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Inverse design of functionally graded porous structures with target dynamic responses

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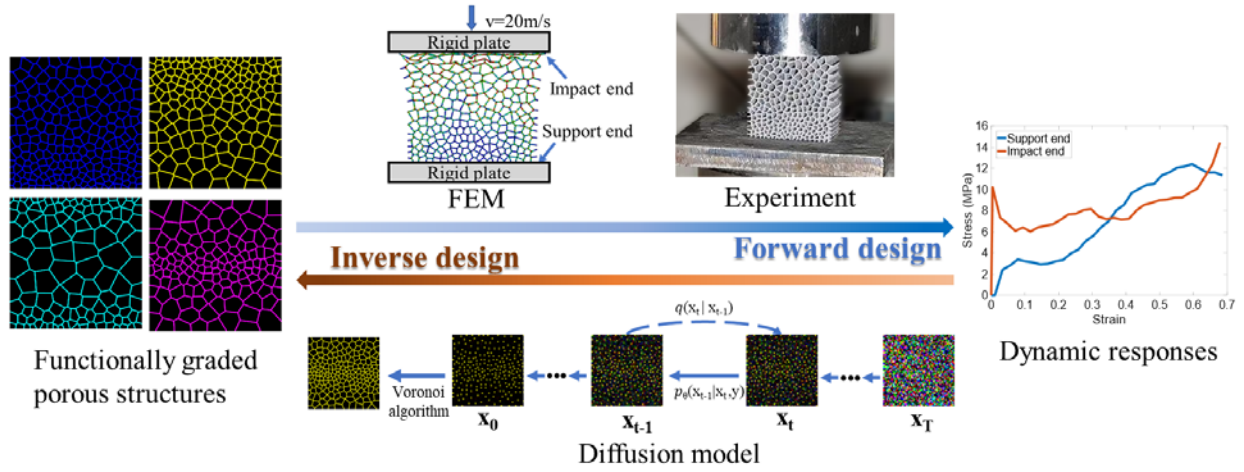
Abstract

Although functionally graded porous structures (FGPS) have been studied comprehensively due to their excellent mechanical and functional properties, the design process of FGPS with target stress response still dependent on continuous trial and error, which is not only time-consuming but also heavily relies on experience and intuition. This study proposes a novel inverse design framework of 2D FGPS with targeted dynamic stress-strain responses via a combination of conditional diffusion model and a residual neural network. Unlike traditional binary pixel representations, this approach utilizes nuclei position maps and color mapping technique to represent the structure configurations and cell wall thicknesses to improve the efficiency and performance of the model. Firstly, various functionally graded porous structures were constructed by employing Voronoi diagram techniques, and finite element simulations were conducted to calculate the nonlinear responses subjected to dynamic loadings. A dataset comprising 2100 FGPS and corresponding nonlinear stress-strain responses was established. Then, an inverse design framework is formulated by integrating a generator that uses a diffusion model to synthesize structures conditioned on specific target responses, with a predictor that employs a residual neural network to assess the responses of these structures. Finally, to demonstrate the effectiveness of the approach, the performance of the predictor and generator was thoroughly investigated. Structures with various target stress-strain responses were generated through the proposed method,

and validated by finite element analysis. A detailed impact experiment was also carried out to verify the effectiveness of the proposed methods. The result shows that the framework can effectively generate new structures with objective nonlinear responses. This work offers a fast and efficient way to design FGPS that meet specific performance objectives.

Keywords: Inverse design, Nonlinear response, Deep learning, Functionally graded porous structure, Voronoi, Diffusion model

Graphical abstract



1. Introduction

Functionally graded porous structures (FGPS) have attracted great attention due to their excellent and customizable properties, such as high strength, light weight, and superior energy absorption capability [1–5]. FGPS have also been discovered in biological materials as shown in Fig.1. By optimizing the distribution of materials, enhanced global properties can be achieved to fit specific requirements with simple materials. While extensive research has been conducted to investigate the mechanical behaviors of different FGPS, nearly all of the research employed forward design approaches, such as theoretical models [6–9], finite element analysis [10,11], topology optimization [12–15] and experimental study [16–19]. Although these studies have achieved great success, designing structures with specific properties still relies heavily on iterative parameters tuning processes and expensive simulations, which are time-consuming, computationally expensive, and often depend on the designers' experience and intuition. Consequently, there is a pressing need for inverse design methods aimed at identifying structures that meet targeted properties.

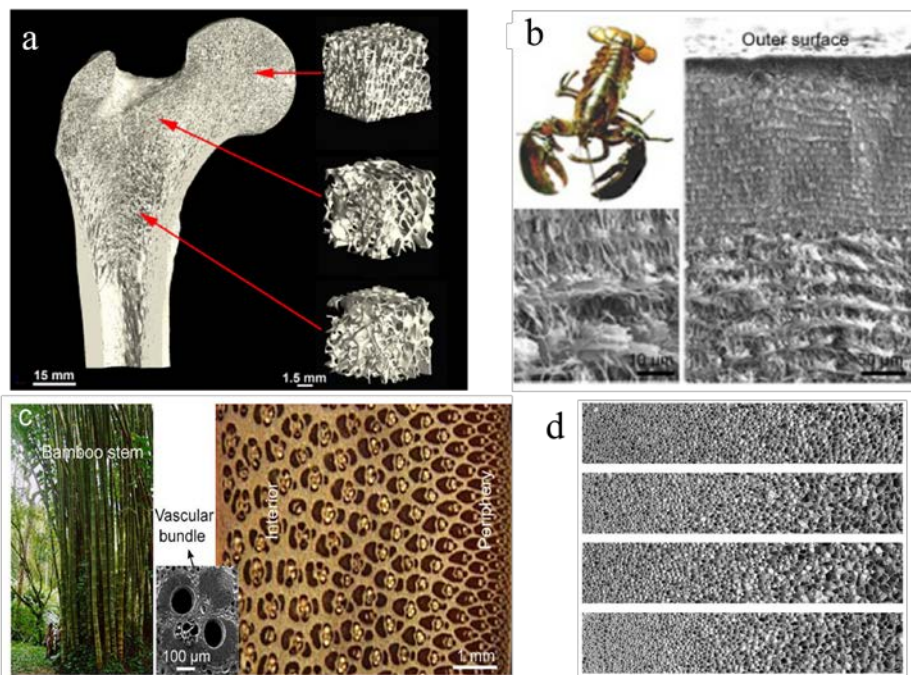


Fig. 1. Functionally graded porous structures in nature. (a) Spatial variations in trabecular bone structure [20]; (b) The exoskeleton of *Homarus americanus* lobster with varied thickness layers [21]; (c) Bamboo stems with graded vascular bundles [21]; (d) Functionally graded aluminum foam [22].

In recent years, deep learning algorithms have been tried to solve these inverse design problems [23–28]. Deep neural networks (DNN) showed great success in designing spinodoid structures [29,30], triply periodic minimal surfaces (TPMS) structures [31–33], and lattice structures [34,35] with specific properties (i.e., Young’s modulus and Poisson’s ratio) thanks to the exceptional ability to learn the mapping relationship from properties to geometrical parameters. Generative adversarial networks (GANs) [36], known for their remarkable ability to synthesize realistic images, have been exploited to handle these challenges by generating pixel-based representative volume elements based on targeted properties. For instance, Tan et al. [37] combined a deep convolutional generative adversarial network (DCGAN) and a convolutional neural network (CNN) to form an inverse design framework that is able to generate metamaterials with the desired compliance tensor. Zheng et al. [38,39] successfully generated both 2D and 3D auxetic structures employing conditional generative adversarial networks (cGAN). Jiang et al. [40] synthesized elastic metamaterials with target dispersion relation by cGAN. Unfortunately, the training difficulty and mode collapse issues impede further application of GAN. Diffusion models [23] with the ability to generate images based on text description offered a new approach to address these challenges. Vlassis and Sun [24] generated heterogeneous microstructures with specific energy responses and topologies employing diffusion models. Bastek and Kochmann [25] utilized a video diffusion model to design metamaterial with targeted stress-strain responses and the design process was physically intuitive. As can be seen from the open literature, similar to the application of diffusion models in the image generation field, the objective properties can serve as guidance for generating targeted structures.

Among the existing research on the inverse design of structures, most of the design objectives were limited to the linear-elastic properties such as Young’s modulus or Poisson’s ratio and rarely considered nonlinear responses [37–42]. Although it is enough to tune structures’ stiffness and Poisson’s ratio under small deformation, extending to nonlinear responses can unlock applications in numerous fields, such as soft robotics [43], impact energy absorption [10], and pressure sensors [44]. However, when consider the nonlinear stage during deformation, the complex material behavior, structure buckling, and contact problem make it challenging to calculate the response immediately, which prevents conventional design methods from

considering nonlinear stages. Efforts have been made to solve this bottleneck by combining evolutionary algorithms and machine-learning-based forward prediction surrogate models that can predict the nonlinear responses rapidly. Examples include shell-based mechanical metamaterials [33] and quadrilateral structures [45]. Despite the advancements of the approach, iterative processes are required to approximate the targeted response and the design space remains limited, which not only increases the design time but also decreases the design diversity. Thus, a direct mapping from the nonlinear stress-strain responses to the configurations of structures with extensive design space is needed.

When employ data-driven methods for structure inverse design, one important issue is how to represent the structures. Some studies utilized geometry parameters that can be used to generate corresponding structures through predefined modelling procedures. Spinodoid metamaterials and TPMS structures [46,47] were implemented via implicit functions and some simple lattice structures [35] have been designed in this way, yet the design space is limited as many kinds of structures can't be represented by simple parameters. Challapalli et al. [48] and Li et al. [49] utilized the nodal adjacency matrix to represent the structures and the inverse design of lattice structures with a wide design domain was realized. Other research [50–52] directly employs 2D pixels or 3D voxels to represent metamaterials and lattice structures. However, this method encounters connectivity issues [50,51] and requires large pixels to represent the structure accurately [38,53], which increases the difficulty of model training. Therefore, a method that can design targeted FGPS with specified nonlinear mechanical behaviors precisely and efficiently is in urgent need.

In this study, we proposed an inverse design framework of FGPS based on the diffusion model. A direct mapping from the nonlinear stress-strain responses to the structures' configurations without iterative processes was established. Moreover, a neural network was trained to predict the responses of the generated structures. Five unique types of FGPS were constructed using Voronoi diagram techniques and their corresponding stress-strain responses were calculated using finite element simulations. The distribution of Voronoi nuclei and color mapping were utilized to represent the structure's configuration and cell wall thickness. The performance of the proposed framework was thoroughly evaluated and structures with varied

nonlinear responses were successfully obtained.

This work is organized as follows. Section 2 provides a brief overview of the proposed inverse design framework. Section 3 introduces the generation and pre-processing methods of the dataset. Section 4 illustrates the models used in the framework. The performance of the well-trained models is discussed in Section 5, and we present several inverse design examples to demonstrate the effectiveness of the approach. Three FGPS were fabricated by SLM and an impact experiment was carried out to verify the method's efficacy. The conclusion is made in Section 6.

2. Overview of the inverse design approach

In this section, we provide a brief overview of the proposed inverse design approach. There are two primary challenges in developing an inverse design framework: firstly, generating structures based on specified conditions (referred to as the 'generator'), and secondly, rapidly evaluating the performance of the generated structures (referred to as the 'predictor'). In this study, we propose a novel framework that uniquely combines a tailored diffusion model with a modified residual neural network (ResNet) to tackle the two challenges. The detailed structures of the two models will be discussed in Sections 4.1 and 4.2. As illustrated in Fig. 2, the two models were integrated to generate porous structures aligned with the predefined stress-strain(S-S) curves. The generator can produce a batch of nuclei maps (detailed in Section 4.1) according to the target responses, and the predictor can predict the S-S responses of the generated nuclei maps. Subsequently, the predicted S-S curves are compared with the target S-S curves, and the discrepancies are quantified by mean absolute percentage error (MAPE), as defined in Eq(21). All the candidate nuclei maps are sorted by the MAPE values, and the map with the lowest MAPE is selected as the target map. Finally, the corresponding porous structure will be reconstructed based on the nuclei's positions and the cell wall thickness using Voronoi diagram techniques. The finite element model can be built to obtain the actual S-S responses following the approach described in Section 3.2.

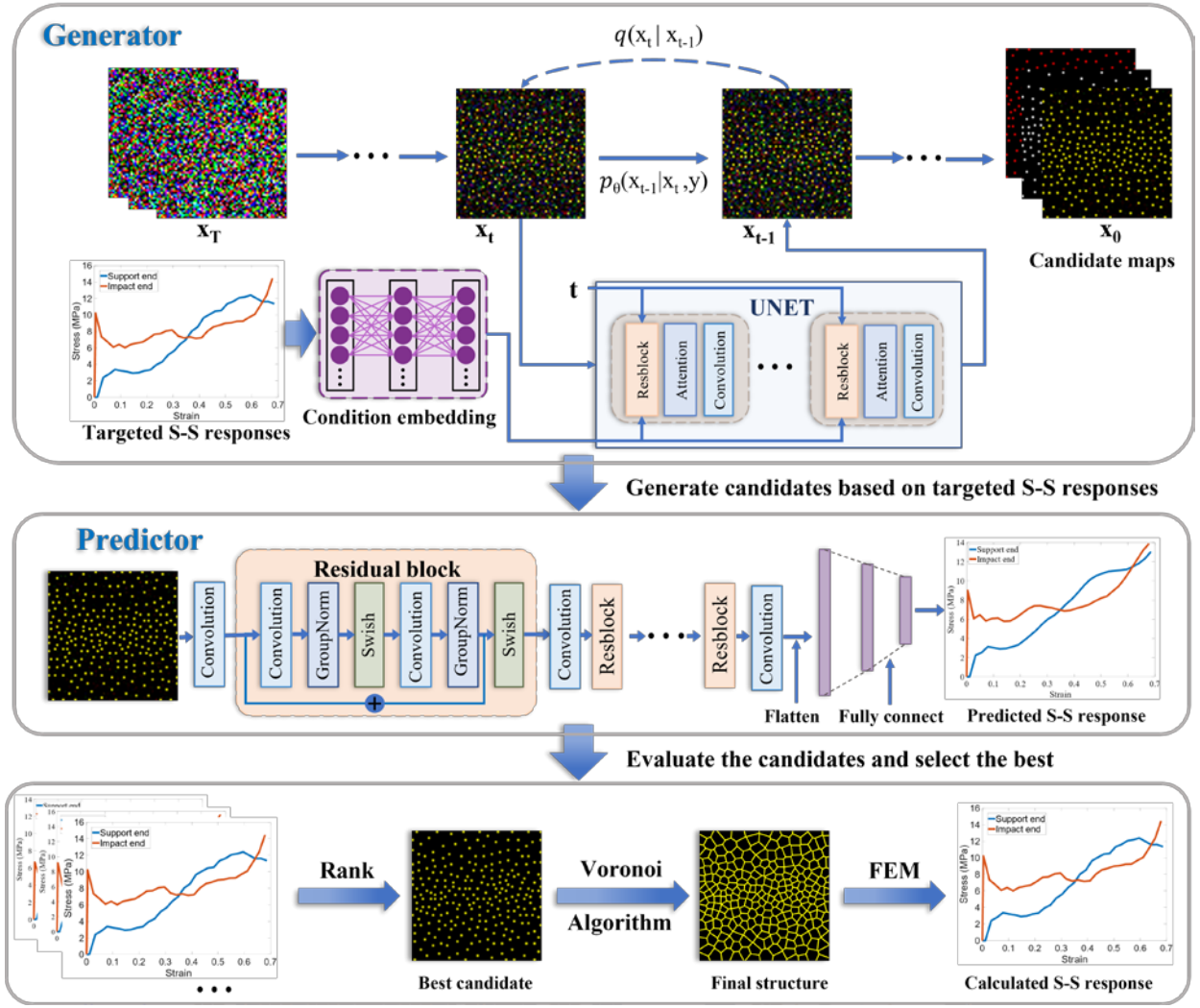


Fig. 2. Overview of the inverse design process.

3. Generation and pre-processing of the dataset

In this section, we introduce the process of building the dataset, including the approach of generating the FGPS, the finite element methods for obtaining the S-S responses of the structures, and the pre-processing models of the data. The S-S responses and the deformation processes of different gradient types of FGPS are illustrated and discussed.

3.1 Implementation of FGPS

As the proposed inverse design framework is based on a data-driven method, a large number of FGPS and their corresponding S-S responses are needed. Here, five distinct gradient types of FGPS' numerical models were built [10]. The structures were established using Voronoi techniques, an effective technique for modeling diverse porous materials [54,55]. As depicted in Fig. 3, the generation of a porous structure involves three steps:

Step 1: Randomly scatter a set of nuclei within a square region $A = 40 \times 40 \text{mm}^2$, ensuring the distance between any two nuclei is larger than the allowable minimal distance δ_{ij} .

Step 2: Generate Voronoi diagrams employing 2D random Voronoi techniques.

Step 3: Thicken the cell wall to the predefined thickness.

The five distinct gradient forms named uniform(U), positive(P), negative(N), middle-high(M-H), and middle-low(M-L), are depicted in Fig. 4. The FGPS were constructed by controlling the minimal distance between neighboring nuclei while keeping the cell wall thickness consistent. The U type structures have the same density along the y-direction, and the minimum distance δ_{ij} equals to $d_{\min}$ for all nuclei. For the P or N graded structures, the upper end has the lowest or highest density, while the lower end has the highest or lowest density. The governing equations for δ_{ij} are defined as Eq.(1) for the P distribution and Eq.(2) for the N distribution. The M-H or M-L distribution is characterized by the highest density in the middle or side region and the lowest density in the side or middle region. The governing equations are defined as Eq.(3) for the M-H form and Eq.(4) for the M-L form relatively.

$$\delta_{ij} = d_{\min} \left[1 + \alpha \frac{(y_i + y_j)}{2L} \right], \quad (1)$$

$$\delta_{ij} = d_{\min} \left(1 + \alpha \left(1 - \frac{y_i + y_j}{2L} \right) \right), \quad (2)$$

$$\delta_{ij} = d_{\min} \left[1 + \alpha \left| \frac{(y_i + y_j)}{2L} - 0.5 \right| \right], \quad (3)$$

$$\delta_{ij} = d_{\min} \left\{ 1 + \alpha \left[0.5 - \left| \frac{(y_i + y_j)}{2L} - 0.5 \right| \right] \right\}, \quad (4)$$

where $d_{\min}$ represents the overall minimum distance, α denotes the degree of gradient variation, y_i and y_j stand for the y-axis coordinates of the two neighboring nuclei, L is the length of the structure in the y-direction and is equal to 40mm here.

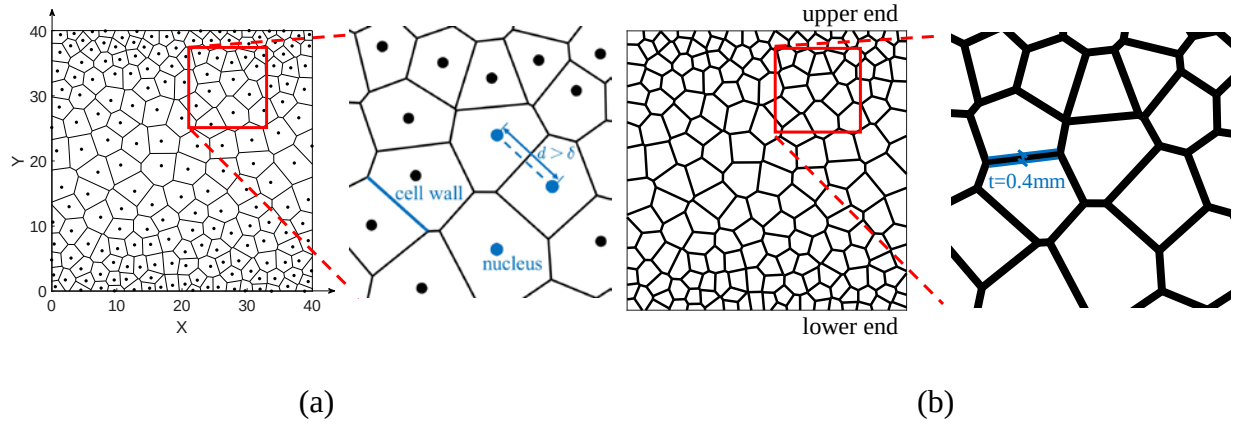


Fig. 3. The processes of generating Voronoi structures. (a) Scatter nuclei and generate a Voronoi diagram. (b) Thicken the cell wall to form the FGPS.

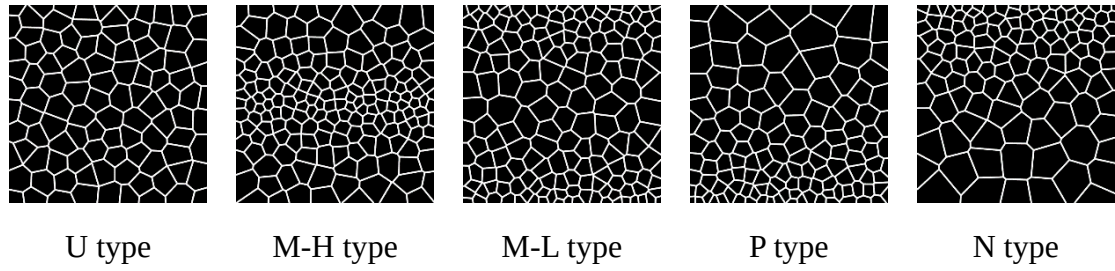


Fig. 4. The schematic diagrams of the five gradient types of FGPS

Table 1

The parameters used to generate FGPS

Gradient type	$d_{\min}$ (mm)	α	Thickness(mm)
U	[1.5:0.1:4]	/	[0.2:0.05:0.5]
M-H	1.5	[1:0.1:4]	[0.2:0.05:0.5]
M-L	1.5	[1:0.1:4]	[0.2:0.05:0.5]
P	1.5	[1:0.1:4]	[0.2:0.05:0.5]
N	1.5	[1:0.1:4]	[0.2:0.05:0.5]

Here, by varying $d_{\min}$, α , and cell wall thickness, a variety of different structures that cover a wide range of design space were generated. The parameters selected for this study are elaborated in Table 1. For the U type porous structures, $d_{\min}$ varies from 1.5 to 4.0, in increments of 0.05, and the cell wall thickness ranges from 0.2 to 0.5, with steps of 0.05. For the gradient porous

structures, $d_{\min}$ is fixed at 1.5 to avoid excessively short cell walls, α varies from 1.0 to 4.0 in increments of 0.1, and cell wall thickness varies from 0.2 to 0.5 with intervals of 0.05. Owing to the stochastic nature of Voronoi structures, structures generated with the exactly same parameters are distinct. Thus, to enrich the dataset, two structures for each parameter configuration were generated. There are 434 U type structures within this database, along with 364 for each of the other four gradient types, resulting in a total of 2100 structures encompassed within the entire dataset. More details about the dataset are provided in Appendix A.

3.2 FE simulation

In order to obtain the S-S responses of the structures within the dataset, finite element models were constructed using batch processing. As illustrated in Fig. 5(b), the porous structure is situated between the impact rigid plate and the support rigid plate, and both plates are modeled using discrete rigid plates attached to reference points. A constant low velocity $v = 20\text{ m/s}$ is applied to the reference point of the impact plate, while the support plate is completely fixed at the bottom of the structure [10]. The structure is discretized using four-node shell elements (S4R) in Abaqus. Only one element is employed in the out-of-plane direction, which is assumed to be rational in the literature [56]. The nodes can only move freely in the plane, whereas the out-of-plane degrees of freedom are constrained. A mesh sensitivity analysis was conducted as shown in Fig. 6. The element size is set to 0.3 mm to balance the computational time and accuracy. The material of cell walls is defined as elastic perfectly plastic with Young's modulus $E = 66\text{ GPa}$, Poison's ratio $\nu = 0.3$, yield stress $\sigma = 175\text{ MPa}$, and mass density $\rho_s = 2700\text{ kg/m}^3$, consistent with the settings in [57]. Self-contact is applied to consider the contact between cell walls during deformation. The contact property was defined as hard contact in the normal direction and penalty friction in the tangential direction. The contact friction coefficient was set to 0.02, allowing for relative slippage with friction between the structure and the plates. The S-S curves obtained by the numerical model is shown in Fig. 5(c) and the deformation process is depicted in Fig. 5(d). The structure initially collapses near the impact end, and subsequently collapses at the support end as well. Since the collapse occurs layer by layer and extends from the low-density area to the high-density area, the stress at both ends continuously increases. At the strain of 0.6, the low-

density regions are compacted, and a shear band forms in the central high-density area of the structure, which leads to a redistribution of stress in the structure. This results in a decrease in support end stress, coupled with an accelerated increase in the impact end stress.

The S-S responses of all the structures in the dataset were all calculated using the previously described model. The stress at both the impact end and support end was extracted, and the range of S-S responses is depicted in Fig. 7. The curves are colored according to their relative densities, ranging from low to high. A wide range of S-S responses has been achieved. For graded porous structures, the S-S responses under impact load are different for the impact end and the stationary end. Stress points are sampled from the S-S curves to be used to represent the S-S responses. Since the initial stresses are all zero, to avoid repetition, sampling starts from the first stress point that is not zero. The impact end begins at the strain of 0.004, and the support end starts at the strain of 0.011, with stress values collected every 0.0225 strain increment, as depicted in Fig. 8. For each end, 31 stress points are sampled, resulting in a total of 62 stress points for each structure. Stress data at both the fixed and impact ends will be utilized as the target responses in the inverse design process simultaneously.

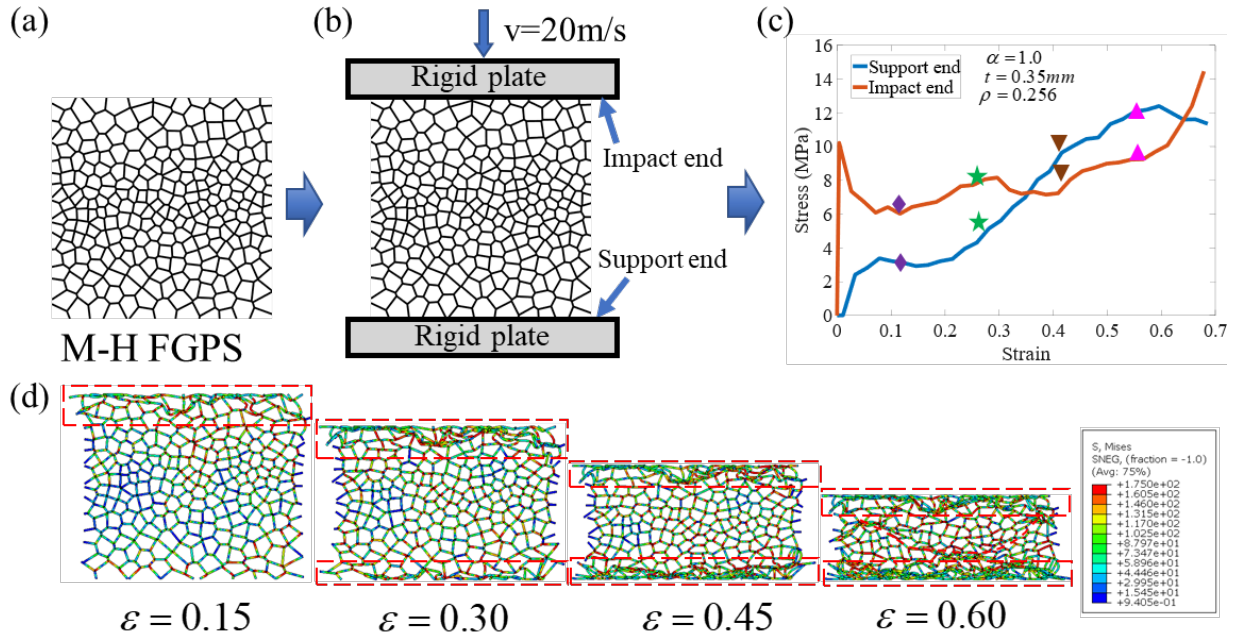


Fig. 5. The calculation flow of FGPS: (a) Configuration of the middle-high porous structure. (b) Boundary condition. (c) The S-S curves at the support end and impact end. (d) Deformation processes and stress cloud of FGPS under compression.

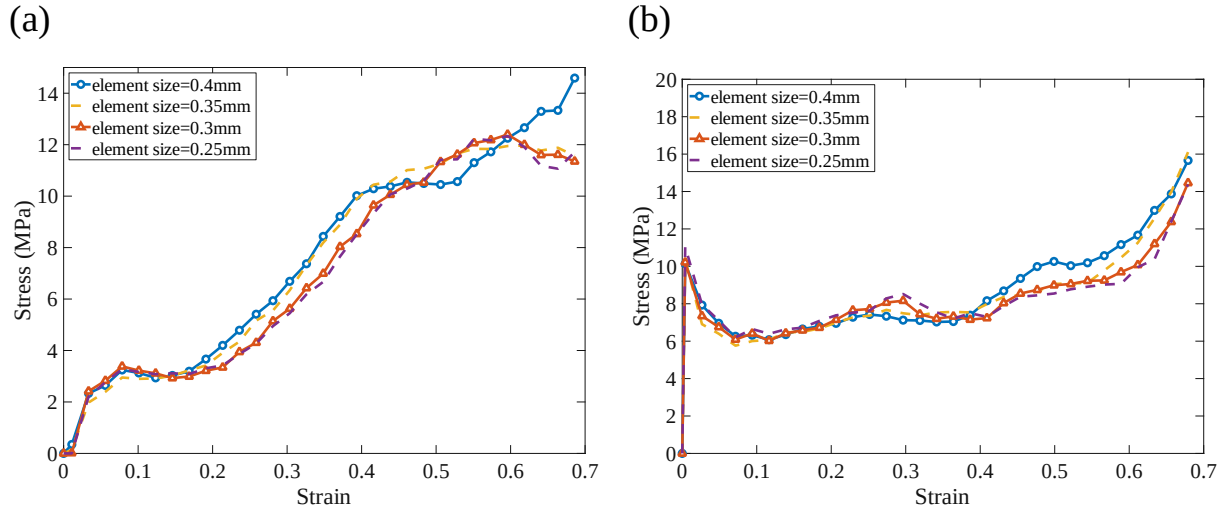


Fig. 6. Mesh sensitivity analysis. (a) Support end. (b) Impact end

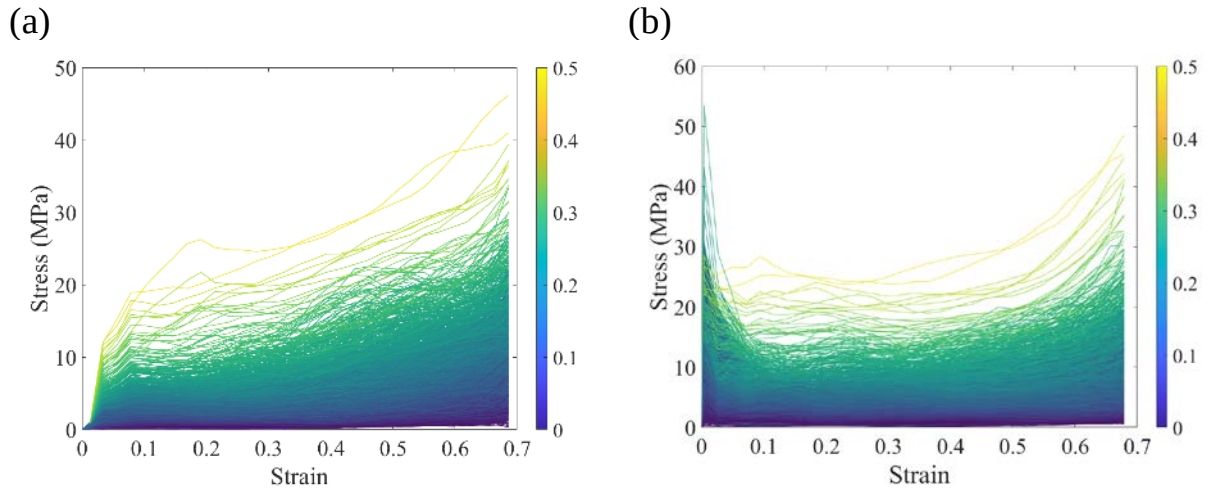


Fig. 7. Summarization of the various S-S curves of the structures in the dataset obtained through FEM. The curves are colored according to their relative densities, ranging from low(blue) to high(yellow). (a) Support end. (b) Impact end.

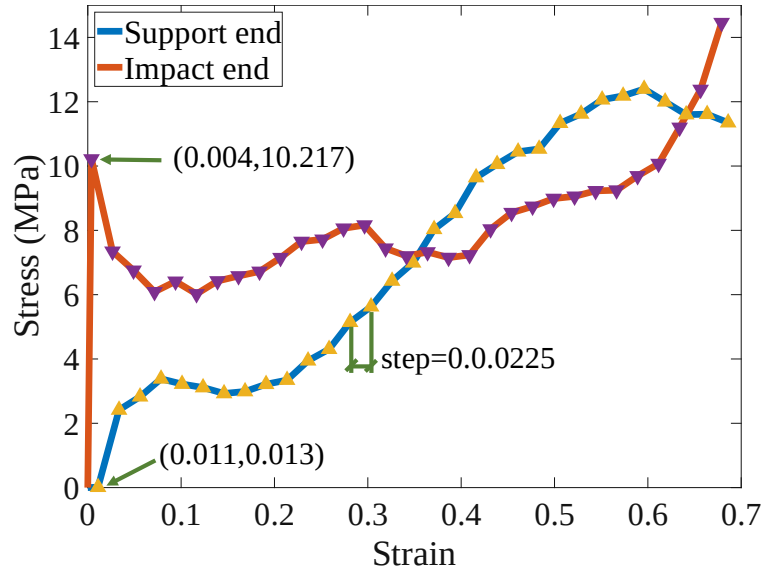
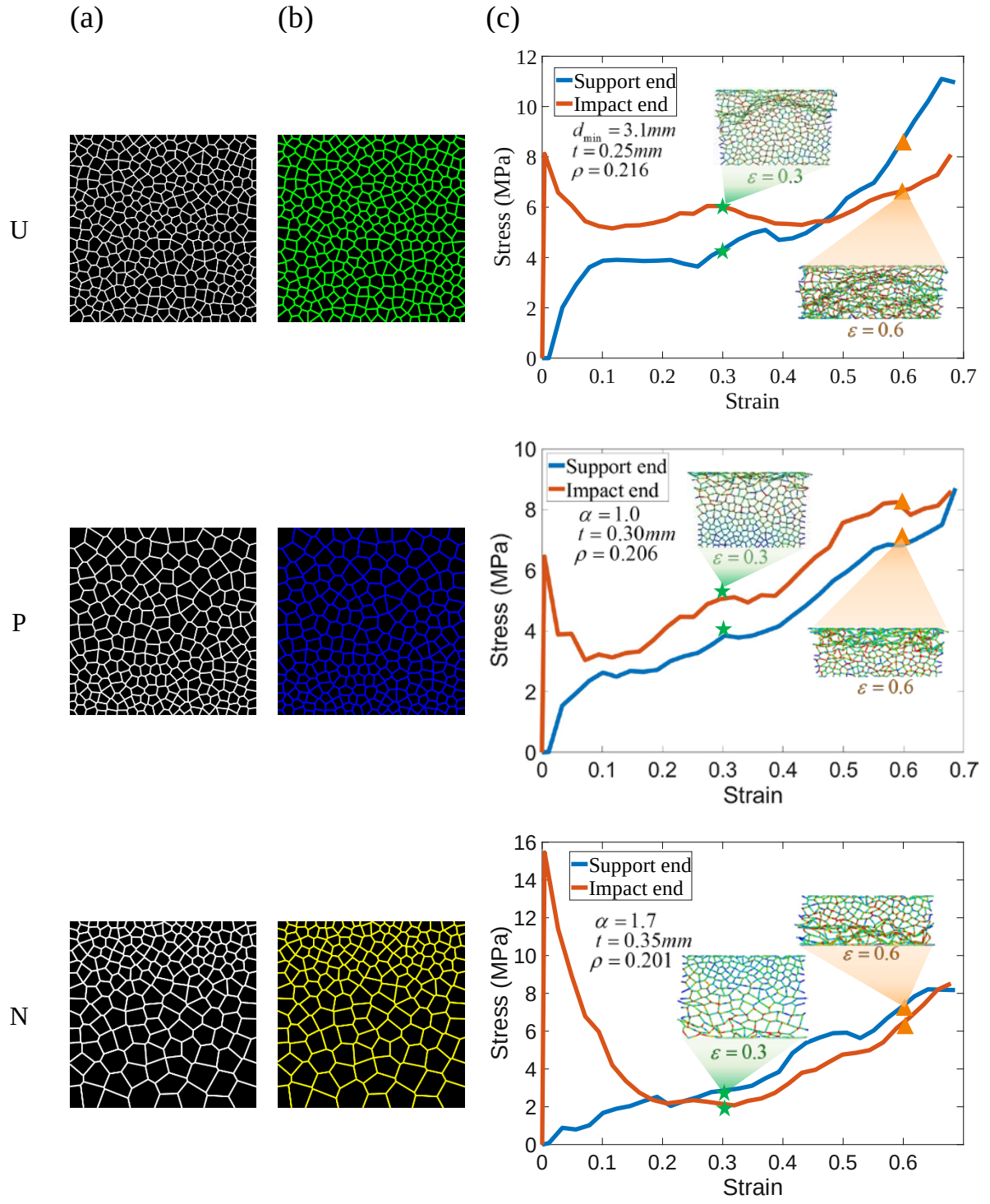


Fig. 8. Sampling method of stress points.

Fig. 9 displays the typical structures of five different gradient types and their S-S responses. Each structure has an approximate relative density of 0.2 and different cell wall thicknesses. The binary and colored images (with color denoting the cell wall thickness, refer to Section 3.3 for more details) are presented. Different gradient types of FGPS exhibit markedly distinct deformation behaviors. The U type structures show random shear bands at the weakest region of the structure under compression. For the graded porous structures, the collapse is firstly observed at the low-density region and gradually propagates to the high-density region, thus a layer-by-layer collapse can be discovered. Nevertheless, for M-L and N gradient FGPS, a slight deformation can be detected at the impact end, even though it is the densest part due to the impact effect. The distinct deformation patterns lead to different S-S responses. The stress at the impact end is greater than that at the support end at the initiation of the deformation. For structures with P and M-H gradients, the initial peak stress at the impact end is relatively small, whereas structures with N and M-L gradients exhibit a notably heightened initial peak stress at the impact end, which is attributed to the high-density region near the impact end. During the deformation process, the stress at the fixed end rises gradually, while the stress at the impact end initially decreases from its initial peak value before rising again. Notably, structures with M-H and U gradients display a period of plateau stress in the initial stages of deformation. The FGPS exhibit various deformation patterns and S-S responses, which reflects their promising applications in many fields.



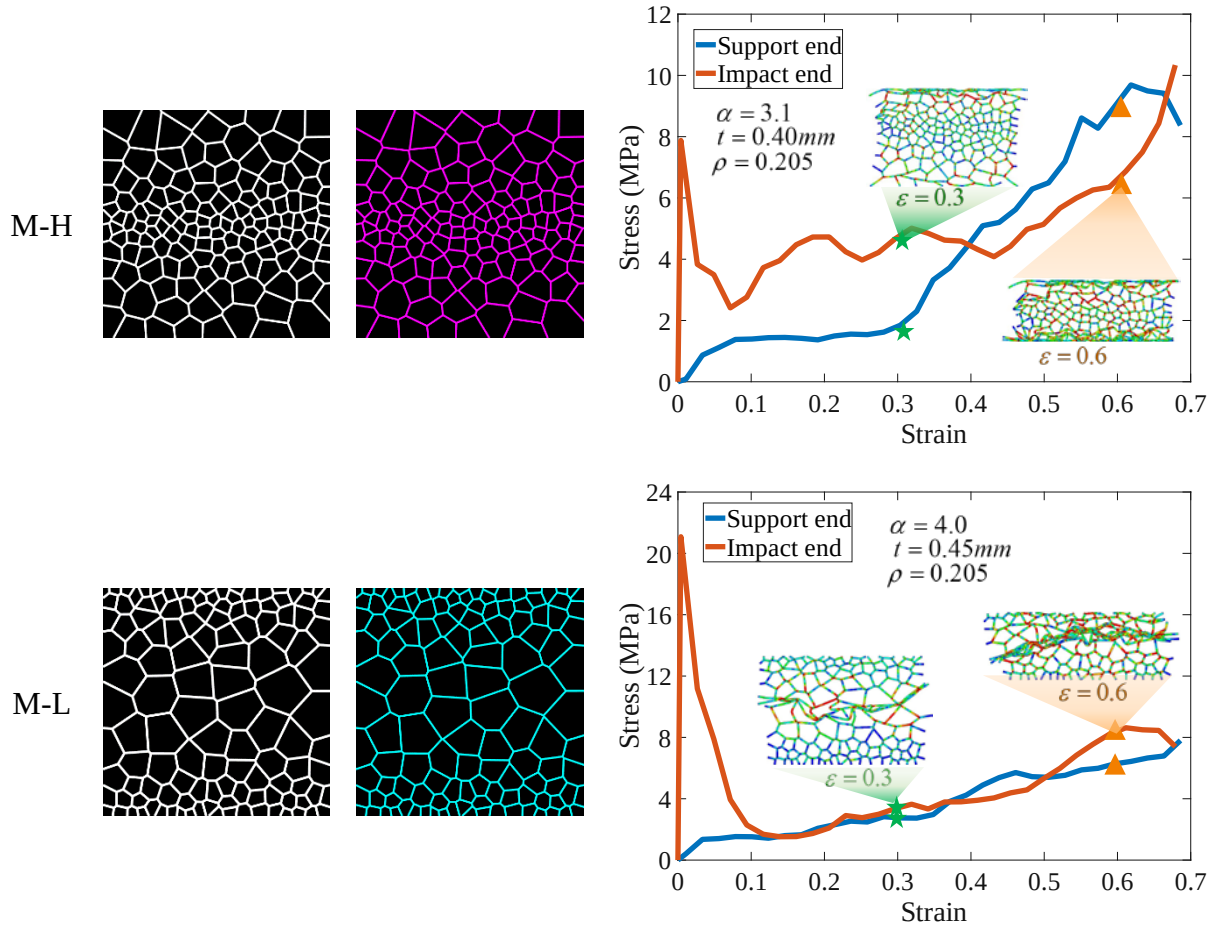


Fig. 9. Structures' configurations and S-S responses of five different gradient types of porous structures, each structure has a close relative density of 0.2. (a) The binary images of the FG structures. (b) The RGB images of the structures, with the color denoting the cell wall thickness. (c) The corresponding parameters and S-S curves of the structures, the deformation at strain 0.3 and 0.6 is presented.

3.3 Data pre-processing

3.3.1 Representation of FGPS

Once the dataset is built, pre-processing is essential for deep learning to effectively interpret the data. Some studies [33,46–48] utilized a sequence of parameters that can be used to generate the corresponding structures to represent the structures. Nevertheless, in this study, identical parameters do not generate the same structure due to the inherent stochastic property of Voronoi structures, and the mechanical responses vary across different structures, making it impractical to use simple parametric representation. Other research [40,52,58–61] directly employed the 2D or

3D binary image of the structure, where different pixels represent different materials or voids. As depicted in previous studies [50,62], the cell walls were observed to be disconnected when adopting this method for representing the gradient porous structures. This is because the generative models are aimed to minimize the pixel difference between the generated images and the original images, so disconnection in the images is acceptable for the model. However, minor structural differences can lead to significant performance variations. Moreover, as the cell wall thickness of the porous structure is very small compared to the whole structure, and the pixels of the image are discrete, it needs exceedingly high-resolution images to accurately depict cell wall thickness. For instance, when using an image with a resolution of 256×256 , each pixel unit represents a length of $d_{\text{pixel}} = 40\text{mm} / 256 = 0.15625\text{mm}$. To represent a structure with a cell wall thickness of 0.3mm , 2 pixels are needed to depict the cell wall thickness. However, the combined length of these two pixels corresponds to an actual length of $d = 0.15625\text{mm} \times 2 = 0.3125\text{mm}$, resulting in a discrepancy. Meanwhile, when representing a structure with a cell wall thickness of 0.25mm , it also needs 2 pixels. This leads to an indistinguishability between structures with a cell wall thickness of 0.25mm and those with a cell wall thickness of 0.3mm , which results in a larger error. Extremely high image resolutions increase the complexity of model training and much more time is needed for training.

To address these problems, as demonstrated in Fig. 10 (a)-(c), we utilize different colors to denote various cell wall thicknesses. Additionally, the positions of the Voronoi nuclei points are used to represent the patterns of the Voronoi structures. Specifically, the entire design domain was discretized into 64×64 grids. By identifying the grid closest to each nucleus point and assigning colors corresponding to the cell wall thickness, a colored ‘map’ that locates each nucleus and contains cell wall thickness information was effectively created. The correlation between cell wall thickness and its color representation is illustrated in Fig. 10 (d). For instance, a structure with a cell wall thickness of 0.2mm is colored red, whereas one with a thickness of 0.25mm is colored green. These maps are then converted into RGB images with a resolution of 64×64 , serving as representations of the structures during the deep learning process. Furthermore, these maps can be easily transformed into the corresponding porous structure through simple steps. Firstly, calculate the coordinates of the nuclei based on the map. Next, employ the Voronoi

algorithm to construct the Voronoi structure. The cell wall thickness of the porous is then determined by the color of the map, enabling the construction of the corresponding porous structure. It should be noted that, to prove a more intuitive understanding of the structure, in this paper, the colored Voronoi structures are used to represent the porous structure as shown in Fig. 9(b).

Through the above steps, we construct an implicit representation of FGPS with different cell wall thicknesses. Utilizing the images of colored nuclei points, it is able to accurately represent FGPS using only 64×64 pixels. Utilizing smaller pixel dimensions can substantially reduce both the parameter count and training time required for the deep learning model, and significantly boost both the model's efficiency and accuracy. Furthermore, as the final structures are created using the Voronoi algorithm based on the generated colored nuclei maps, the connectivity issues are thus eliminated.

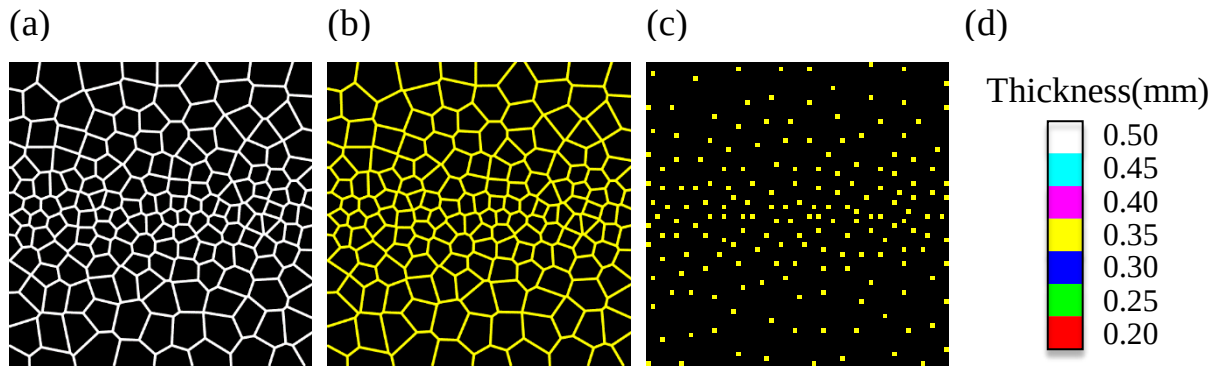


Fig. 10. (a) The binary images of the functionally graded structures. (b) The RGB images of the structures, with the color denoting the cell wall thickness. (c) The colored nuclei map, with the point denoting the location of the nuclei and the color denoting the cell wall thickness. (d) The correlation between cell wall thickness and its color representation.

3.3.2 Data normalization

To enhance the convergence speed and accuracy of the model, it is generally necessary to normalize the input data. All stress data are linearly mapped to the range of $[-1,1]$, and the function for the linear mapping is provided as

$$y_i = \frac{2Y_i - (Y_{i\max} + Y_{i\min})}{Y_{i\max} - Y_{i\min}}. \quad (5)$$

Furthermore, a standardization process is applied to all map images. This process adjusts the

pixel values of each image channel to conform to a distribution with a mean of 0 and a variance of 1. The mapping equation used for this standardization is

$$output_{[channel]} = \frac{input_{[channel]} - mean_{[channel]}}{std_{[channel]}}. \quad (6)$$

Here, the mean represents the average value of each channel in the image, and std denotes the standard deviation of each channel, which is determined through sampling.

4. Models used in the framework

In this section, we first make a brief introduction to the conditional diffusion model. Then, the model structures of the generator implemented by diffusion model and predictor implemented by residual neural network are presented. And the training protocols and sampling strategies are also described.

4.1 The generator of FGPS

4.1.1 Conditional diffusion model

The aim of the generator is to generate nuclei map pictures under specific S-S conditions. To accomplish this task, the recently developed generative models known as the diffusion models [63] were employed. Diffusion models establish a Markov chain process that progressively introduces random noise into the data and then learns in reverse to reconstruct the data samples from the noise, which is defined as forward process and reverse process respectively. In the forward process, a data point sampled from a distribution is incrementally perturbed by a small amount of Gaussian noise over T diffusion time steps, resulting in a series of noisy samples $x_1, \dots, x_T$. The noise process is described by a Markov chain and is defined as

$$q(x_t | x_{t-1}) = N(x_t; \sqrt{1 - \beta_t} x_{t-1}, \beta_t I), \quad (7)$$

where $\beta_t \in (0,1)$ represents a variance schedule. By defining $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{i=1}^t \alpha_i$, the sample at any time step t can be written as

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \mathbf{0}, \quad (8)$$

where $\mathbf{x}_{t-1}, \mathbf{x}_{t-2}, \dots \sim (0, I)$, and the distribution in Eq.(7) at the time step t can be given by

$$q(x_t | x_0) = \mathcal{N}(x_t; \sqrt{\alpha_t} x_0, (1 - \alpha_t) \mathbf{I}). \quad (9)$$

As long as the T is large enough and β_t is small enough, the initial picture will be transformed into a Gaussian noise distribution after the forward process.

By reversing the process and sample from $q(\mathbf{x}_{t-1} | \mathbf{x}_t)$, the origin sample can be created from a Gaussian noise input. Beginning with pure Gaussian noise, a model is trained to learn the joint distribution as

$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t), \quad (10)$$

$$p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)), \quad (11)$$

where the time-dependent parameters of Gaussian transitions are learned. The diffusion model p_θ is optimized by maximizing the likelihood of the training data, and in practice, we choose to minimize the variational lower bound (L_{VLB}) of the negative log-likelihood which is expressed as

$$L_{\text{VLB}} = \mathbb{E}_{q(\mathbf{x}_{0:T})} \left[\log \frac{q(\mathbf{x}_{1:T} | \mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})} \right]. \quad (12)$$

And this can be rewritten in terms of Kullback-Leibler (KL) Divergences as

$$L(\theta) = E_q \left[\underbrace{D_{\text{KL}}(q(\mathbf{x}_T | \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T \underbrace{D_{\text{KL}}(q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t))}_{L_{t-1}} - \log p_\theta(\mathbf{x}_0 | \mathbf{x}_1) \right]. \quad (13)$$

Using Bayes theorem, the post posterior can be tractable when conditioned on $\mathbf{x}_0$:

$$q(x_{t-1} | x_t, x_0) = \mathcal{N}(x_{t-1}; \tilde{\mu}(x_t, x_0), \tilde{\beta}_t I),$$

$$\text{where } \tilde{\mu}_t(x_t, x_0) := \frac{\sqrt{\alpha_{t-1}} \beta_t}{1 - \alpha_t} x_0 + \frac{\sqrt{\alpha_t} (1 - \alpha_{t-1})}{1 - \alpha_t} x_t \quad \text{and} \quad \tilde{\beta}_t := \frac{1 - \alpha_{t-1}}{1 - \alpha_t} \beta_t. \quad (14)$$

Thus L_{t-1} can be calculated in closed form and by setting the variances of $p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$ to be equivalent to the forward process variance schedule, L_{t-1} can transformed into:

$$L_{t-1} \propto \|\tilde{\mu}_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2. \quad (15)$$

Ho et al.[63] found that training μ_θ to predict the noise component at any given time step leads to improved outcomes. And the training objective can be simplified as

$$L_{\text{simple}}(\theta) := \mathbb{E}_{t, \mathbf{x}_0, \epsilon} [\|\epsilon - \epsilon_\theta(\sqrt{\alpha_t} \mathbf{x}_0 + \sqrt{1 - \alpha_t} \epsilon, t)\|^2]. \quad (16)$$

To generate nuclei maps corresponding to the S-S condition, the classifier-free diffusion guidance strategy [64] is used. A conditional diffusion model $p(x|y)$ is trained with conditioning information dropout randomly at a given probability (10%). The noise predictor can be transformed into a linear combination of the conditional and unconditional noise predictor:

$$\bar{\epsilon}_\theta = (\mathbf{x}_t, t, y) = (w + 1)\epsilon_\theta(\mathbf{x}_t, t, y) - w\epsilon_\theta(\mathbf{x}_t, t), \quad (17)$$

where w is called guidance weight. It can be adjusted to make a trade-off between diversity and fidelity and is set to 5 here.

4.1.2 Architecture of the diffusion model

The U-Net architecture [65] is commonly chosen for constructing the diffusion model due to its identical input and output dimensionality. The U-Net architecture consists of an encoder and a decoder, each containing four steps. Each step incorporates residual blocks, attention blocks, and a down-sampling or up-sampling convolution block. The middle block connecting the encoder and the decoder consists of two residual blocks and one attention block. The residual blocks are comprised of a set of convolutional layers and employ the SiLU [66] activation function. The U-Net architecture employs channel widths of $[C, 2C, 4C, 8C]$ from higher to lower resolutions, with the base channel size set as $C = 64$. The relevant hyperparameters are summarized in Table 2. To incorporate the S-S responses into the model, the 62 normalized stress values are transformed into a condition embedding using a learnable two-layer network. The network consists of two dense layers with a SiLU activation function. Both the condition and time embeddings are straightforwardly incorporated into the residual blocks. The condition dropout probability is chosen as 0.1, and the number of time steps T is set to 1000. The AdamW [67] optimizer is employed, with the initial learning rate equals $2e^{-4}$ and the batch size established as 16. When sampling from the diffusion model, the DDIM [68] strategy is utilized to expedite the process by reducing the number of sampling steps. Here, the number of DDIM sample steps

is set to 100, which can enable the model to generate high-quality images more rapidly.

Table 2

The parameters used in the diffusion model

Parameter	Value
Number of residual blocks per step	2
Normalization	Group Normalization
Number of attention blocks per step	1
Activation function	SiLU [66]
Feature map resolutions (down sample)	[64,32,16,8]
Feature map dimensions (down sample)	[64,128,256,512]

4.2 The predictor of FGPS

The diffusion model introduces randomness in the generation process, enabling the generator to produce diverse structural configurations under identical input conditions. Concurrently, the intricate mapping relationship between the S-S responses and the structure configuration makes the generation of a structure that exactly aligns with the target S-S responses almost unattainable. Therefore, it is imperative to get the S-S responses quickly and discern the variance between the responses of the generated structures and the target response. To achieve this, a surrogate model for rapid prediction of the S-S curves of the generated structures was trained. Given a map of the nuclei points of the structure, the model predicts the S-S responses at both the impact end and support end. These predictions can serve as substitutes for the FEM results, and the structure's response can be obtained with an acceptable margin of error. Notably, finite element simulations are also employed to validate the final generated porous structures.

A modified ResNet architecture followed by three fully connected layers was employed as the surrogate model. The residual block comprises two convolution layers, preceded by a group normalization layer, with Swish [69] serving as the activation function. In the fully connected blocks, the dropout method was incorporated to enhance model generalization, and Tanh was used as the activation function. The model's output is a 62-element vector, where the initial 31 points represent the stress points at the support end, and the remaining 31 points correspond to the stress

points at the impact end. The detailed structure of the network is depicted in Fig. 11. The dataset was randomly split into the training set (90%) and the test set (10%). Mean Absolute Error (MAE) was employed as the loss function and Stochastic Gradient Descent (SGD) was used as the optimizer. Note that the vertically inverted gradient porous structure has the same S-S response as the original structure, so data augmentation was applied by randomly flipping the structures left-to-right with a 50% probability to enhance the performance of the model. The model was trained for 300 epochs, with a batch size of 8. The initial learning rate was set at 0.1, and it was reduced by a factor of 0.1 every 100 epochs. The training loss and validation loss during the training process are illustrated in Fig. 12. The losses were further minimized after reducing the learning rate. Both losses converged at nearly epoch 250 and they are nearly identical which indicates that it was not overfitted.

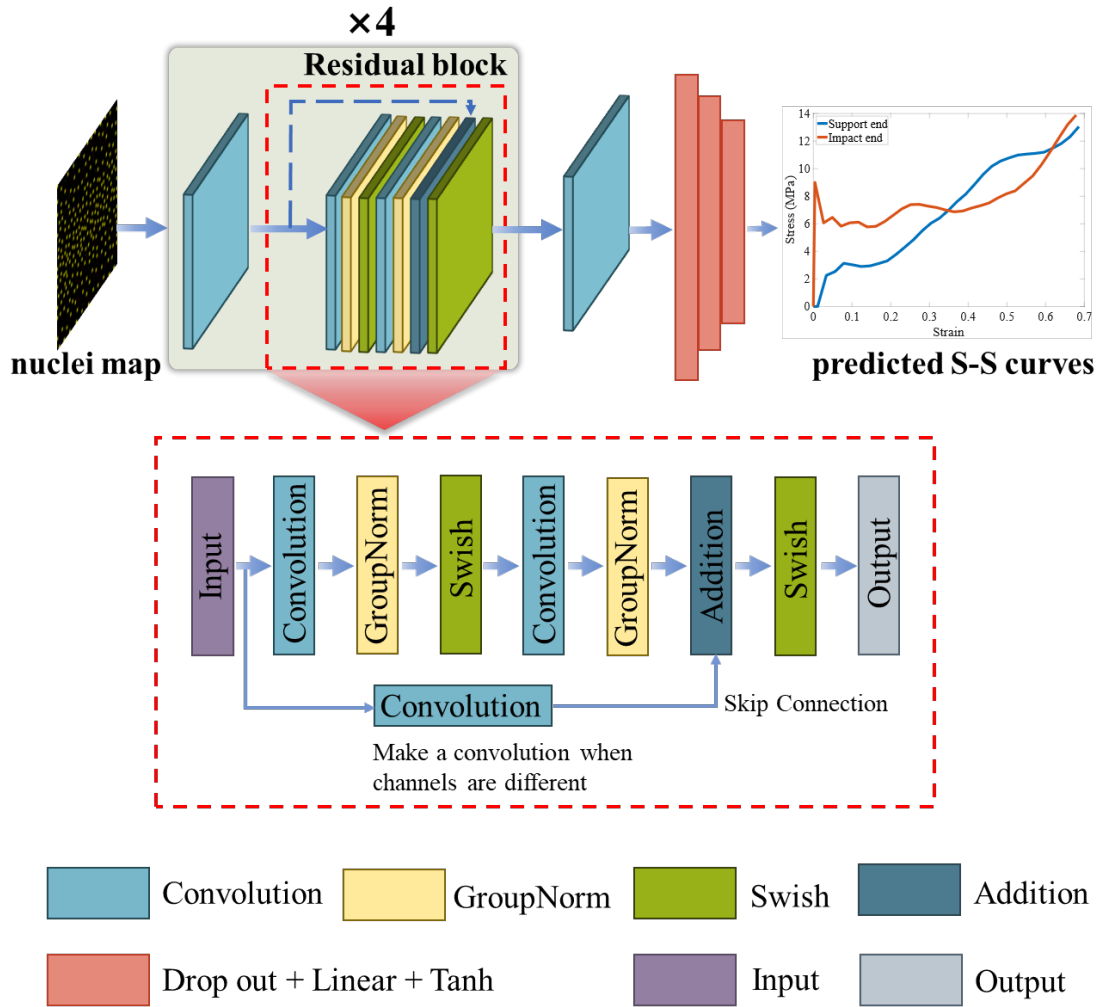


Fig. 11. The architecture of the predictor.

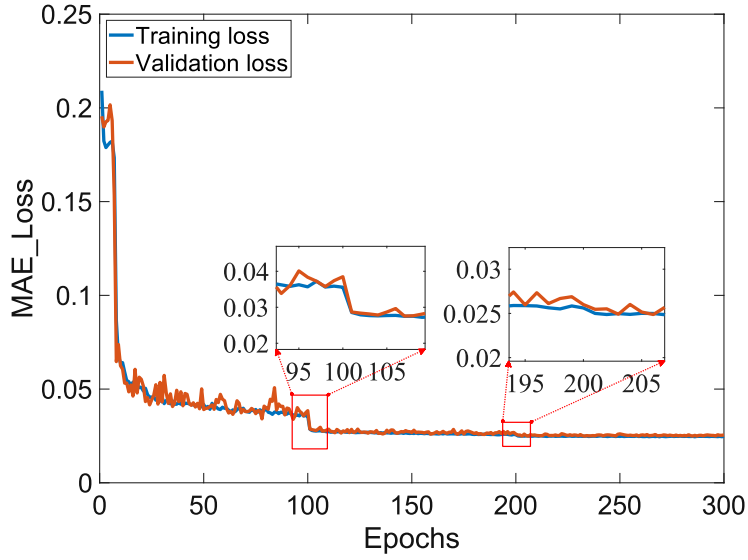


Fig. 12. Training and validation losses of the predictor

5. Result and discussion

In this section, the performance of the predictor is evaluated statistically and the prediction error on specific FGPS is illustrated. Then, to demonstrate the effectiveness of the generator, the generator is utilized to generate diverse FGPS targeted on the same S-S responses. Lastly, structures with different S-S responses are generated through the proposed inverse design framework. Impact experiments are also conducted to further verify the effectiveness of the FEM and the proposed inverse design methods.

5.1 Performance of the predictor

The predictor estimates the S-S curves based on the generated nuclei map images and serves as an evaluator in the inverse design process, thus the accuracy of the predictor can significantly determine the ultimate effectiveness of the model. In this section, the performance of the predictor is assessed on the test dataset. The correlation plot between the finite element modeling (FEM) results (on the x-axis) and predicted values (on the y-axis) is presented in Fig.13(a). The spread and distribution of points provide insight into the accuracy and precision of the predictions. A closer alignment of points to the bisection line ($y=x$) suggests more accurate predictions. Statistically, the coefficient of determination (R^2) defined as

$$R^2 = \frac{\sum_{i=1}^n (y_{pred_i} - \bar{y}_{ref})^2}{\sum_{i=1}^n (y_{ref_i} - \bar{y}_{ref})^2} \quad (18)$$

is calculated to be 0.9898, which indicates a strong linear relationship between the predicted values and FEM results. Here, y_{pred} represents the predicted values, y_{ref} denotes the reference results calculated by FEM and $\bar{y}_{ref}$ is the mean of the reference results.

The relative error (RE) is also adopted to evaluate the prediction accuracy of the predictor and is defined as

$$RE = \frac{y_{pred} - y_{ref}}{y_{ref}} \times 100\%. \quad (19)$$

The RE between FEM results and predicted values in the test dataset is statistically illustrated in Fig. 13(b) to learn the distribution characteristics. The probability density function (PDF) is estimated using kernel density estimation (KDE), which is a non-parametric method to evaluate the probability density function of a random variable. The cumulative distribution function (CDF) of the distribution is calculated by integrating the probability density function. The probability of relative error between -10% and 10% is 0.8696, suggesting most of the relative error points fall within an acceptable range.

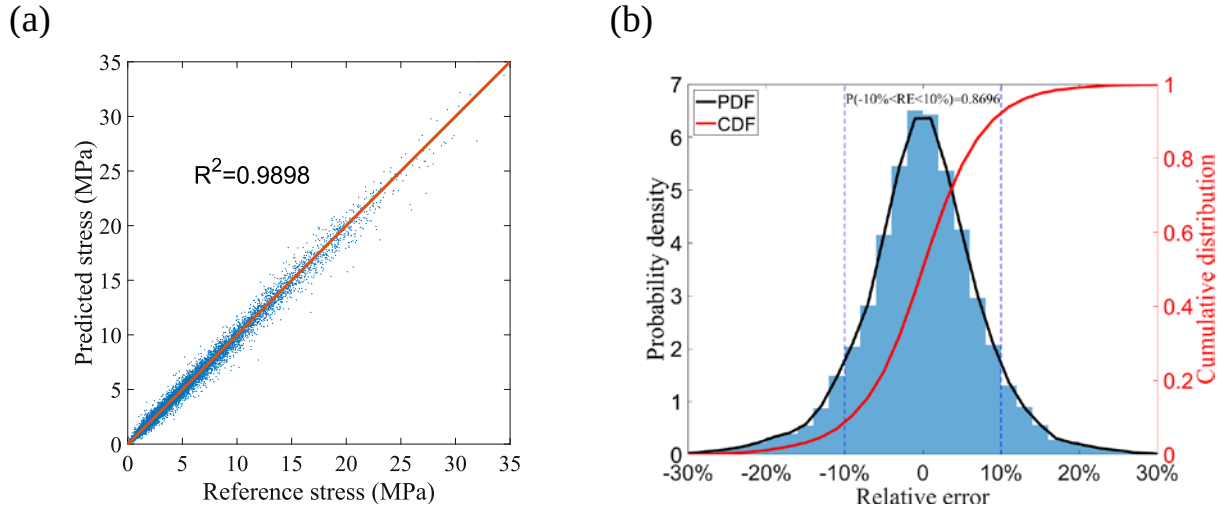


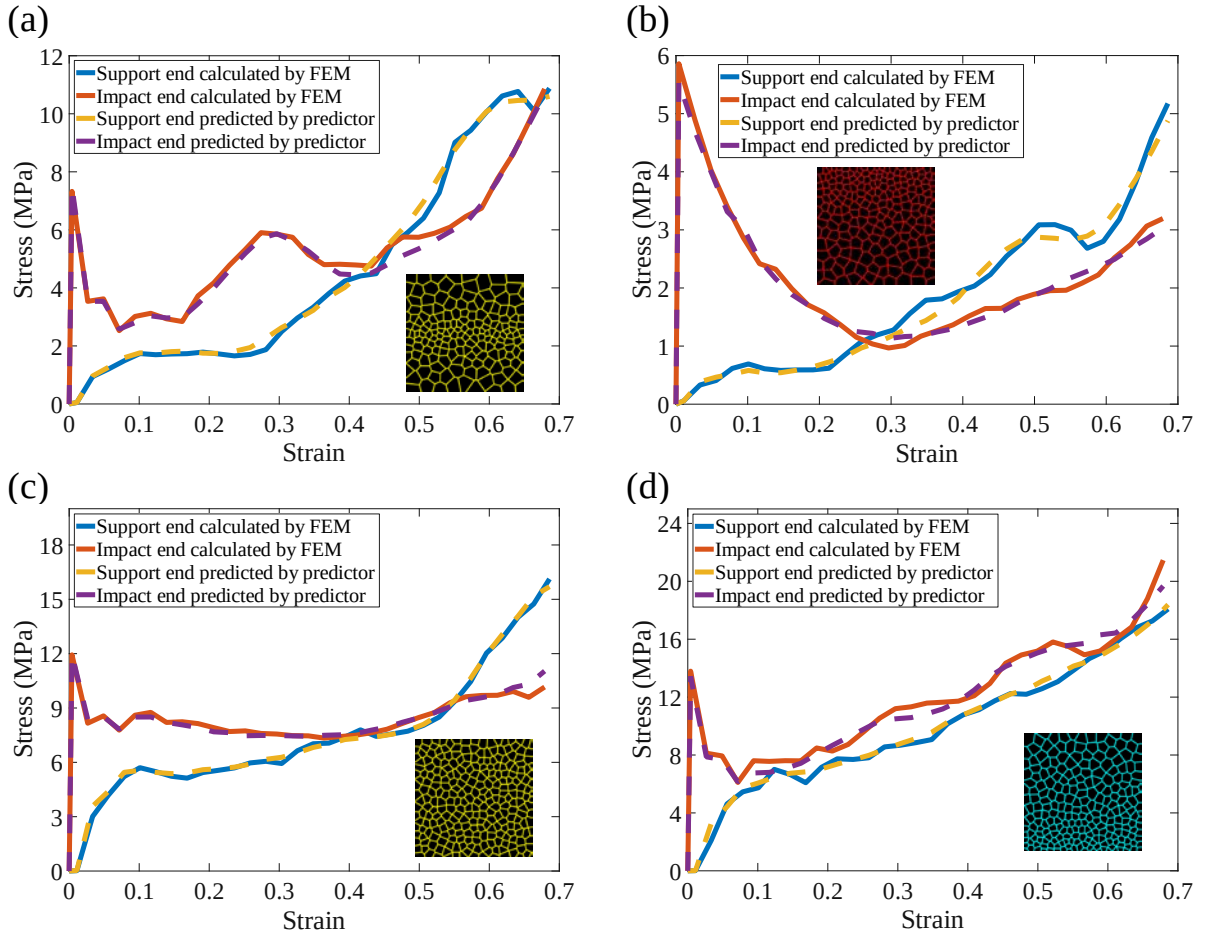
Fig. 13. (a) The relationship between S-S curves predicted by predictor and FEM. (b) The distribution characteristics of the relative error between FEM results and predicted results.

Fig. 14 displays four randomly selected porous structures from the test dataset with their S-S curves obtained through FEM and the predictor respectively. The error was quantified using mean average percentage error (MAPE) as defined as

466

$$\text{MAPE} = \frac{100\%}{n} \sum_{i=1}^n \left| \frac{\hat{y}_i - y_i}{y_i} \right|, \quad (20)$$

467 where $\hat{y}_i$ represents the predicted values and y_i denotes the ground truth. A lower error
 468 indicating a more precise approximation of the ground truth. The predicted S-S curves align
 469 closely with results from finite element analysis, with the initial elastic phase and the initial peak
 470 stress being almost identical. Errors are mainly observed in the nonlinear stage, especially when
 471 the stress changes suddenly. As the strain increases, the material nonlinearity and the complex
 472 contacts between cell walls lead to a highly intricate S-S response, which makes it hard to predict
 473 the precise S-S responses. Based on the above results, it can be concluded that the well-trained
 474 predictor can obtain the S-S responses of structures within a tolerable margin of error.

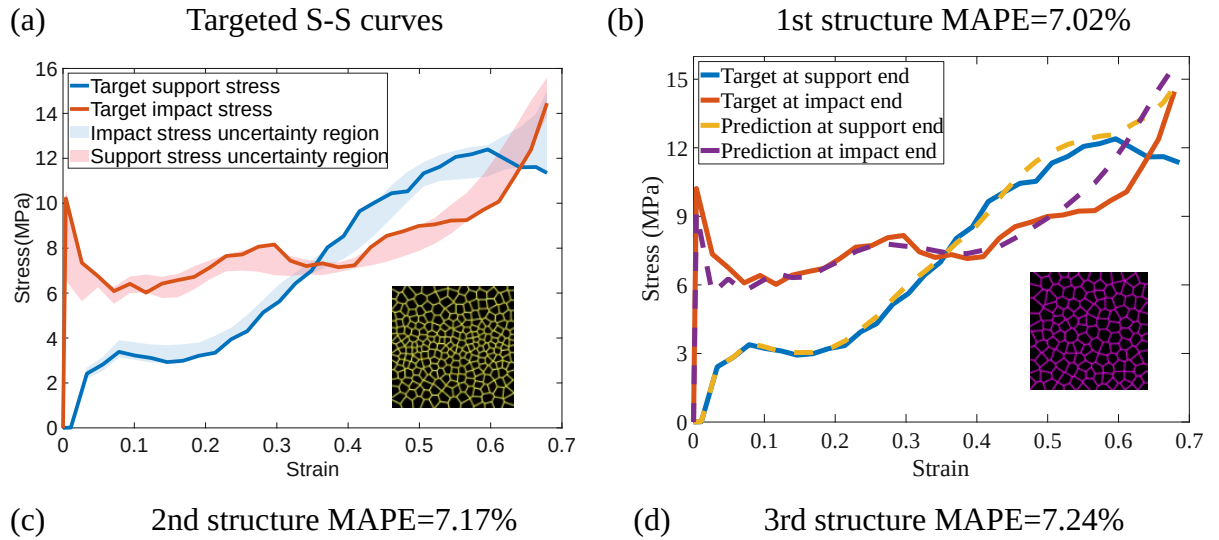


475 **Fig. 14.** Comparison between S-S curves of four randomly selected FGPs obtained by FEM and
 476 predictor and MAPE is calculated. (a) MAPE=4.23%. (b) MAPE=7.19%. (c) MAPE=2.86%. (d)
 477 MAPE=4.59%.

5.2 Performance of the generator

The generator aims to generate structures that match closely to the desired S-S profile. To assess the generator's effectiveness in condition-based generation, a structure was randomly chosen from the test set and the inverse design framework was utilized to generate structures with the same S-S responses as the selected structure. A total of 100 candidate structures were generated using the generator and their corresponding S-S responses were estimated by the predictor.

As shown in Fig. 15, the top 3 structures with minimal error were identified and the MAPE was compared. The uncertainty region in Fig. 15(a) covers the distribution of five selected S-S curves and illustrate the deviation of S-S responses between the generated structures and the target. The S-S curves of the generated structures closely align with the target profile, and the structures exhibited variations in shape and cell wall thickness, reflecting that the generator has the capacity to generate diverse structures. Notably, the generated structures are all M-H gradient structures, which suggests that the generator's proficiency in learning S-S characteristics associated with varying gradient types. Nevertheless, owing to the stochastic nature of the diffusion model's generation process and the complex mapping between S-S responses and structures, it is challenging to obtain a structure that is exactly consistent with the target S-S profile, yet the generator performs excellently within an acceptable error margin.



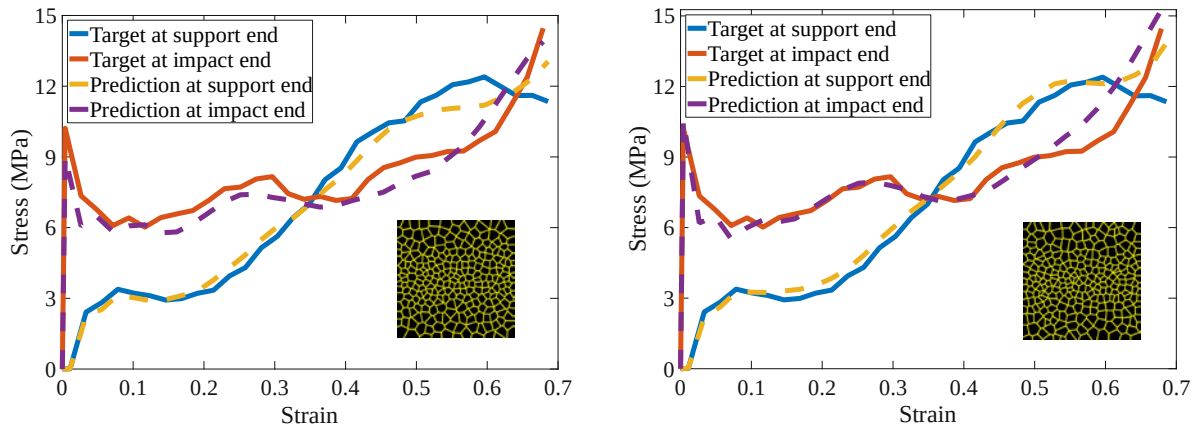


Fig. 15. (a) The target S-S curve and the stress range of the five generated structures. (b)-(d) The generated structures and the predicted S-S curves conditioned on the same S-S in (a).

5.3 Generate structures on target-conditioned responses

To assess the generalization ability of the model, a set of S-S profiles which not included in the dataset were proposed as targeted conditions. The inverse design framework is utilized to generate structures corresponding to the conditions. For each case, the targeted S-S curves, the S-S curves predicted by the predictor, the S-S curves calculated by FEM, and the closest match S-S curves in the dataset were compared. The MAPE was calculated to evaluate the deviation from the targeted S-S.

5.3.1 Target 1: S-S responses not included in the dataset

Firstly, to get a S-S profile that doesn't exist in the dataset yet conforms to the mechanical response characteristics of FGPS, a P gradient structure and a N gradient structure were randomly selected from the dataset, with the mean of their stress values serving as the input condition for the model, as shown in Fig. 16. The generated structure, its deformation process and the comparison of S-S curves are illustrated in Fig. 17. A M-L gradient FGPS was generated, collapse first occurs in the middle of the structure where the density is the lowest. Then, an oblique shear band is formed, and finally, the entire structure is compacted. Although the S-S curves of the generated structure exhibited some deviation from the targeted S-S curves (MAPE = 11.261%), it outperforms the closest match identified in the training dataset (MAPE=14.237%), which underlines it certainly produces novel target-oriented structures.

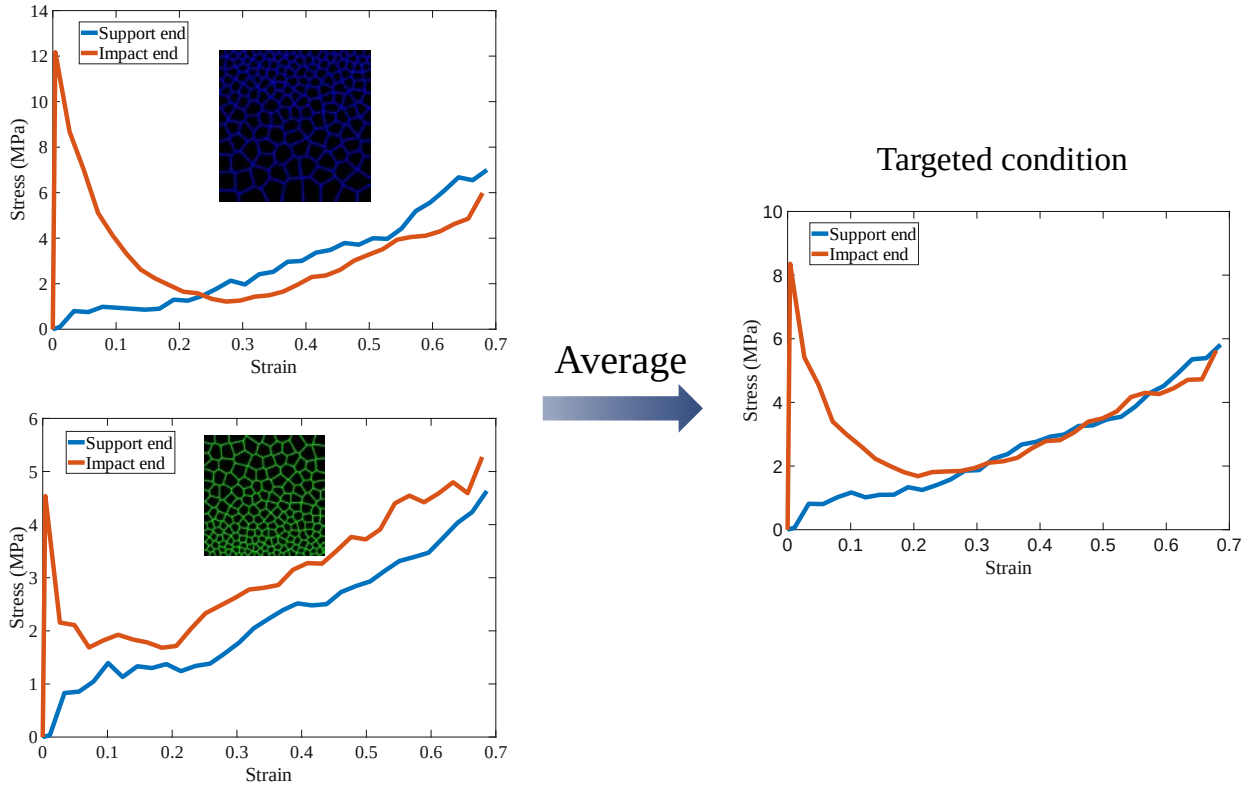


Fig. 16. The S-S curves obtained by average two S-S curves of a N type FGPS and a P type FGPS.

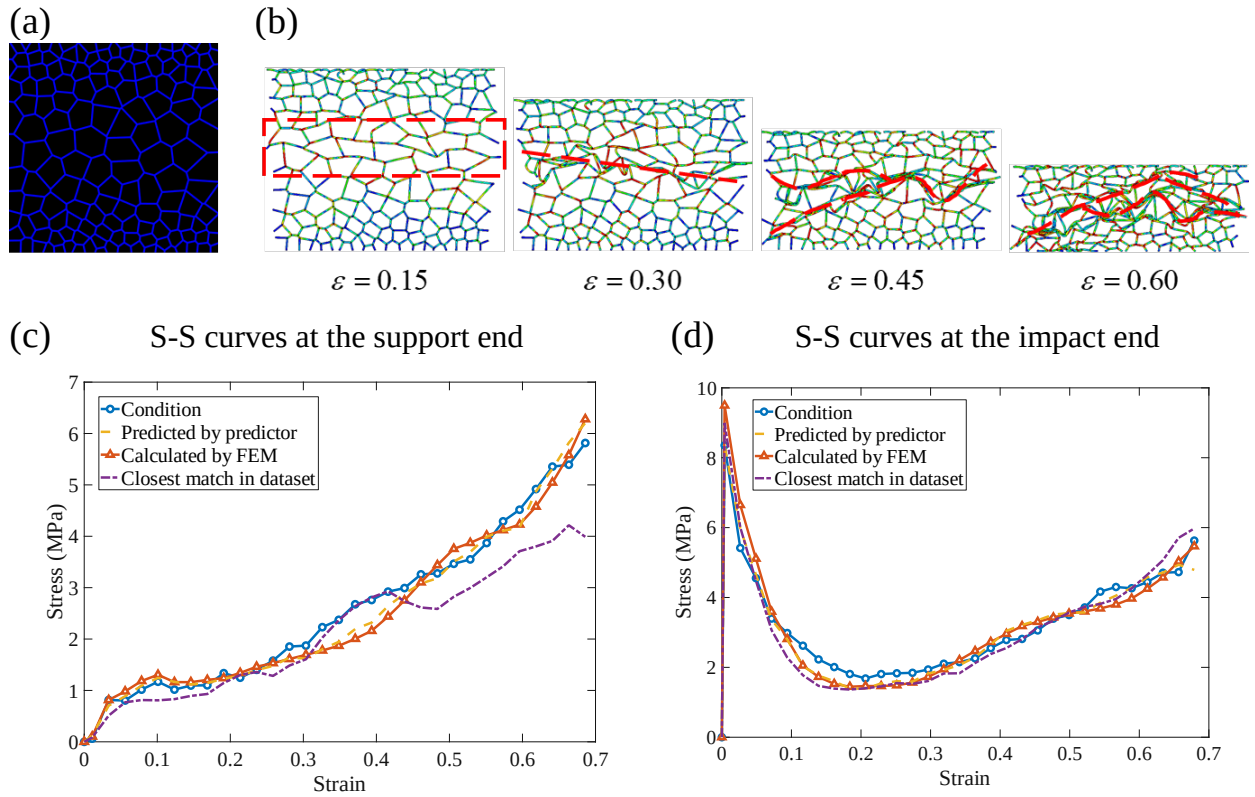


Fig. 17. (a) The generated FGPS based on the condition. (b) The deformation process of the generated structure. (c)-(d) Comparison of the condition S-S curves, the S-S curves predicted by

the predictor (MAPE=9.613%), the S-S curves calculated by FEM (MAPE=11.261%), the closest match S-S curves in the dataset (MAPE=14.237%).

5.3.2 Target 2: S-S profile for energy absorber

Secondly, the engineering application of the real S-S profile is investigated. For example, as depicted in Fig. 18, the energy absorption device of railway passenger vehicles and cars is recommended to incorporate several energy-absorbing components[70,71], each activated by varying levels of impact stress. In this context, the targeted S-S curve is characterized by a two-stage plateau stress at the support end to meet the dual-stage energy absorption requirement, while the stress at the impact end remains constant to maximize the energy absorption efficiency [72]. As shown in Fig. 19, a M-H FGPS was produced. The deformation localization initially occurs at the impact end, resulting in a relative low plateau stress. Subsequently, the support end starts to be compacted while the collapse at the impact end keeps propagating, and this leads to the increasing stress at the support end. After the regions at both ends become compacted, the high-density region in the middle starts to collapse. The results illustrated in Fig. 19(c)-(d) reveal that the generated structure (MAPE = 10.516%) exceeds the closest match in the training dataset (MAPE = 11.396%). As can be seen, the S-S curve shows an abrupt deviation when the strain exceeds 0.5. This behavior arises because the proposed target S-S curves may not align with the mechanical response characteristics of FGPS, and porous structures often demonstrate strain hardening at large strains, which results in the sudden increase in stress and a better energy absorption capacity of FGPS. However, it is worth noting that the predicted results are very close to the FEM results, which reflects the effectiveness of the proposed methods.

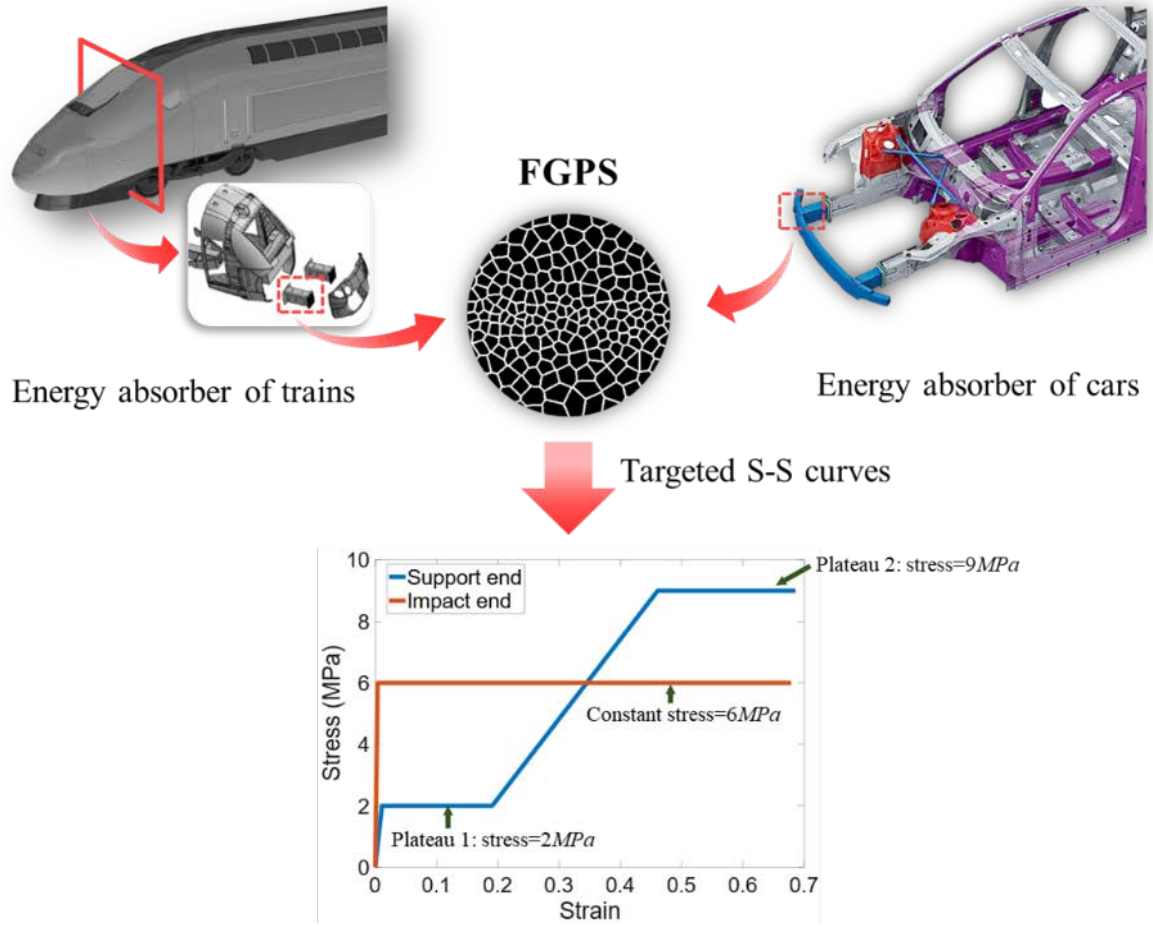
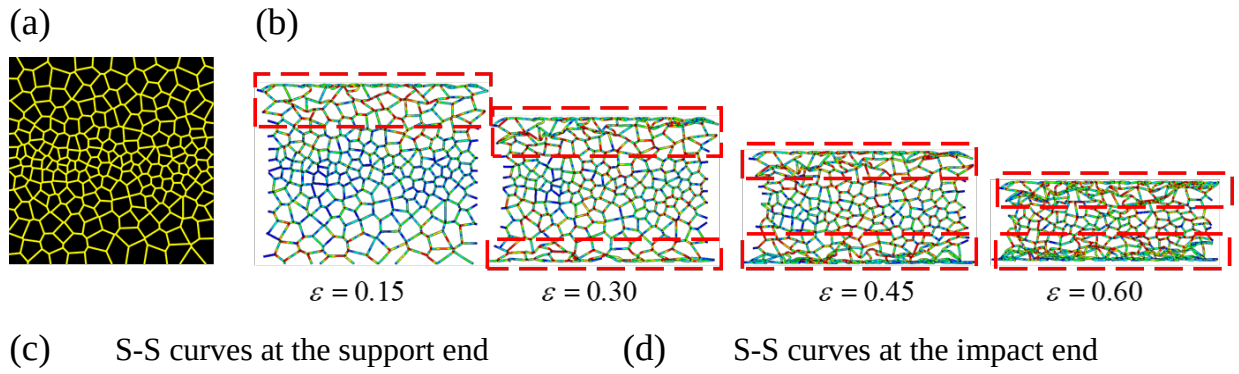


Fig. 18. The energy absorber used in trains [73,74] and vehicles [75] and the targeted S-S curves for FGPS.



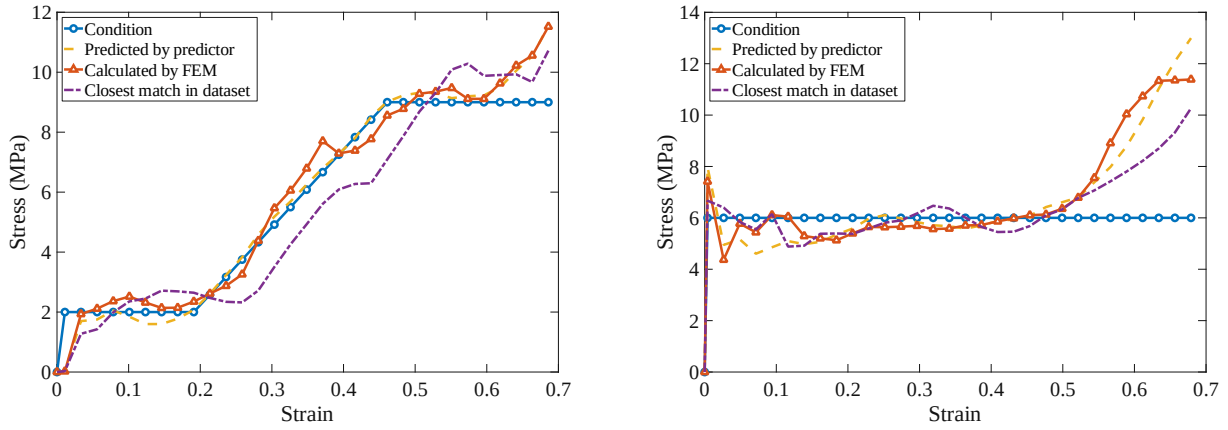


Fig. 19. (a) The generated FGPS based on the condition. (b)The deformation process of the generated structure. (c)-(d) Comparison of the condition stress, the S-S curves predicted by the predictor (MAPE=9.989%), the S-S curves calculated by FEM (MAPE=10.516%), the closest match S-S curves in the dataset (MAPE=11.396%)

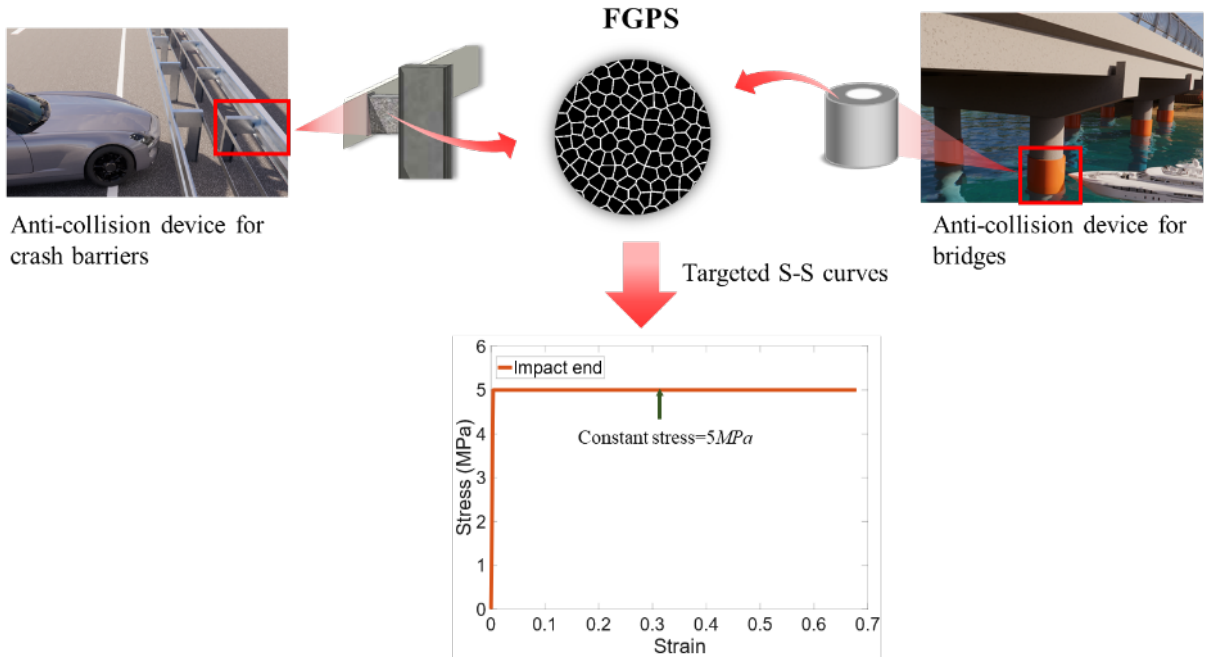
5.3.3 Target 3: S-S profile for anti-collision protective device

Another engineering practice is anti-collision protective devices, for bridges and crash barriers as shown in Fig. 20. By filling porous material in the thin-walled components, the FGPS can absorb adequate impact energy to protect the safety of specific targets and save people's lives. Given this scenario, the design objective is to find the structure with specific energy absorption per unit volume (SEAv) as calculated by Eq. (22). Regarding this scenario, the stress at the impact end is set to a constant value of 5 MPa, while the stress at the support end, which is not the primary concern, is not presented. Subsequently, the generator produced 100 candidate structures under the conditions. During the evaluation process for the optimal structure, the evaluation function was shifted to mean percentage error (MPE) as defined in Eq. (23). The assessment and ranking process focused solely on the stress at the impact end. MPE ensures the generated structure is closest to the target SEAv by minimizing the area between the S-S curve of the generated structure and the target S-S curve. The generated structure is demonstrated in Fig. 21, a structure with slight gradient is formed. It shows a uniform deformation under impact, leading to the constant stress at the impact end. Additionally, the comparison of the S-S curves is also illustrated in Fig. 21(c), with the SEAv of each curve calculated. The results demonstrate that this approach can easily and effectively generate structures with the desired SEAv.

$$SEAv = \int_0^{\delta} \sigma d\delta \quad (21)$$

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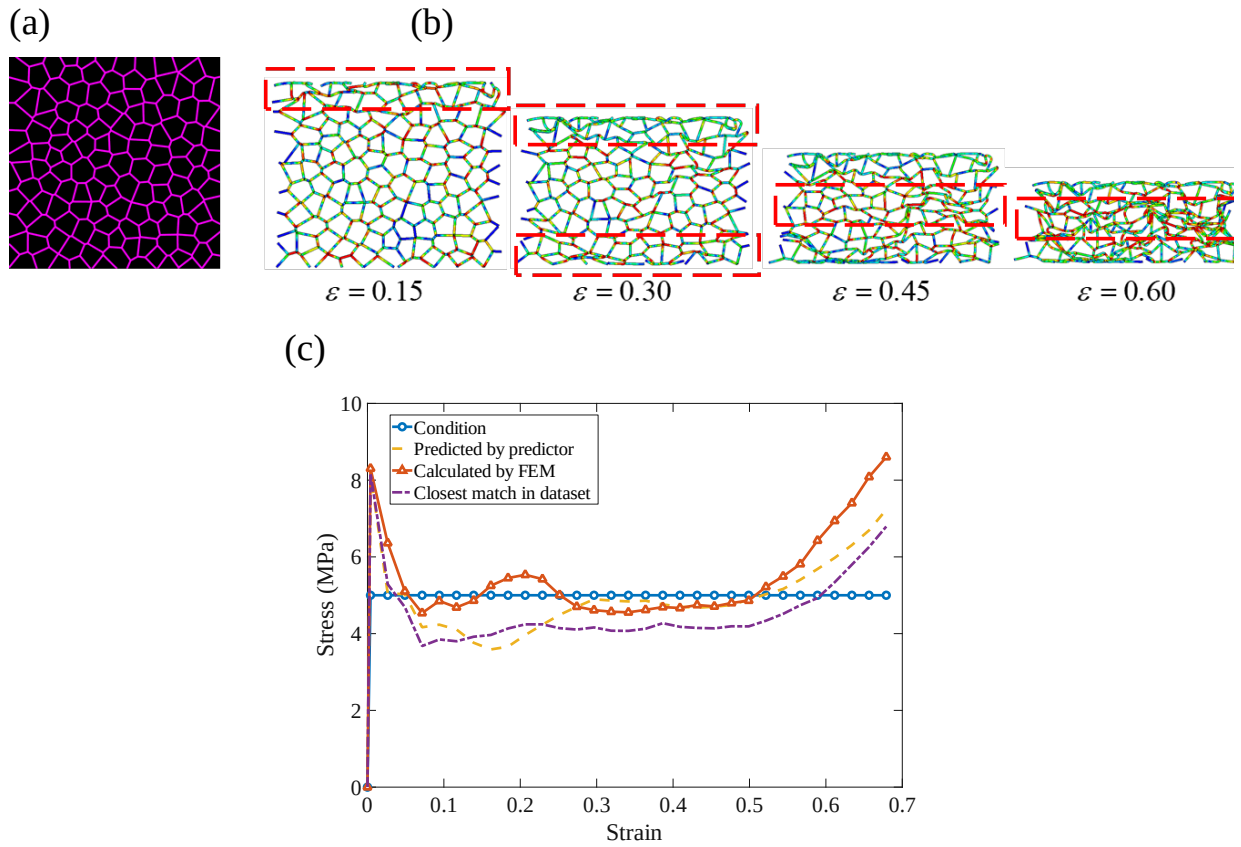
$$\text{MPE} = \frac{100\%}{n} \sum_{i=1}^n \frac{\hat{y}_i - y_i}{y_i} \quad (22)$$



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Fig. 20. The anti-collision protective device for bridges or crash barriers.



570

Fig. 21. (a) The generated FGPS with target SEAv. (b) The deformation process of the generated

structure. (c) Comparison of condition S-S curves ($SEAv=3.385 \text{ MJ/m}^3$), the S-S curves predicted by the predictor ($SEAv=3.321 \text{ MJ/m}^3$), the S-S curves calculated by FEM ($SEAv=3.671 \text{ MJ/m}^3$), the closest match S-S curves in the dataset ($SEAv=3.054 \text{ MJ/m}^3$).

5.4 Experimental verification

To validate the effectiveness of the proposed inverse design methods as well as the accuracy of the finite element model, relevant dynamic impact experiments were conducted. The structures generated in Section 5.3.2, along with a uniform structure and a positive gradient structure, were printed by SLM (Selective laser melting) method, as shown in Fig. 22. The base material is aluminum alloy AlSi10Mg which is commonly used in 3D printing [76–79]. The in-plane dimensions of the structure are 40mm x 40mm, and the out-of-plane dimension is 20mm to prevent buckling. Three dog-bone specimens were also printed using the same material and printing method to assess the material property. The uniaxial tensile test was conducted by using Instron 3367 testing machine and the stress-strain curves are shown in Fig. 23. The material property is listed in Table 3, and is similar to the property defined in the FEM in Section 3.2. The impact experiment was conducted on the Instron Ceast 9350 drop tower. A flat square shaped impactor was attached to the load cell, and a velocity of 20m/s was applied to the impactor. It should be noted that, only the force at the impact end was measured due to experimental limitations. The deformation patterns of the crushed specimens were recorded at 30,000 frames per second with a high-speed camera.

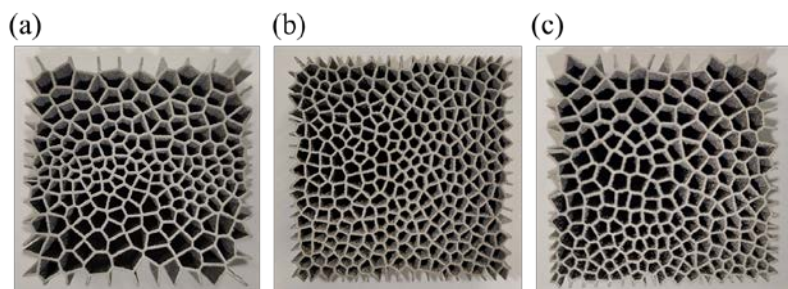


Fig. 22. The manufactured specimens. (a) The specimen generated in Section 5.3.2. (b) The uniform specimen. (c) The positive gradient type specimen.

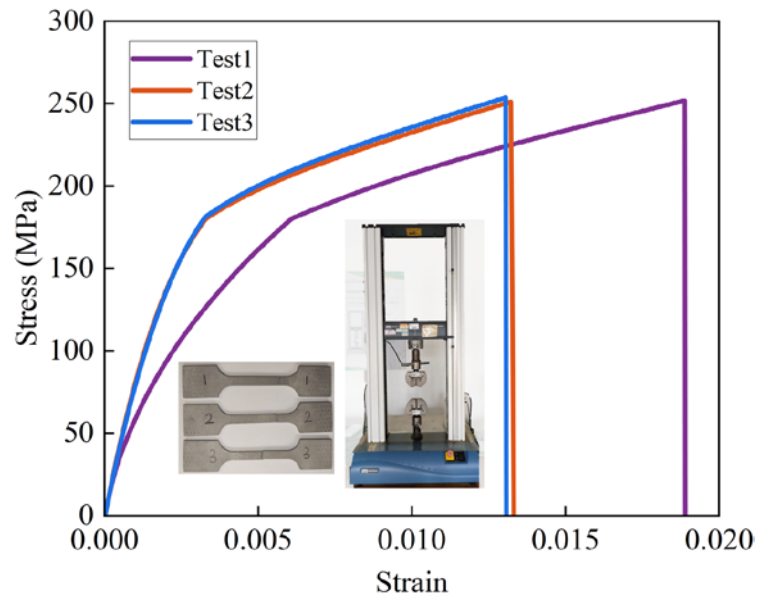


Fig. 23. Stress-strain curves of test specimens printed by AlSi10Mg.

Table 3

The material property of AlSi10Mg.

Density (g/cm ³)	Young's modulus (GPa)	Yield stress (MPa)	Poisson's ratio
2.7	70	80	0.31

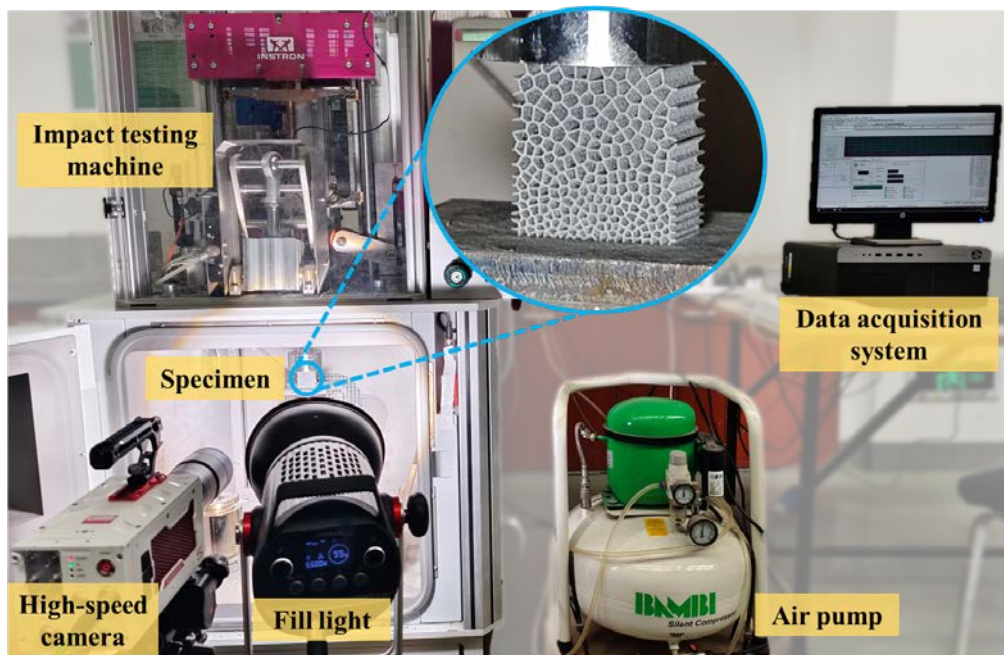
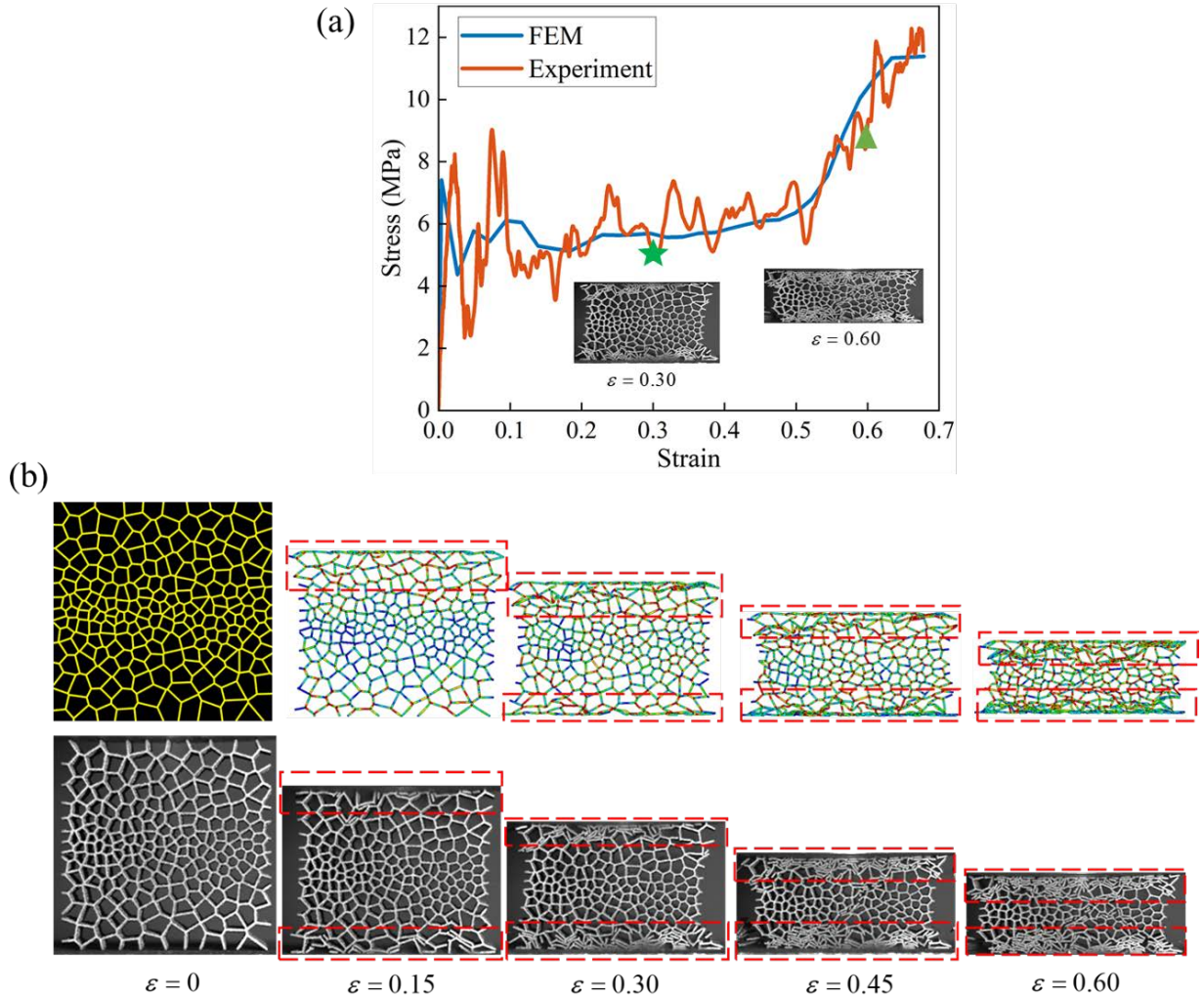
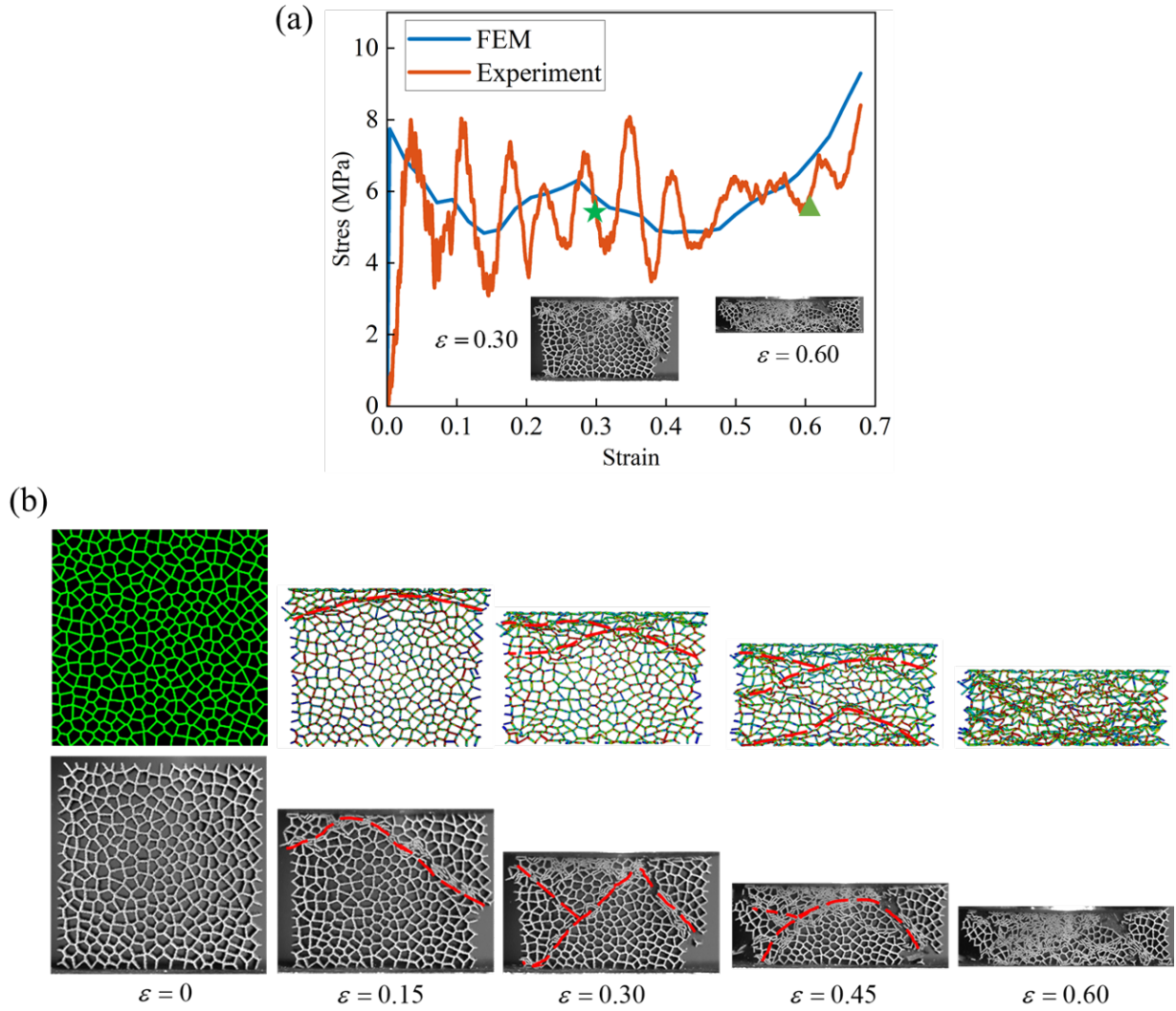


Fig. 24. Schematic of the impact test set-up using Ceast 9350 drop tower and high-speed camera.

The deformation patterns and the stress-strain curves of three specimens obtained by experiment and FEM are compared in Fig.25-27. In the beginning, the stress increases linearly and reach to the initial peak stress due to the material elasticity. Then, as illustrated in Fig. 25 the M-H type structure is crushed layer by layer at the both impact end and support end, which is constant with the FEM results. As shown in Fig. 26, shear bands first appear at the weak locations in the U type structure. As deformation progresses, the shear bands keep expanding, and the cell walls at the impact end are progressively crushed, leading to a continuous increase in stress. The discrepancy in the locations of shear bands observed in the experiment and FEM may attributed to 3D printing errors which leads to the inconsistencies in the weak locations of the structure. In the case of the P type structure, the structure exhibits layer-by-layer crushing deformation from the impact end to the support end, which is consistent with the FEM results. The numerical results are in good agreement with the experimental results at both the stress level and deformation process, which conforms the validity of the proposed methods and the finite element models.



615 **Fig. 25.** Comparison of (a) stress-strain curves and (b) deformation process obtained by
 616 experiment and FEM. The structure is generated by the proposed inverse design approaches as
 617 shown in Section 5.3.2.



618
 619 **Fig. 26.** Comparison of (a) stress-strain curves and (b) deformation process obtained by FEM and
 620 experiment. The structure is selected from the dataset with uniform type.

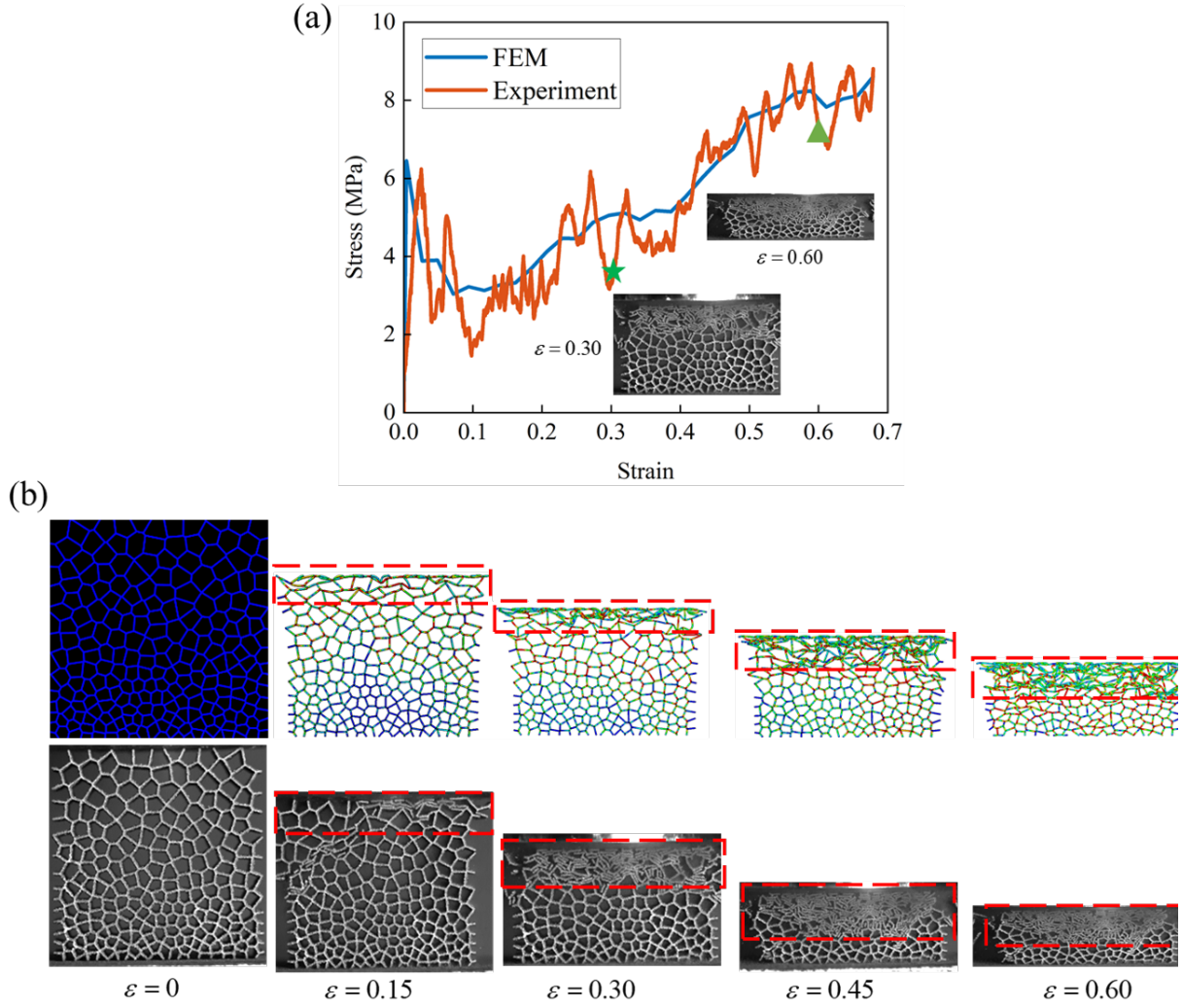


Fig. 27. Comparison of (a) stress-strain curves and (b) deformation process obtained by experiment and FEM. The structure is selected from the dataset with positive gradient type.

6. Conclusions

In this study, an inverse design framework to generate targeted FGPS based on deep learning is proposed. Five distinct types of graded porous structures are implemented by controlling the minimal distances of neighboring nuclei. By utilizing the colored nuclei maps to represent the structures, the efficiency and preciseness of the model can be improved, and the connectivity issues are eliminated. A dataset composed of 2100 structures with their S-S responses was established, the proposed FGPS with different gradient configurations exhibit varying S-S responses and deformation characteristics, thus providing a vast design space and application scenarios. The inverse design framework involves a generator that synthesizes structures based

on the target S-S responses, and a predictor which predicts the S-S responses of the generated structures. In spite of the highly complex relationship between the structure configurations and S-S responses, the developed predictor makes an accurate prediction of the S-S responses for FGPS. The inverse design capability of the proposed method is thoroughly investigated by three examples, the stochastic S-S curves not existing in the dataset, the classic S-S curves with two-stage plateau stress at the support end and a constant stress at the impact end, as well as the anti-collision structures with specific energy absorption per unit volume. The impact experiments were conducted to verify the accuracy of the finite element models and the proposed methods. The results show that the present method can generate optimal FGPSs based on the target responses rapidly and efficiently.

The framework can be further extended to other applications like multi-scale optimization, soft robotics, and biomedical implants. Future work may involve using larger and more comprehensive datasets to achieve better results. Incorporating physical information during model training could lead to better outcomes. Additionally, it is important to explore improved representation methods to incorporate various structures within a single model, and graph neural networks could be a promising candidate for this purpose.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgment

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Appendix A

In this appendix, more details of the dataset are discussed. Relative density has the most significant effect on mechanical response among the parameters of Voronoi structures [80], and it is calculated as

$$\rho = \frac{\rho_0}{\rho_s} = \frac{t}{S} \sum l_i, \quad (\text{A.1})$$

where t represents the thickness of the cell wall, S denotes the area of the design domain and l_i is the length of i -th cell wall.

The relative density distribution for the whole dataset is illustrated in Fig. A. 28, indicating that the relative densities of most of the structures range between 0.05 and 0.35. As shown in Fig. A. 29, various FGPS with different thicknesses are presented, and the relative density distribution for different thicknesses are depicted in the right. FGPS with thicker cell walls exhibit higher relative density and more dispersed distribution.

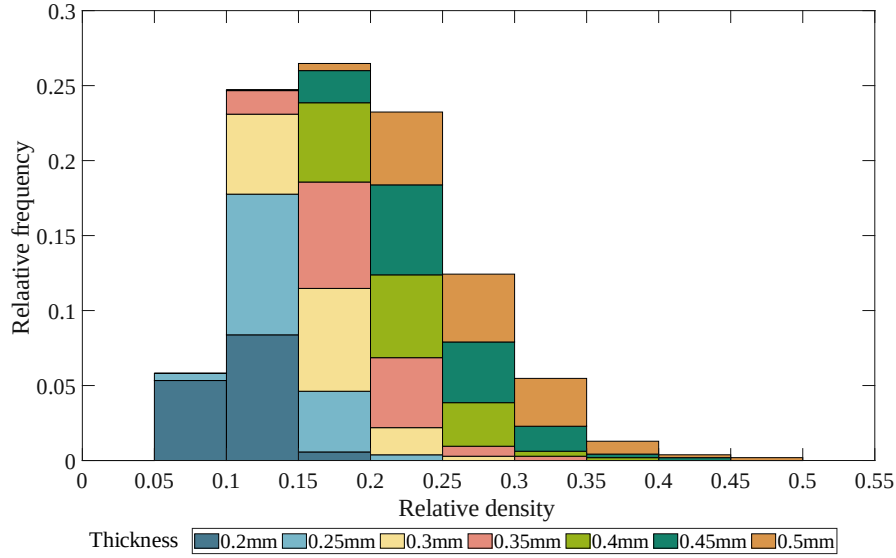
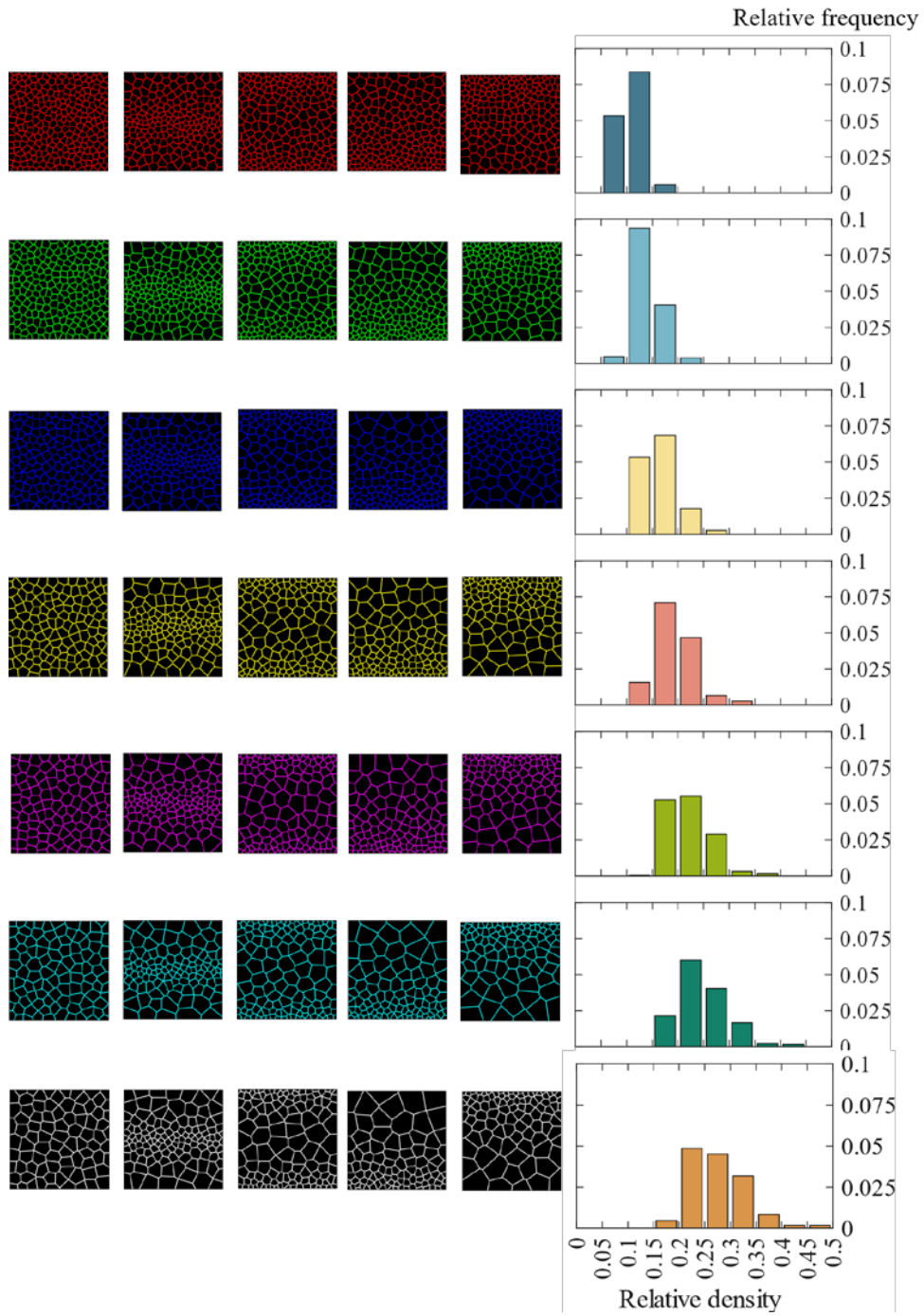


Fig. A. 28. The relative density distribution of FGPS in the dataset



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675 **Fig. A. 29.** Examples of the FPGS with different thicknesses, along with the relative density
 676 distribution for each thickness.

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