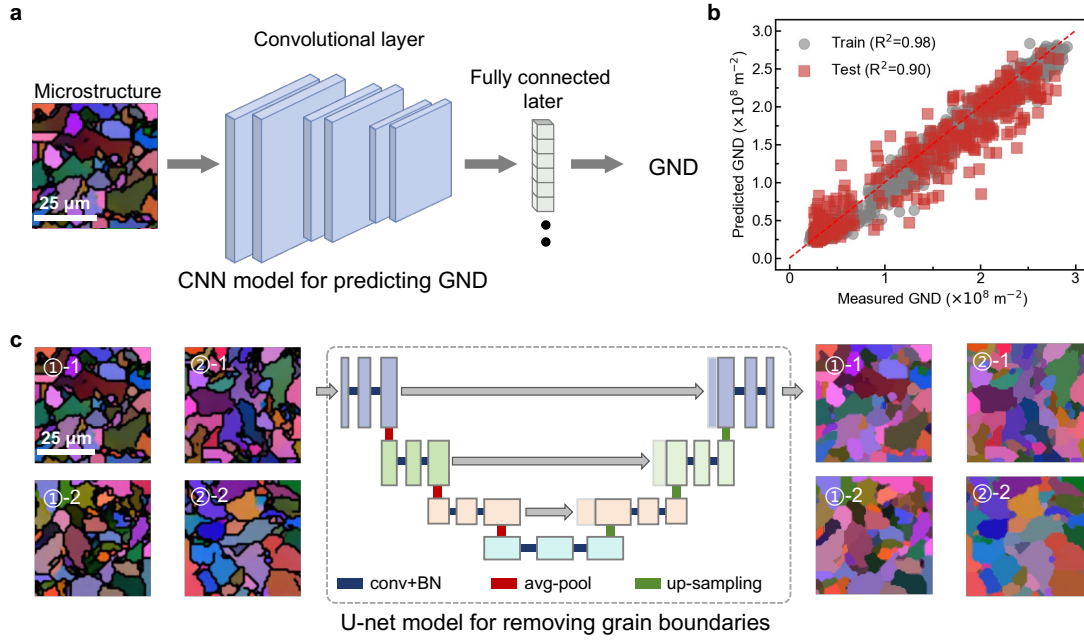
Supplementary Note 7: Image processing of generated microstructures for CPFE simulation

To convert the generated microstructures into finite element models suitable for crystal plasticity finite element (CPFE) simulations, a sequence of image-processing and data-mapping procedures is implemented. First, a convolutional neural network (CNN) is trained to predict the geometrically necessary dislocation (GND) density of the generated microstructures, which is subsequently used as an input for CPFE simulations (Supplementary Figure 13a). A pretrained ResNet-18 architecture is adopted as the backbone for feature extraction from microstructural images. To enable property regression, the original classification head is replaced with a fully connected regression layer, allowing direct mapping from image features to GND density.

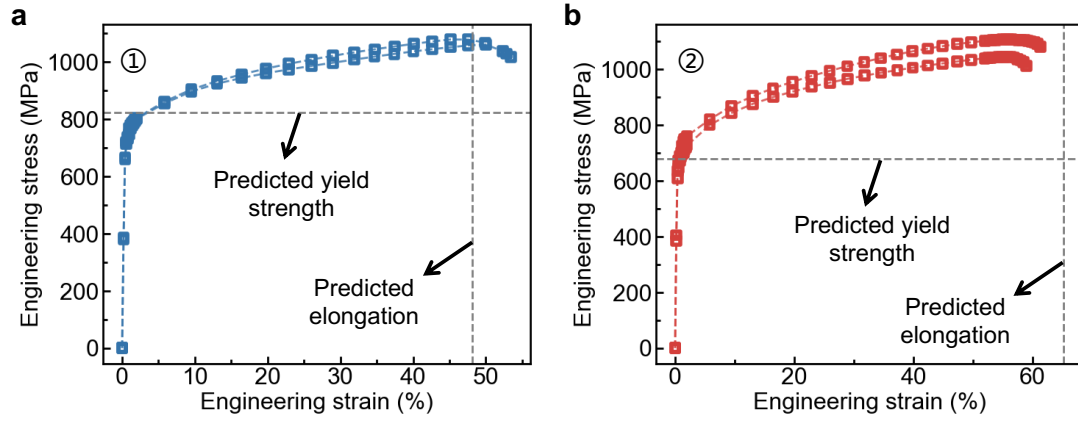
The training dataset is constructed by extracting GND maps from 2,000 cropped experimental microstructures using the Channel 5 software package, with 80% of the data allocated for training and the remaining 20% reserved for testing. During training, both the convolutional layers and the regression head are jointly fine-tuned to optimize the predictive performance of the CNN. The resulting model achieves a coefficient of determination $R^2 = 0.90$ on the test set, as shown in Supplementary Figure 13b. The predicted GND densities are then employed as the initial dislocation density field in the CPFE simulations.

To further prepare the generated microstructures for CPFE input, a U-net model is trained to remove grain boundaries from the microstructural images (Supplementary Figure 13c), thereby isolating intragranular orientation information. The architecture of the U-net model is summarized in Supplementary Table 6. The training dataset is constructed by extracting grain-boundary-free microstructures from the same set of 2,000 cropped experimental images using Channel 5. These images are used as ground truth targets for supervised training of the grain-boundary removal network. Representative results of grain boundary removal for selected microstructures corresponding to optimized points ① and ② are shown in Supplementary Figure 13c.

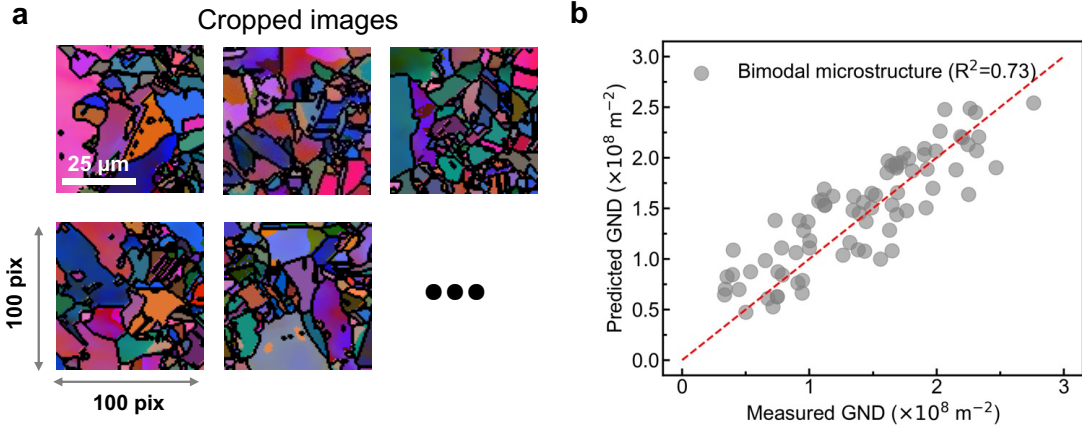
Following grain boundary removal, the pixel values within each grain are averaged and mapped to the three Euler angles which corresponding to the three image channels, yielding the crystallographic orientation field of the microstructure. The reconstructed orientation data are then discretized into finite elements and directly imported into the CPFE framework for subsequent simulation and validation of mechanical properties.



Supplementary Figure 13: Preprocessing workflow for microstructural images used in CPFE simulations. **a**, Convolutional neural network (CNN) employed to predict geometrically necessary dislocation (GND) density from microstructural images. **b**, Prediction performance of the GND model, where grey and red points correspond to the test and training sets, respectively. **c**, A U-net model used to remove grain boundaries from candidate microstructural images prior to CPFE modeling.



Supplementary Figure 14: CPFE simulation of generated optimized microstructures. a and b, Simulated tensile responses of the optimized microstructures (point ① and ② of Supplementary Figure 12a). The horizontal and vertical gray dashed lines indicate the predicted yield strength and elongation of machine learning models, respectively.



Supplementary Figure 15: Validation of the CNN model's predictive performance on out-of-distribution data. **a**, The experimentally obtained bimodal microstructure image is cropped into 100×100-pixel patches. **b**, The predicted GND density from the CNN model is compared with the actual GND density.

Supplementary Table 1: The 25 samples with different processing and measured yield strength and elongation.

ID	Heat treatment temperature (°C)	Heat treatment time (h)	Hot rolling deformation at 900°C (%)	Yield strength (MPa)	Elongation (%)
1	650	1	0	470.23	69.32
2	750	5	0	468.47	68.70
3	850	10	0	434.94	72.51
4	950	15	0	394.53	78.29
5	1050	20	0	362.26	82.18
6	1050	15	20	377.75	78.15
7	950	10	20	399.05	75.03
8	850	5	20	613.19	53.39
9	750	1	20	700.46	49.44
10	650	20	20	827.46	40.76
11	650	15	30	897.42	35.42
12	750	10	30	793.37	40.48
13	850	20	30	594.08	50.53
14	950	1	30	441.99	69.56
15	1050	5	30	395.19	74.56
16	1050	1	40	429.82	67.24
17	950	5	40	451.36	66.30
18	850	15	40	593.98	45.55
19	750	20	40	790.98	39.15
20	650	10	40	983.38	33.63
21	650	5	50	938.12	32.69
22	750	15	50	844.78	36.77
23	850	1	50	807.42	35.94
24	950	20	50	462.32	64.45
25	1050	10	50	373.67	70.09

Supplementary Table 2: Crystal plasticity constitutive parameters

Parameters	Symbol	Value	Unit	Source
Elastic modulus	C_{11}	172	GPa	[10]
	C_{12}	77.38	GPa	[10]
	C_{44}	114	GPa	[10]
Reference shear rate	$\dot{\gamma}_0$	0.001	s ⁻¹	Identified
Rate sensitivity parameter	m	0.1	-	Identified
Initial slip resistance	g_0	73.3	MPa	[1]
Similitude coefficient	K	11	-	[11]
Dynamic recovery coefficient	k_b	14	nm	[12]
Burger's vector	b	2.67e-7	mm	Measured
Shear modulus	μ	72	GPa	Measured

Supplementary Table 3: Components of the interaction matrixes $A^{\alpha\beta}$ and $H^{\alpha\beta}$

$A^{\alpha\beta}$	a_0	a_1	a_2	a_3	a_4	a_5
[12]	0.122	0.122	0.657	0.084	0.137	0.118
$H^{\alpha\beta}$	h_0	h_1	h_2	h_3	h_4	h_5
[13]	0.0	0.038	0.38	0.27	0.02	1

Supplementary Table 4: Parameters of the damage model

Parameters	Symbol	Value	Unit	Source
Damage initiation threshold	κ_{ini}	1200	mJ/mm ³	Identified
Damage saturation threshold	κ_{max}	2200	mJ/mm ³	Identified
Material constants	q	3	-	Identified
	c	1	-	Identified
	d	1	-	Identified

Supplementary Table 5: Architecture of the VAE model

Model	Functions	Parameters (in_channels, out_channels, kernel_size, stride, padding)	Output shape
Encoder	Input	-	(50, 3, 128, 128)
	Conv2d + ReLU	(3, 32, 3, 1, 1)	(50, 32, 128, 128)
	Conv2d + ReLU	(32, 64, 4, 2, 1)	(50, 64, 64, 64)
	Conv2d + ReLU	(64, 128, 5, 2, 2)	(50, 128, 32, 32)
	Flatten		(50, 131072)
	Linear $\times 2$		(50, 128) $\times 2$
Decoder	Linear		(50, 128)
	UnFlatten		(50, 128, 32, 32)
	ConvTranspose2d + ReLU	(128, 64, 6, 2, 2)	(50, 64, 64, 64)
	ConvTranspose2d + ReLU	(64, 32, 6, 2, 2)	(50, 32, 128, 128)
	ConvTranspose2d + Sigmoid	(32, 3, 5, 1, 2)	(50, 3, 128, 128)

Supplementary Table 6: Architecture of the U-net model.

Model	Functions	Parameters (in_channels, out_channels, kernel_size, stride, padding)	Output shape
Encoder	Input	-	(50, 3, 128, 128)
	Conv2d	(3, 32, 3, 1, 1)	(50, 32, 128, 128)
	Conv2d + BatchNorm2d + SiLU + Residual Block	(32, 32, 3, 1, 1)	(50, 32, 128, 128)
	AvgPool2d	-	(50, 32, 64, 64)
	Conv2d + BatchNorm2d + SiLU + Residual Block	(32, 64, 3, 1, 1)	(50, 64, 64, 64)
	AvgPool2d	-	(50, 64, 32, 32)
	Conv2d + BatchNorm2d + SiLU + Residual Block	(64, 96, 3, 1, 1)	(50, 96, 32, 32)
	AvgPool2d	-	(50, 96, 16, 16)
	Conv2d + BatchNorm2d + SiLU + Residual Block	(96, 128, 3, 1, 1)	(50, 128, 16, 16)
	UpsamplingBilinear2d	-	(50, 128, 32, 32)
	Conv2d + BatchNorm2d + SiLU + Residual Block	(128, 96, 3, 1, 1)	(50, 96, 32, 32)
	UpsamplingBilinear2d	-	(50, 96, 64, 64)
Decoder	Conv2d + BatchNorm2d + SiLU + Residual Block	(96, 64, 3, 1, 1)	(50, 64, 64, 64)
	UpsamplingBilinear2d	-	(50, 64, 128, 128)
	Conv2d + BatchNorm2d + SiLU + Residual Block	(64, 32, 3, 1, 1)	(50, 32, 128, 128)
	Conv2d	(32, 3, 3, 1, 1)	(50, 3, 128, 128)

Supplementary Table 7: Architecture of the GANs model

Model	Functions	Parameters (in_channels, out_channels, kernel_size, stride, padding)	Output shape
Generator	Input	-	(50, 128, 1, 1)
	ConvTranspose2d + BatchNorm2d + ReLU	(128, 1024, 4, 1, 0)	(50, 1024, 4, 4)
	ConvTranspose2d + BatchNorm2d + ReLU	(1024, 512, 4, 2, 1)	(50, 512, 8, 8)
	ConvTranspose2d + BatchNorm2d + ReLU	(512, 256, 4, 2, 1)	(50, 256, 16, 16)
	ConvTranspose2d + BatchNorm2d + ReLU	(256, 128, 4, 2, 1)	(50, 128, 32, 32)
	ConvTranspose2d + BatchNorm2d + ReLU	(128, 64, 4, 2, 1)	(50, 64, 64, 64)
	ConvTranspose2d + Tanh	(64, 3, 4, 2, 1)	(50, 3, 128, 128)
	Input	-	(50, 3, 128, 128)
	Conv2d + LeakyReLU	(3, 64, 4, 2, 1)	(50, 64, 64, 64)
	Conv2d + InstanceNorm2d + LeakyReLU	(64, 128, 4, 2, 1)	(50, 128, 32, 32)
	Conv2d + InstanceNorm2d + LeakyReLU	(128, 256, 4, 2, 1)	(50, 256, 16, 16)
	Conv2d + InstanceNorm2d + LeakyReLU	(256, 512, 4, 2, 1)	(50, 512, 8, 8)
Critic	Conv2d + InstanceNorm2d + LeakyReLU	(512, 1024, 4, 2, 1)	(50, 1024, 4, 4)
	Conv2d	(1024, 1, 4, 1, 0)	(50, 1, 1, 1)
	Flatten	-	(50, 1)

Supplementary References

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