

Inverse design of cellular structures with the geometry of triply periodic minimal surfaces using generative artificial intelligence algorithms

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Abstract

Triply periodic minimal surfaces (TPMS) exhibit excellent mechanical and energy absorption properties due to their structural advantages. However, existing porous TPMS structural design methods are constrained to a forward process from structural parameters to mechanical properties. This study proposed an inverse design method that combines bidirectional generative adversarial networks (BiGAN) and mechanical performance targets, resulting in a combined TPMS structure of Primitive and IWP types with superior buffering and energy absorption capabilities. The results show that under a single load value target condition of the designed structure, the minimum deviation index (R^2) between the load value corresponding to the displacement point and the target load value is only 0.987, and the maximum mean absolute percentage error (MAPE) is only 5.92 %. When considering the elastic modulus target, the approach successfully conducts two sets of combined structural designs meeting the requirements of both high and low elastic moduli. When targeting the specified load-displacement curve conditions, specifically when combining high elastic modulus with ascending plasticity, the designed structures exhibit an error of only 2.2 % compared to the target property. Moreover, the quasi-static uniaxial compression experiments conducted on additively manufactured designed structures confirm that the experimental curves match the target curves in terms of deformation trends and load value ranges. The success of this inverse

design approach for cellular TPMS structures has the potential to expedite new structural material development processes.

Keywords : Triply periodic minimal surface; Generative artificial intelligence algorithms; Additive manufacturing; Inverse design; Numerical simulation

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Nomenclature			
N	Number of data points	s	Dimension of the latent data
$Loss_D$	Discriminator loss	D	Discriminator network
$Loss_G$	Generator loss	G	Generator network
$Loss_E$	Encoder loss	E	Encoder network
D_E	Discrimination of the Encoder by the Discriminator	D_G	Discrimination of the Generator by the Discriminator
IF_i	Structural parameter	$\overline{IF}_i$	Generated structural parameter
OS_i	Structural property	L_i	Latent distribution data
δ	Weight of the property error term	PM	Physical model network
m	Size of the dataset	p	Sigmoid function parameter
T	TPMS structural period	k	Gradient function parameter
c_1	Thickness parameter on the Primitive side	c_2	Thickness parameter on the IWP side

1 Introduction

Triply periodic minimal surfaces (TPMS) are a class of cellular structures inspired by natural organisms, characterized by smooth surfaces, excellent properties, biocompatibility, and self-supporting properties. These structures can be accurately controlled by mathematical implicit functions for structural characterization [1-5]. Due to their structural advantages, the excellent mechanical properties of TPMS, including high energy absorption, large deformation capacity, and high specific strength, have facilitated their widespread adoption across various sectors such as the automotive industry, aerospace, and medical fields [6-12]. This advantage is especially evident when various types of TPMS structures are integrated or when TPMS structures are combined with other structural forms. For instance, a combined structure incorporating both the octet-truss lattice and TPMS structures was developed, resulting in a significantly higher specific energy absorption [13]. Additionally, a novel TPMS structure combining Gyroid and Diamond configurations was proposed, demonstrating superior energy absorption capabilities [14]. Recent advancements in metal additive manufacturing technology have significantly enhanced manufacturing efficiency and reduced production costs, further enhancing the potential for manufacturing and utilizing complex combined porous TPMS structures [15-16]. However, despite these technological advancements, optimizing structural design remains challenging due to the multi-parameter and multi-type characteristics of TPMS structures [17-18]. The complexity of identifying specific mechanical demands highlights the ongoing need for innovative computational approaches and advanced manufacturing techniques.

Some researchers have traditionally relied on established methods such as genetic algorithms, topology optimization, mathematical modeling, voxel optimization, and particle swarm optimization to design TPMS structures. While these approaches have proven effective, they often require extensive experimental testing, adherence to specific rules, and reliance on

work experience, resulting in significant computational effort and manual labor [19-26]. In contrast, recent advances in machine learning algorithms have introduced alternative strategies for addressing structural design challenges. These approaches leverage prior data to obtain optimal solutions, thereby circumventing the need for specific rules or experiential knowledge, [27]. Typically, these methods focused on forward property prediction, mapping structural parameters directly to their corresponding mechanical properties. The advent of generative artificial intelligence (AI) algorithms, represented by generative adversarial networks (GANs), autoencoders, and diffusion models, has further revolutionized the field, enabling structural inverse design methodologies where desired mechanical properties guide the generation of optimal structural configurations [28-31]. This integration of forward prediction and generative AI represents a significant advancement in structural inverse design, where the generative AI model is responsible for establishing the mapping from original structural parameters to desired ones. For instance, the integration of original GAN with a forward regression network has enabled the generation of lattice unit cells exhibiting compression strength 40 %-120 % higher than those of conventional cubic unit cells [32]. Similarly, autoencoders, when combined with forward convolutional networks, have facilitated the creation of gradient TPMS structures with a 20 % enhancement in yield strength compared to uniform structures, which were successfully applied to the reconstruction of bone scaffolds in New Zealand rabbits [33]. While GANs have made substantial contributions to the field of unsupervised learning, often producing higher-quality outputs, they still encounter several significant challenges. Firstly, there is the issue of mode collapse, where the generator may only learn partial patterns of the given training data, neglecting other important patterns and regularities [34-35]. Secondly, training instability is a common problem, often leading to difficulties in conducting training [36]. Lastly, GANs sometimes struggle with generation accuracy, particularly when dealing with large datasets or complex data distributions, which can result in blurry generated results [37].

To address those issues, an improved algorithm known as the bidirectional generative adversarial network (BiGAN) has been proposed. BiGAN extends the traditional GAN framework by introducing an encoder that maps data from the original distribution to a latent distribution. The generator samples from this latent space to produce a generated distribution, encompassing both the original data space and the latent data space, and ensures cyclical consistency between them. The discriminator in BiGAN can simultaneously distinguish between the generated distribution, original distribution, random sampling, and latent distribution, making the bidirectional feedback mechanism stabilize training [38]. Additionally, by leveraging the expression of the latent space, the interpretability of the network can also be enhanced, facilitating the evaluation of the training process and the understanding of training information [39]. Therefore, this study aims to generate new combinations of Primitive and IWP porous TPMS structures using the IOA-Model, an advanced inverse design framework that integrates a forward prediction model (physical model) with a generative AI model (BiGAN). The ability of IOA-Model to accomplish mechanical property targets is evaluated from the perspective of neural network interpretability. Additionally, the training process of the IOA-Model framework is also highly controllable, ensuring that the final training structures more effectively achieve the desired structural parameter design targets. The model enables efficient structural generation through the complete automation of geometric modeling and finite element analysis. These generated structures will integrate the excellent energy absorption capability of the Primitive structure and the good buffering capacity of the IWP structure, achieving the optimization of buffering and energy absorption characteristics for the combined TPMS structure [40-42]. The methods and techniques proposed in this study will provide the theoretical foundation and technical support for AI-based reverse design and additive manufacturing of TPMS complex components with excellent properties for industrialized applications.

2 Methods

2.1 Inverse design method based on the IOA-Model framework

The nomenclature of the IOA-Model framework proposed here is derived from the sequential steps of network data exchange. Firstly, in the input (I) step, the framework accepts structural parameters and mechanical properties during training (only the desired structural properties are required during generation). Subsequently, in the output (O) step, the framework outputs structural parameters under the condition of structural property. Finally, in the analyse (A) step, the training process is evaluated through the analysis of the distribution of latent data.

The detailed structure of the IOA-Model framework is shown in Fig. 1. The entire framework consists of a physical model depicting the relationships between structural parameters and mechanical properties, and BiGAN. The input of the physical model is structural parameter IF_i as shown in Eq. (1) and the output is structural property OS_i as shown in Eq. (2). The physical model is trained in advance to provide the BiGAN network with the mechanical properties corresponding to the structural parameters. The BiGAN network consists of an Encoder, a Generator and a Discriminator. The Encoder input is the structural parameter IF_i , and the output is the dimensionality-decreased latent distribution L_i as shown in Eq. (3). The monitoring of the latent distribution L_i allows to understand the training information and grasp the training process. The Generator input consists of two parts, one part is the random noise n_i with the same dimension as the latent distribution, and the other part is the structural property condition label OS_i corresponding to the structural parameter IF_i . The output is the generated structural parameter $\overline{IF}_i$. The Discriminator receives all the inputs and outputs from both the Encoder and the Generator: IF_i , L_i , n_i , $\overline{IF}_i$, OS_i , and the output is the probability of the real structure. The specific equations are as follows:

$$IF_i = [k_i, c_{1i}, c_{2i}] \quad (1)$$

$$OS_i = [os_{i1}, os_{i2}, \dots, os_{iN}] \quad (2)$$

$$L_i = [l_{i1}, l_{i2}, \dots, l_{is}] \quad (3)$$

where N is the number of data points for structural property data, s is the dimension of the latent distribution data, IF_i is the structural parameter, OS_i is the structural property, and L_i is the latent distribution data.

From the perspective of the loss function, the operation principle of the entire network is associated with the Discriminator. Eq. (4) represents the loss function of the Encoder, expecting the Discriminator to judge the output of the Encoder as real information. Eq. (5) represents the loss function of the Generator. Specifically, the loss function of the Generator consists of two parts: one part is the discrimination by the Discriminator of the output of the Generator, expecting the Discriminator to judge the output of the Generator as real information, and the other part is the structural mechanical property loss. The structural parameters $\overline{IF}_i$ generated by the Generator will obtain the corresponding structural property $\overline{OS}_i$ through the physical model. By constructing the difference between $\overline{OS}_i$ and OS_i through mean squared error (MSE) loss, the goal is to ensure that the generated structural parameters $\overline{IF}_i$ meet the property criteria OS_i . Eq. (6) represents the loss function of the Discriminator. Conversely, the Discriminator expects to judge the information from the Encoder as real information and the information from the Generator as fake information. The specific equations are as follows:

$$Loss_E \rightarrow \min - \{\sum_{i=0}^m [\log(1 - D_E(IF_i, E(IF_i), OS_i))]\} \quad (4)$$

$$Loss_G \rightarrow \min - \{\sum_{i=0}^m [\log(D_G(G(L_i, OS_i), OS_i))] - \delta [PM(\overline{IF}_i) - OS_i]^2\} \quad (5)$$

$$Loss_D \rightarrow \min - \{\sum_{i=0}^m [\log(D_E(IF_i, E(IF_i), OS_i)) + \log(1 - D_G(G(L_i, OS_i), OS_i))]\} \quad (6)$$

where $Loss_D$ represents the Discriminator loss, $Loss_G$ represents the Generator loss, $Loss_E$ represents the Encoder loss, G denotes the Generator network, D denotes the Discriminator network, E denotes the Encoder network, D_E represents the discrimination of the Encoder by the Discriminator, D_G represents the discrimination of the Generator by the Discriminator, $\overline{IF}_i$ represents the generated structural parameter, δ is the weight of the

property error term, PM represents the physical model network, and m is the size of the dataset.

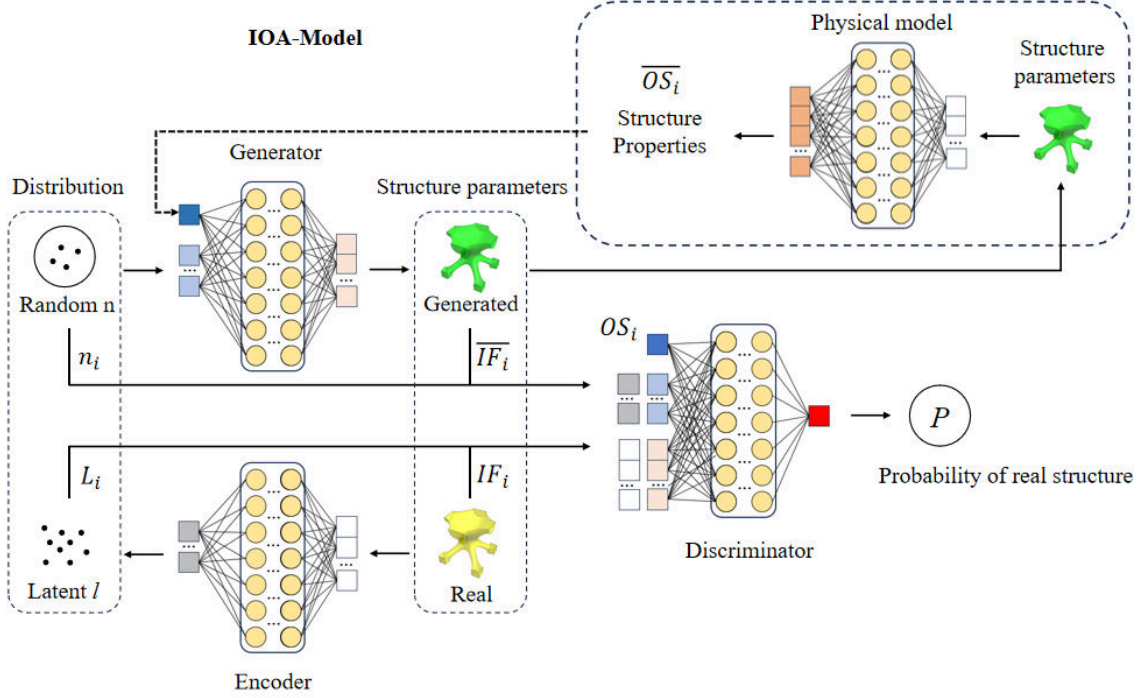


Fig. 1 Detailed structure and input/output information of the IOA-Model framework.

Moreover, the inverse design method of combined TPMS structures based on the IOA-Model mainly includes four processes, as shown in Fig. 2. Firstly, the combined structure of Primitive and IWP is parameterized, and a gradient structure is constructed to cover more feature distributions in the training dataset. Through the nested loops between the maximum and minimum values of each structural parameter, different combinations of structural parameters are constructed to obtain the structural parameter dataset. Secondly, based on the structural parameters of the dataset, automated geometric modeling is performed using Mathematica software. The finite element method (FEM) software ANSYS automatically reads the generated geometric model files. The contact type is frictional contact with a friction coefficient of 0.1, and the contact formulation and stiffness are in the programmed automatic control mode of ANSYS. The mesh type is tetrahedral element with intermediate nodes. The material model, gathered from standard tensile tests, capture the nonlinearity of the material using a bilinear isotropic hardening model. This model includes two elastic and plastic stages

with different slopes, along with the yield strength. The Ti6Al4V material used in this study has an elastic modulus of 100300 MPa, a tangent modulus of 1675 MPa, and a yield strength of 1003 MPa. The 50 solution points are fixed to ensure consistency in the length of structural property data during training, obtaining elastic modulus data and load-displacement property curves. The above finite element calculation process is fully automated through socket programming and real-time communication with ANSYS. Thirdly, combining 1000 sets of structural datasets (80 % training sets and 20 % test sets) with the structural parameters and mechanical property mapping provided by the physical model, the distribution of structural parameters is learned to train the IOA-Model using BiGAN. During training, the latent variable distribution generated by the Encoder in the IOA-Model is monitored. The structural parameters output by the Generator in the IOA-Model under specific target properties are used for geometric modeling. Inputting into the FEM automation program for simulation obtains numerical property, and simultaneously inputting the structural parameters into the physical model obtains the predicted structural property. If the gap between the target mechanical property and FEM mechanical property is within a certain range, the structure is considered the ideal structure.

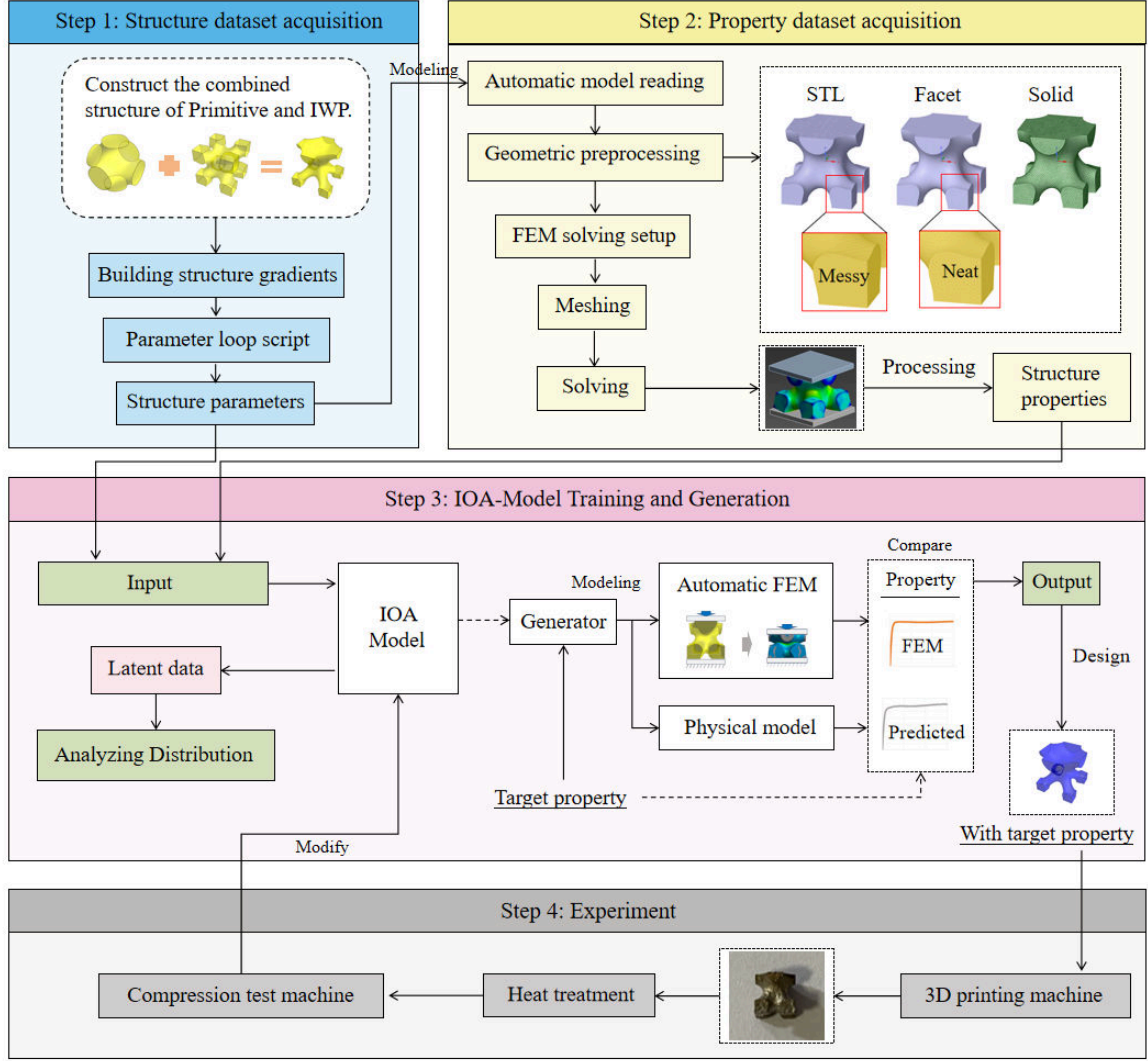


Fig. 2 Inverse design method of combined TPMS structure based on the proposed IOA-Model.

Finally, the structural geometric model is manufactured to obtain the mechanical property data, verifying the feasibility of the IOA-Model. If there is a significant difference between the experimental property and the target property, the IOA-Model needs to be adjusted, including neural network parameters, the prediction accuracy of the physical model, and simulation models.

2.2 Primitive and IWP combined structures

The Primitive and IWP structures are constructed by Eqs. (7) and (8), respectively. The combination structure of the two structures is built by Eq. (9), and the Primitive and IWP structures are connected through the Sigmoid equation. The specific equations are as follows:

$$P(X, Y, Z) = \cos(X) + \cos(Y) + \cos(Z) \quad (7)$$

$$I(X, Y, Z) = 2(\cos(X)\cos(Y) + \cos(X)\cos(Z) + \cos(Y)\cos(Z)) - (\cos(2X) + \cos(2Y) + \cos(2Z)) \quad (8)$$

$$\begin{cases} S(z)[P(X, Y, Z)] + (1 - S(z))[I(X, Y, Z)] > t \\ S(z) = \frac{1}{1+e^{-pz}} \end{cases} \quad (9)$$

where X, Y, Z are independent variables, and $X=2\pi x/T$, $Y=2\pi y/T$, and $Z=2\pi z/T$; T is the period, controlling the size of the structural units; the parameter p controls the rate of structural size change at the junction, i.e., the smoothness, with smaller p resulting in smoother connections; the parameter t controls the thickness of the structure, i.e., the volume of the solid region. In addition, the equation of the Primitive structure is shifted along the Z -axis by 0.5 cycles T to modify the position of the junction plane during the combination, as shown in Fig. 3(a).

The graded variation of TPMS thickness is advantageous for customizing the structural stress and deformation response [43], while maintaining relative energy absorption capacity. There are many types of TPMS gradients, and the cosine function gradient type, which has been proven to enhance the compressive strength of structures [44], is selected. The thickness of the combined structure varies gradient along the Z -axis, with the specific function as follows:

$$\begin{cases} t(z) = k \cos\left(\frac{\pi}{T}z\right) \\ P(X, Y, Z) + c_1 \\ I(X, Y, Z) + c_2 \end{cases} \quad (10)$$

where the structural parameter of k controls the magnitude of thickness gradient variation, and the structural parameters of c_1 and c_2 independently control the thickness values at both parts of the Primitive and IWP, respectively, determining action positions of the gradient function. Through different combinations and transformations of k, c_1 and c_2 , various combination structures can be constructed, forming a structural parameter dataset, as shown in Fig. 3(b).

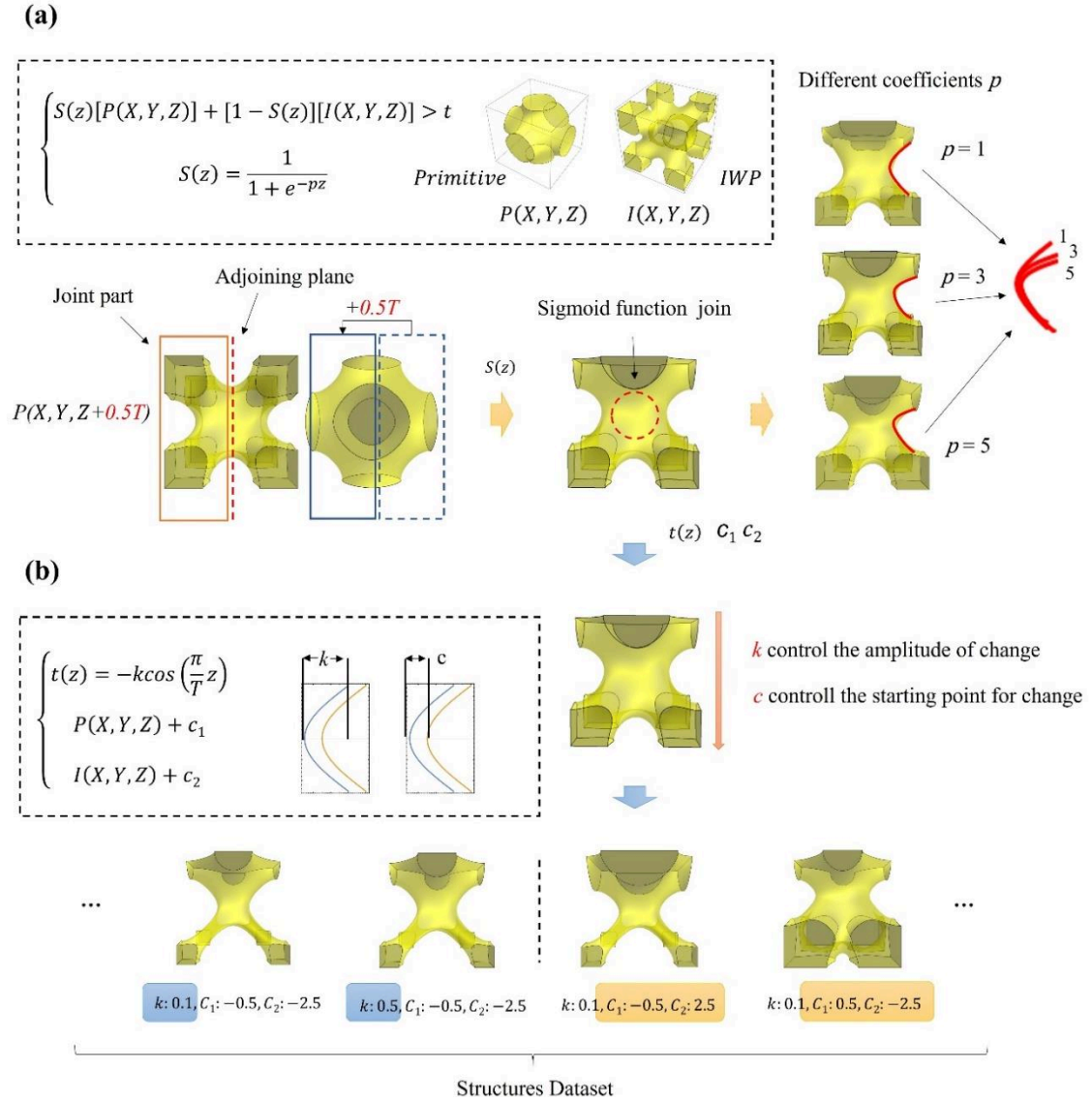


Fig. 3 Combined TPMS structure of Primitive and IWP types: **(a)** method of combining Primitive and IWP, and **(b)** method of gradientization of combination structure.

2.3 Experimental methods

Based on Selective Laser Melting (SLM), the excellent performance Ti6Al4V printing material is selected, and the designed structure is additively manufactured using the FS121M-D printer, with a structural unit size of $5 \text{ mm} \times 5 \text{ mm} \times 5 \text{ mm}$. Subsequently, the samples are heat-treated at 850°C under argon protection for 2 hours and cooled in the heating furnace, as shown in Fig. 4(a). Subsequently, the SUST CMT5105 machine is used to conduct compression tests. The compression tests are conducted at a quasi-static compression rate of 0.001 s^{-1} , and the load-displacement curve data of the experimental specimens are obtained. Fig. 4(b) shows

the initial manufactured experimental specimens. Considering the small size of the samples, to facilitate distinction and improve printing efficiency, every three specimens are grouped and connected by small inter-structure supports during manufacturing. Fig. 4(c) shows the experimental specimens after heat treatment, with the removal of inter-structure supports.

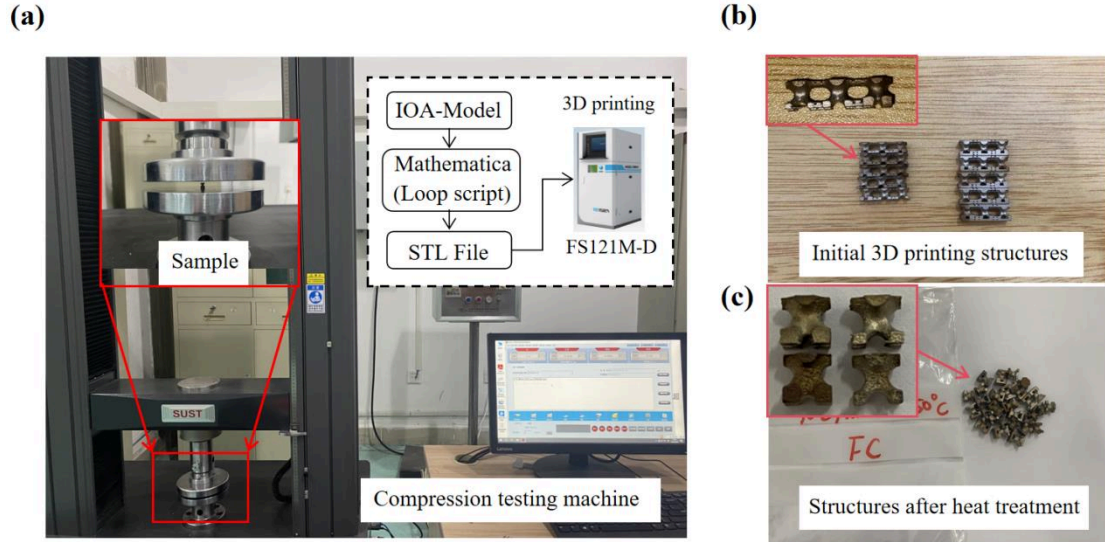


Fig. 4 (a) Additive manufacturing process from IOA-Model to compressed experimental machine, (b) untreated printing initial structural specimens, and (c) structural specimens with the removal of supports after heat treatment.

3 Results and discussion

3.1 Influence of structural parameters on mechanical properties of combined structures

Fig. 5(a) presents the load-displacement curves obtained from both experimental testing and FEM simulation for the combined structure, along with FEM simulation curves for the individual Primitive and IWP structures under compression. A comparison between the red FEM curve and the purple experimental curve reveals a close alignment in both deformation trends and load values, demonstrating a strong correlation between the FEM and experimental results. Additionally, the inset in Fig. 5(a) shows that within the compression range of 0-1.4 mm, the load-displacement curve of the combined structure lies between the curves of the individual Primitive and IWP structures. Its elastic modulus is 24.78 % lower than that of the Primitive structure when the combined structure has parameters $c_1 = -0.5$, $c_2 = -1.3$, and $k = -0.1$, exhibiting lower initial resistance and better buffering capability. In the subsequent plastic

stage, the curve is higher than that of the IWP structure, with a larger area under the curve, indicating better energy absorption capability. Therefore, the buffering and energy-absorbing effects of the combined structure can be modulated by adjusting the thicknesses of the two parts of Primitive and IWP structures, respectively.

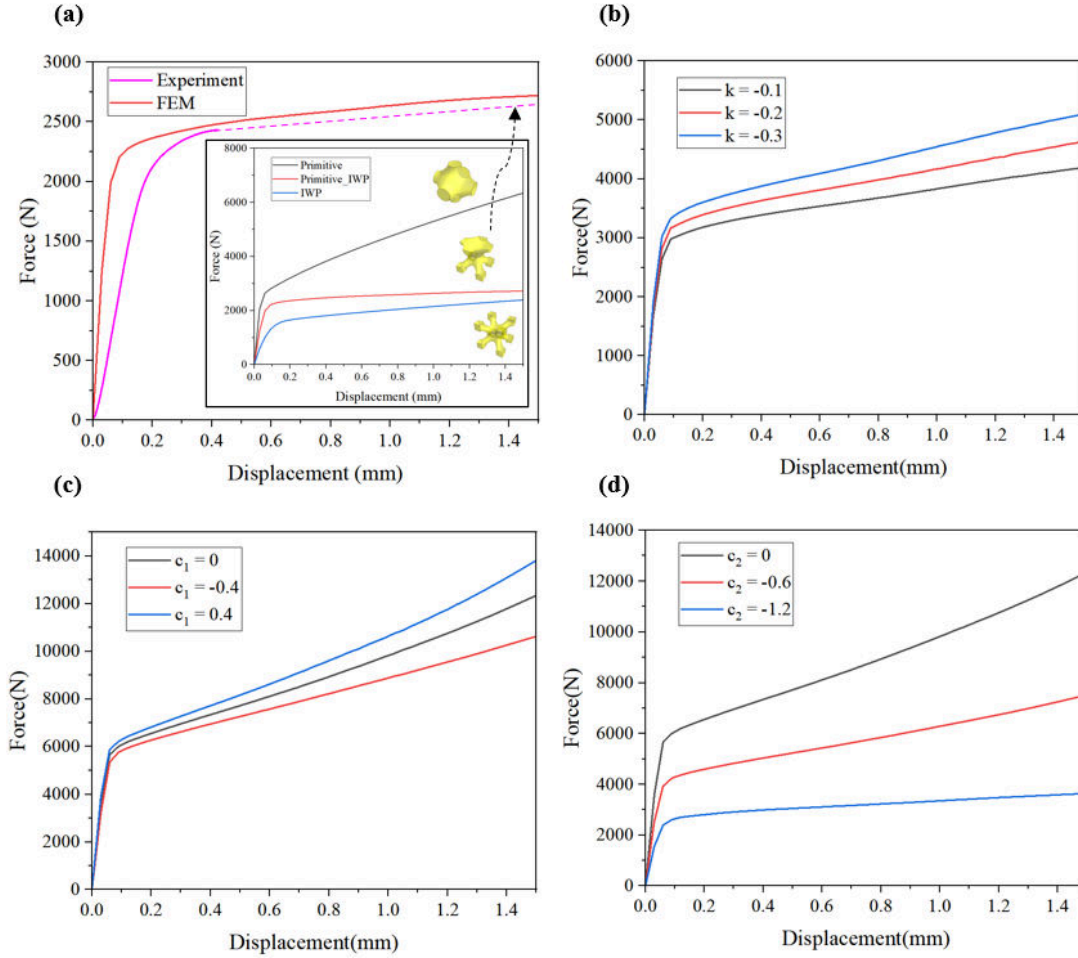


Fig. 5 Effect of structural parameters on the mechanical property of the combined Primitive and IWP structures: **(a)** experimental and simulation load-displacement curves for the combined structure, and simulation load-displacement curves for the individual Primitive and IWP structures, **(b)** effect of structural parameter k , **(c)** effect of structural parameter c_1 , and **(d)** effect of structural parameter c_2 .

Additionally, Figs. 5(b)-(d) show the effects of structural parameters k , c_1 and c_2 on the mechanical property of the combined structure, respectively. As shown in Fig. 5(b), keeping both c_1 and c_2 consistent ($c_1 = -0.5$, $c_2 = -1$), the parameter k has a smaller effect on the elastic modulus but a greater influence on the plastic stage of the load-displacement curve. As the absolute value of k increases, the load in the plastic stage and the area under the curve

both increase, enhancing the energy absorption of combined structure. As shown in Fig. 5(c), keeping both k and c_2 consistent ($k = -0.1, c_2 = 0$), the effect of parameter c_1 on the property curve is similar to that of parameter k , but the characteristic of the parameter c_1 effect on the plastic stage is different. The change in k has a more gradual effect on the plastic stage, and the entire curve tends to move parallelly, while the change in c_1 has a more abrupt effect on the plastic stage, causing the entire curve to change in slope. With the increase in c_1 , the energy absorption capability of the structure gradually improves. As shown in Fig. 5(d), keeping both k and c_1 consistent ($k = -0.1, c_1 = 0$), the parameter c_2 has a significant impact on both the elastic and plastic stages. With the increase in c_2 , the energy absorption capability of the structure improves rapidly. In general, the structural parameters k and c_1 have a greater impact on the plastic stage property, facilitating the independent adjustment of energy absorption capability, while the parameter c_2 has a significant impact on both the elastic and plastic stages, enabling the simultaneous adjustment of buffering and energy absorption capabilities. From another perspective, the IWP part has a greater impact on the structural mechanical properties in both the elastic and plastic stages, while the Primitive part has a greater impact on the structural properties in the plastic stage.

3.2. Combined structure design under varying single specific loads

In some application scenarios, mechanical property requirements may not necessitate the customization of the entire curve. Instead, it may suffice for the curve to meet the required load value at a specific displacement point. For instance, the load-displacement curve might need to pass through a specific demand point, such as the yield strength requirement, or the initial peaking force requirement point. Figs. 6(a)-(c) show the training responses of the IOA-Model framework when the displacement points selected from the dataset are 0.06 mm, 0.6 mm, and 1.2 mm as target demands, respectively. The true response in the figure is the load value corresponding to the displacement point in the dataset, and the generated response is the load

value of the structure generated by the IOA-Model framework corresponding to the displacement point (predicted by the physical model in the IOA-Model). From the response chart, it can be seen that the generated response and the true response are highly matched. The coefficient of determination R^2 values are all above 0.98, ranging from a maximum of 0.994 to a minimum of 0.987. The values of mean absolute percentage error (MAPE) are all below 10 %, ranging from a maximum of 5.92 % to a minimum of 3.02 %. It can be inferred that the accuracy of the IOA-Model framework is very high.

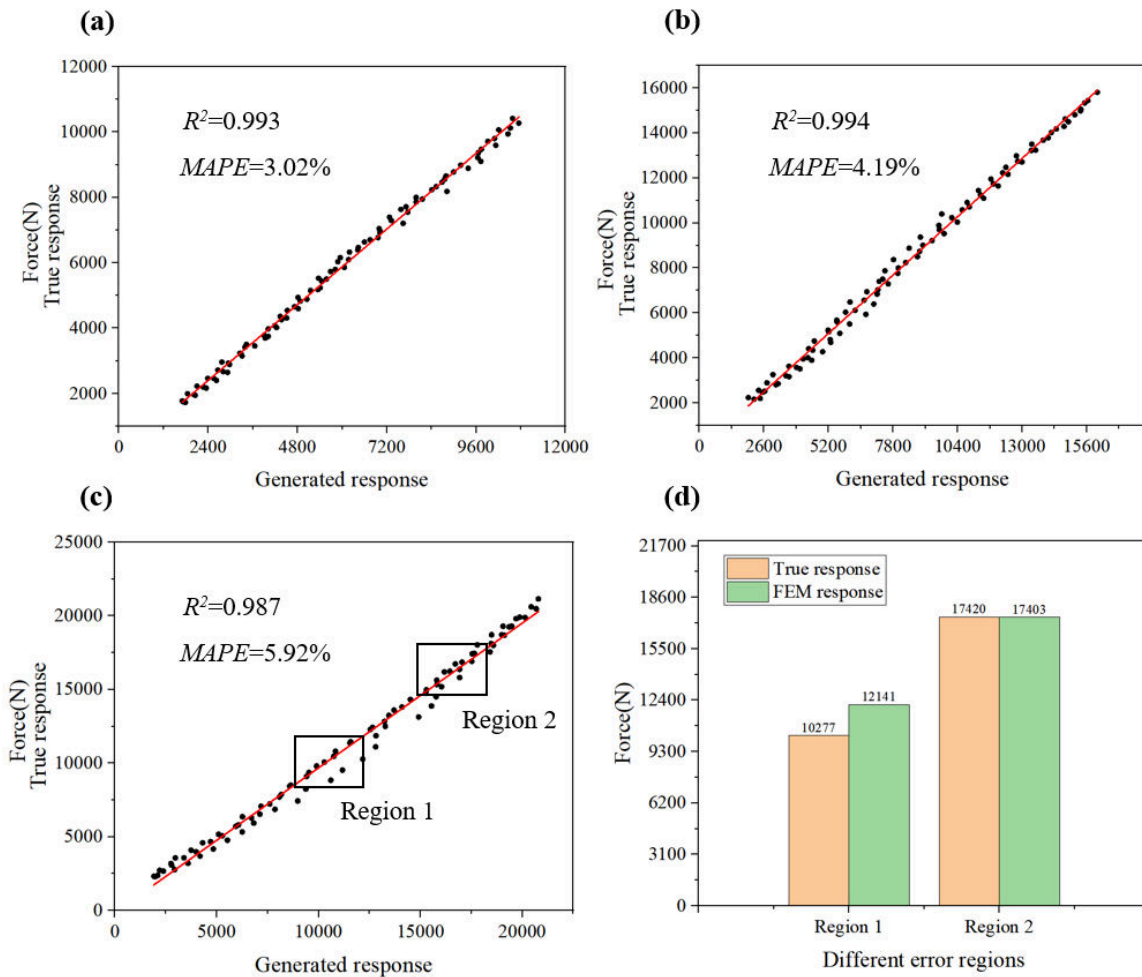


Fig. 6 Training responses for the displacement points at: **(a)** 0.06 mm, **(b)** 0.6 mm, and **(c)** 1.2 mm, respectively, and **(d)** comparison between FEM results of the IOA-Model framework at different precision levels and dataset results for the displacement point at 1.2 mm.

Moreover, two regions in Fig. 6(c) are randomly selected to verify the design accuracy of the IOA-Model. The first region has a scattered data distribution (marked as Region 1), indicating a low design accuracy of the IOA-Model framework in this area, while the second

region has a concentrated data distribution (marked as Region 2), indicating a high design accuracy of the IOA-Model framework in this area. Fig. 6(d) shows the comparison of the FEM results and the true results of the loads in those two regions. At the load point, it can be observed that the load obtained by FEM in Region 1 is 10277N, while the result in the load dataset is 12141N, indicating a large gap, corresponding to the design accuracy in Region 1. The load obtained by FEM in Region 2 is 17420N, while the result in the load dataset is 17403N, indicating a very small gap, corresponding to the design accuracy in Region 2. Therefore, it can be found that the design accuracy of the IOA-Model framework determines the magnitude of the error between the true mechanical property and the target mechanical property of the designed structure.

To validate the generalization ability and working capability of the IOA-Model, it is required to meet mechanical properties that differ from the load values in the training dataset. For instance, the curve might need to pass through load points of 5000 N and 8000 N at a displacement of 0.06 mm. For each load target, three combined structures of Primitive and IWP are designed using the IOA-Model framework. After each structural design, the physical model is trained and optimized to enhance its prediction accuracy before the next design. Fig. 7(a) illustrates the three structural designs under the 5000 N target. The load-displacement curves all pass through the 5000 N load point at a displacement of 0.06 mm, but there are significant differences in the curves. The load-displacement curve of the third structure differs significantly from the curves of the first two structures in the plastic segment. Upon observing the geometric features from the first structure to the third structure, the thicknesses of both the Primitive and IWP parts are decreased. Fig. 7(b) shows the three structural designs under the load of 8000 N target, and the load-displacement curves all pass through the 8000 N load point when the displacement is 0.6 mm. The three sets of curves closely match the 5000 N target but display different characteristics in the plastic stage. The slope of the load-displacement curve

for the second structure differs from that of the third structure, while the slope of the plastic stage between the first and second structures is basically consistent. Observing the geometric features from the first structure to the third one, there is an increase in the thickness of the Primitive part and a decrease in the thickness of the IWP part. Therefore, whether from the analysis of the load-displacement curve characteristics or the structural geometric features, designing based on a single point allows for significant freedom in the results. The designed combined structures have different energy absorption capabilities, and the diversity of the generated results also confirms the strong generative ability of the IOA-Model framework.

Fig. 7(c) shows the load values obtained by FEM and the load results predicted by the physical model under two previous load targets, where “Net” represents the prediction result of the physical model. It can be seen that the FEM load and the predicted load of the physical model under each structural design are basically consistent and change together. The physical model affects the generative performance of entire IOA-Model framework, and optimizing the accuracy of the physical model can make the true FEM calculated load of the structure closer to the target load. It can also be seen that through the training optimization of the physical model, the structural design error (the error between the target result and the FEM result) under the 5000 N target decreases from 9.06 % to 3.93 %, and the design error under the 8000 N target decreases from 5.06 % to 0.26 %. Fig. 7(d) shows the values of the structural parameters k , c_1 , and c_2 designed under two load targets. As the target load increases from 5000 N to 8000 N, the increase in parameter c_2 surpasses that of c_1 , indicating that the load value at 0.6 mm is more sensitive to the parameter c_2 . Adjusting the parameter c_2 makes it easier to achieve significant changes in the elastic stage. For the parameter k , the magnitude of change is relatively smaller compared to c_1 and c_2 , serving for finer adjustments in structural mechanical property, which aligns with the discussion in *Section 3.1*.

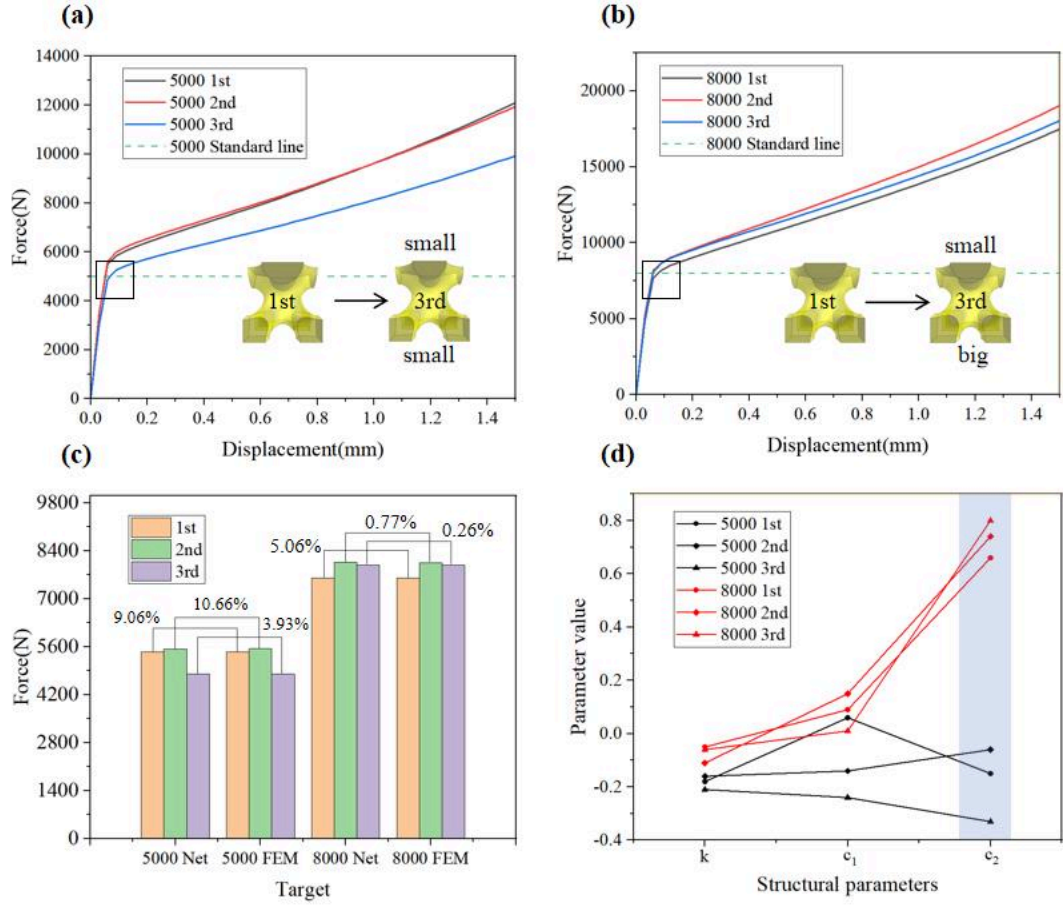


Fig. 7 Results of IOA-Model designs under 5000 N and 8000 N targets when the displacement value is 0.06 mm: (a) three designs under the 5000 N target, (b) three designs under the 8000 N target, (c) the design errors between FEM mechanical property and physical model prediction results of the structures, and (d) structural parameters designed under two load targets.

In the training framework corresponding to the aforementioned Figs. 6 (a)-(c) and Figs. 7 (a)-(b), IOA-Model learns the distribution of the original dataset during training, while its Encoder continuously generates the latent distribution l . Therefore, in order to observe the relationship between the distribution of the original training data and the latent distribution l , and analyze the changes and features of the two-dimensional latent distribution l output by the Encoder during training, the training process of the framework corresponding to Fig. 6 (c) is selected for monitoring. As shown in Fig. 8 (a), based on the parameter c_2 , continuous distributions of original data are selected from the dataset at a displacement of 1.2 mm with load value ranges of 1000-5000 N, 6000-12000 N, and 12000-20000 N for monitoring, with each distribution containing 10 data points. During 1 epoch of training in Fig. 8 (b), the latent

distribution is in a random state, and the three types of data are irregularly distributed together. After 3 epochs of training in Fig. 8 (c), the three sets of data begin to gradually separate, forming three continuous distributions. After 5 epochs of training in Fig. 8 (d), the three curves are independently and continuously distributed in space, with latent distributions 1 and 2 closer in space, consistent with the original distribution characteristics shown in Fig. 8 (a). At this time, the structural designs of the IOA-Model correspond to Fig. 6 (c). The latent distribution l gradually forms a distribution similar to the original data during continuous training. Hence, through the BiGAN-based IOA-Model framework, analyzing the latent distribution output by the Encoder, and comparing the spatial characteristics of the latent distribution with the original data distribution, the training status ultimately achieved by the IOA-Model can more accurately complete the structural design based on load targets.

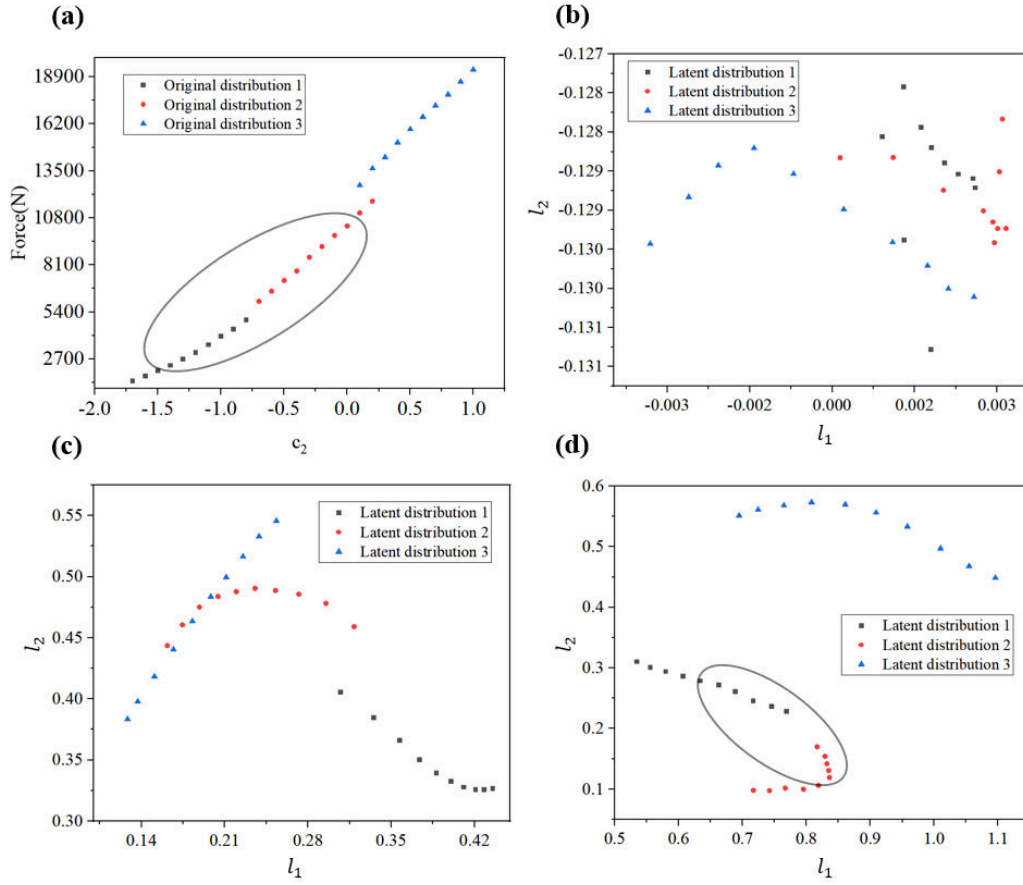


Fig. 8 (a) Three sets of continuous data distributions in the original training dataset, (b) latent data distribution at 1 epoch of training, with curve colors corresponding to the original data, (c) at 3 epochs of training, and (d) at 5 epochs of training.

3.3. Effect of elastic modulus variation on combined structure design

The elastic modulus is a significant parameter used to gauge the ability of structure to undergo elastic deformation. By customizing the high or low elastic modulus values, different characteristics of the structure in the elastic state can be obtained to adjust the structural buffering capacity [45]. Without introducing a physical model, using data with equal structural parameter k in the dataset, the IOA-Model framework with only the BiGAN network is trained to generate 180 sets and 500 sets of structures respectively without mechanical property requirements. The elastic modulus values of the generated Primitive and IWP combined structures are calculated, and a threshold of 24000 MPa is chosen to divide them into high and low elastic modulus categories here. Figs. 9(a)-(b) show the parameter distribution of two types of elastic modulus. It can be seen that there are obvious distribution areas and boundaries between the two types of elastic modulus (red data and black data are clearly differentiated), indicating that the IOA-Model framework using the BiGAN network has strong generation capability. It can also learn some relationship hidden in the dataset between structural parameters and structural mechanical property, such as the relationship between c_1 , c_2 , and elastic modulus. This enables the generated structural parameters c_1 and c_2 to fall into different elastic modulus regions.

To ensure the accuracy of the data training, the physical model for classification utilizes the above data. Six algorithms including artificial neural network (ANN), logistic regression, decision tree, random forest, support vector machine (SVM), and k-nearest neighbors (KNN) are employed for this purpose. The training accuracies are shown in Table 1. For the 180 sets of data, the decision tree achieves a higher training accuracy of 0.944, and the decision boundary is shown in Fig. 9(a). For the 500 sets of data, the training accuracy of ANN is better, perfectly separating the two types of elastic modulus, and the decision boundary is shown in Fig. 9(b).

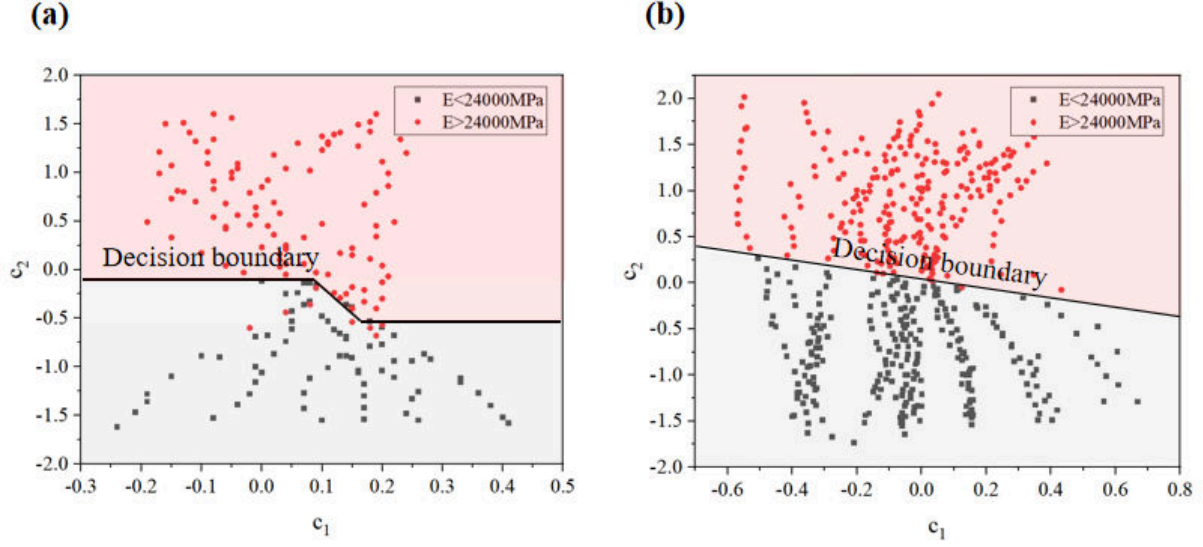


Fig. 9 Parameter distributions and decision boundaries schematic of the classification model with 24000 MPa as the elastic modulus threshold for: **(a)** 180 datasets, and **(b)** 500 datasets.

Table 1. Classification accuracy of 180 and 500 data sets generated by the IOA-Model, respectively.

Algorithm	Train set accuracy	Test set accuracy
	(180/500)	(180/500)
Logistic regression	0.917/0.990	0.910/0.998
Decision tree	0.944/0.970	0.951/0.983
SVM	0.917/0.980	0.903/0.988
Random forest	0.861/0.990	0.993/0.988
KNN	0.861/0.990	1.000/1.000
ANN	0.889/1.000	0.944/1.000

Using the aforementioned optimal classification physical model, the IOA-Model framework is trained. Fig. 10(a) shows the structural mechanical property curves designed by the IOA-Model framework under two targets, namely high and low elastic moduli. Each target is designed three times, and the results of each design are grouped together to obtain three groups. It is observed that under the requirement of high elastic modulus, the elastic moduli of all three structural designs exceed 24000 MPa, meeting the design specifications. Similarly, under the requirement of low elastic modulus, the elastic moduli of all three structural designs are lower than 24000 MPa, also meeting the requirement.

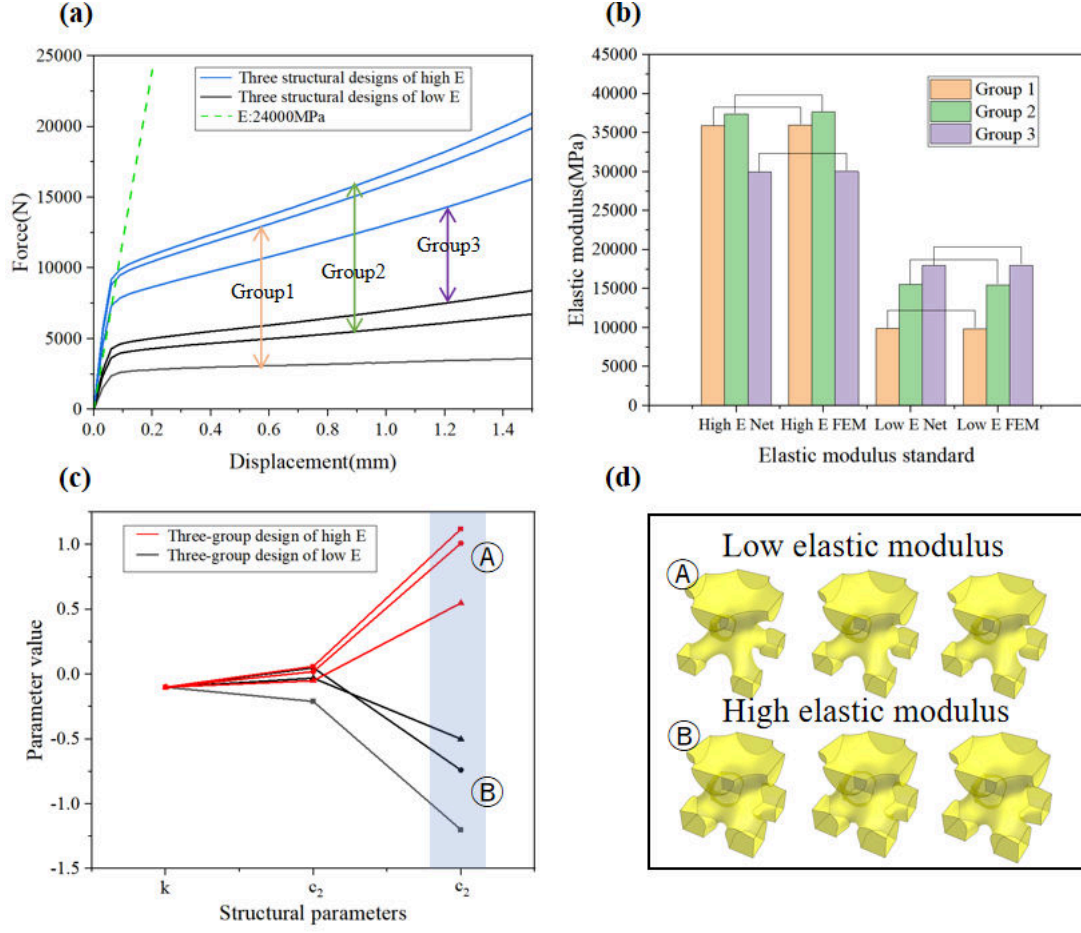


Fig.10 Structural mechanical property curves, elastic modulus values, and structural parameters designed under two different types of elastic modulus targets: **(a)** three sets of structural property curves designed by the IOA-Model framework, **(b)** FEM results and physical model predicted results for structures, **(c)** values of structural parameters, and **(d)** designed geometric structures.

Fig. 10(b) shows the elastic moduli obtained by FEM simulation and predicted by the physical model for three structural designs under high and low elastic modulus targets, respectively. The elastic modulus values of FEM simulation tend to be consistent with the predictions of the physical model, and the prediction error (the error between the target result and the predicted result) affects the magnitude of the design error. Fig. 10(c) shows the values of structural parameters designed under two types of elastic modulus targets. Similarly, the property in the elastic state is more sensitive to the parameter c_2 , consistent with the discussions in *Sections 3.1* and *3.2*. Fig. 10(d) shows the true combined structures corresponding to the structural parameters designed under two types of elastic modulus targets. It can be observed

that the structures designed under high elastic modulus are more robust compared to those under low elastic modulus, consistent with physical laws.

In order to achieve better training results, the training process of the corresponding framework in Fig. 10(a) is monitored, and the changes in the two-dimensional latent distribution l are analyzed during the training process of 500 sets of elastic modulus data. As shown in Fig. 11(a), the structure parameters of the original 500 datasets are divided based on the elastic modulus of 24000 MPa, showing clear boundaries. When monitoring the corresponding latent distribution generated by the Encoder during the training at 1 epoch, illustrated in Fig. 11(b), the initial latent data form clustered distributions, but they overlap with each other. Subsequently, during the training at 3 epochs, as shown in Fig. 11(c), the separation begins to show boundaries, and after enlarging the image, there are still some overlaps. Continuing with the training at 5 epochs, as shown in Fig. 11(d), clear boundaries appear with almost no overlaps, consistent with the distribution of the original data, showing two types of clustered distributions. This demonstrates a common pattern with Fig. 8, indicating that the latent distribution has a certain connection with the corresponding original distribution. Therefore, although the latent distribution lacks a specific physical meaning, and it is not exactly the same as the original distribution in space, the data characteristics of both distributions are related and similar, such as the quantity of data, spatial distance, and continuity features. By analyzing the changes in these features, the training information can be grasped, and the completion ability of the IOA-Model framework for downstream target tasks can be evaluated in the Nash equilibrium state.

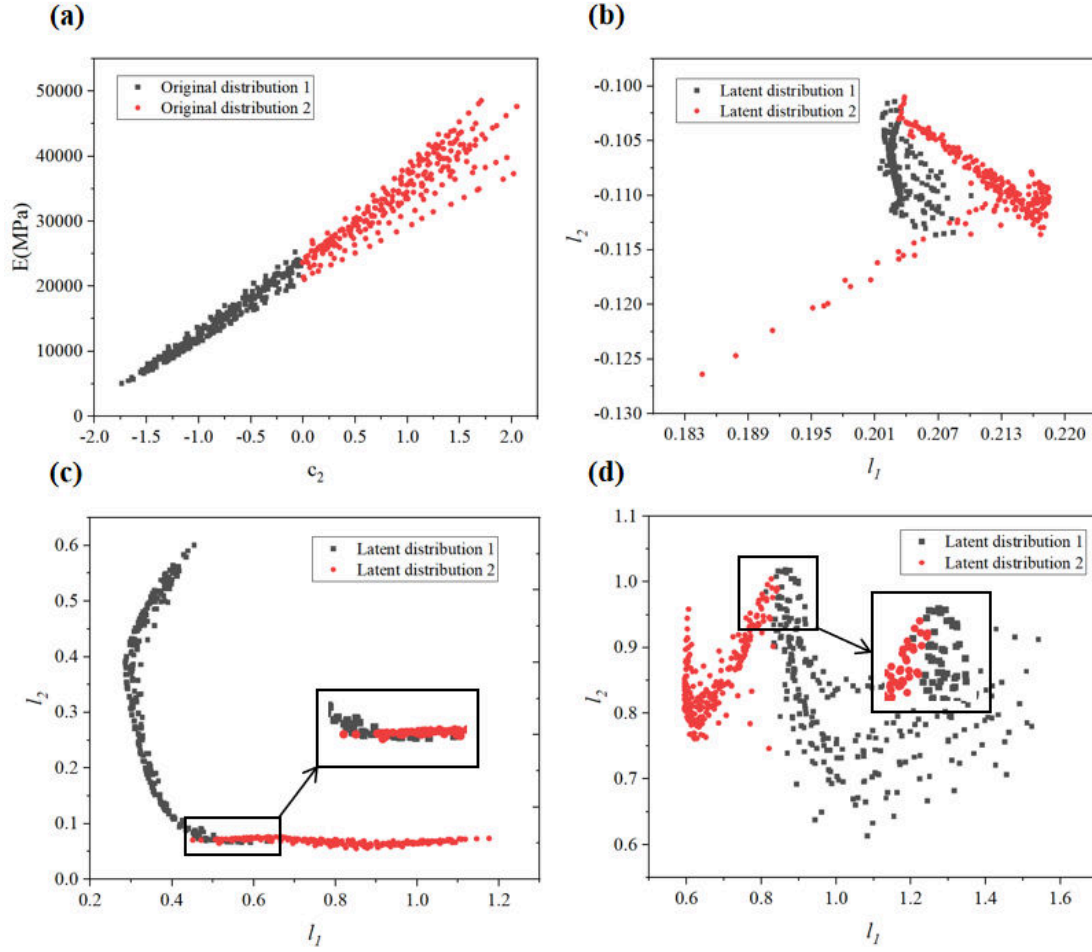


Fig.11 Original data distribution and corresponding latent distribution change during training: (a) original data distribution, (b) distribution of latent data at 1 epoch, (c) distribution of latent data at 3 epochs, and (d) distribution of latent data at 5 epochs.

3.4. Combined structure design under varying load-displacement curves

Figs. 12 (a)-(b) illustrate the load-displacement curves of Primitive and IWP combined structures generated by the IOA-Model framework under two different target load-displacement curves (namely target curves ① and ②), obtained by FEM simulation and predicted by the physical model. The error is calculated by comparing the L_2 norm of the difference between the two curves with the L_2 norm of the target curve. The target curve ① in Fig. 12 (a) features a relatively high elastic modulus combined with ascending plasticity. The error between the FEM curve of combined structures designed by the IOA-Model framework and the target curve is 2.2 %, indicating a very small design error. Additionally, the error between the predicted curve of the physical model and the target curve is 2.15 %, which is also

very small. The target curve ② in Fig. 12(b) is characterized by a relatively low elastic modulus, with features of initial softening and gentle plastic deformation stage. The error between the target curve and the FEM curve of the designed structure is 9.20 %, relatively larger than that of ①. The error between the predicted curve of the physical model and the target curve is 5.08 %, which is also relatively large. It can be seen that although the errors of inverse design under two different characteristic target curves may vary, the changes in the load-displacement curves of the two types are well matched. This facilitates effective structural designs for different characteristic target demands. Comparing the prediction error and design error under the two targets, there is a positive correlation between prediction error and design error. The prediction error corresponds to the prediction accuracy of the physical model in the IOA-Model. Thus, the physical model determines the overall performance of the IOA-Model framework.

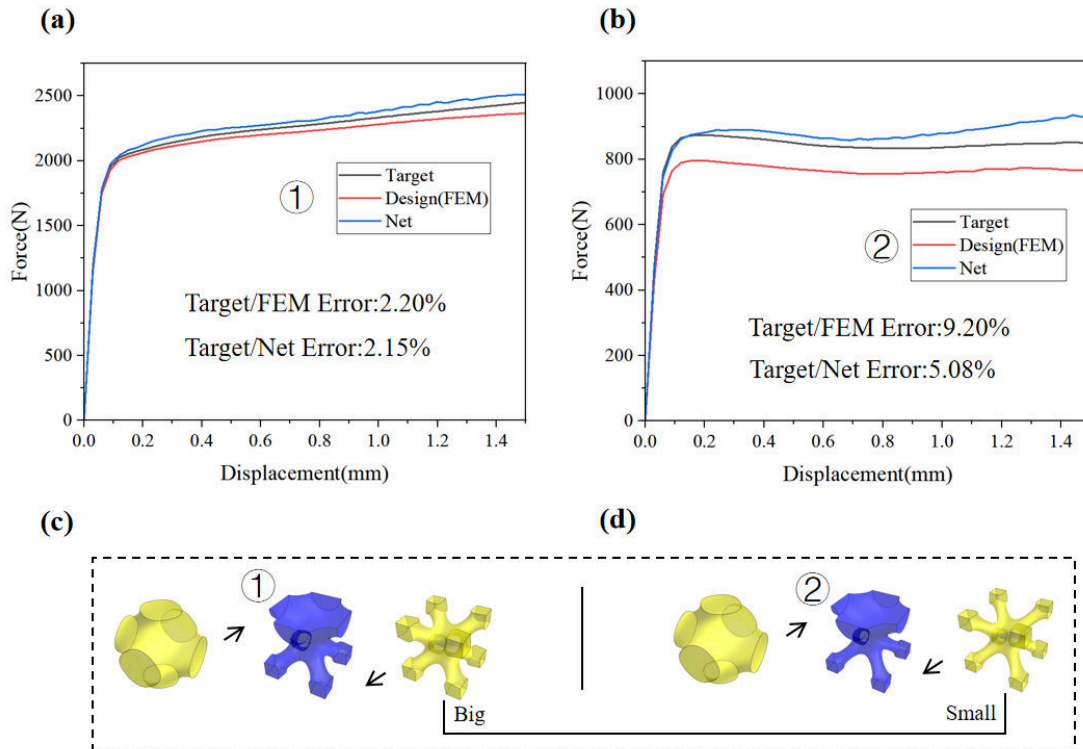


Fig.12 Property curves and corresponding actual geometric structures obtained through reverse design under two different target load-displacement curves: **(a)** design based on target curve ①, **(b)** design based on target curve ②, **(c)**geometric structure generated by the IOA-Model corresponding to target ①, and **(d)** geometric structure generated by the IOA-Model corresponding to target ②.

Figs. 12(c)-(d) illustrate the true Primitive and IWP combined structures obtained through inverse design under two different load-displacement target curves (corresponding to numerical indices in Figs. 12(a)- (b)). Comparing the dimensions of structures based on target curves ① and ②, the thickness variation of the IWP part is more pronounced, and the load-displacement mechanical property curve of the overall combined TPMS structure is more sensitive to the changes in the IWP part. A more robust IWP is chosen for combination in Target ①, resulting in a property curve with a larger elastic modulus, and a steeper slope in the plastic stage. Meanwhile, a slimmer IWP is opted in target ②, resulting in a lower elastic modulus of the property curve, with the plastic stage exhibiting a more gradual change. This observation aligns with the discussion in *Section 3.1* regarding the impact characteristics of structural parameters on the load-displacement mechanical curves of combined structures.

To observe the relationship between the original data distribution and the latent distribution l , three groups of structural parameters with different spatial distribution characteristics are selected from the original training dataset, each containing 20 data points, as shown in Fig. 13(a). In terms of spatial distance, original distributions 1 and 3 are close in spatial distribution, while both are distant from original distribution 2. Concerning data characteristics, all three sets of original data exhibit approximately linear continuous distributions. During the training, the latent distribution l is monitored corresponding to the Encoder outputs.

Figs. 13(b)-(d) depict the latent two-dimensional distribution l corresponding to the original data during the training process, with curve colors matching the original data. After 1 epoch of training, the three groups of latent distributions are in a mixed and disordered state, intersecting with each other without clear boundary distinctions. After 3 epochs of training, the latent distribution corresponding to original distribution 2 begins to separate from the other two groups of data. After 5 epochs of training, latent distributions 1 and 3 become closer to each

other, while being farther from latent distribution 2. At the same time, all three tend to exhibit approximately linear continuous distributions, consistent with the characteristics of the original data distribution. This further validates the same pattern observed in Fig. 8 and Fig. 10 regarding the relationship between the original distribution and the corresponding latent distribution.

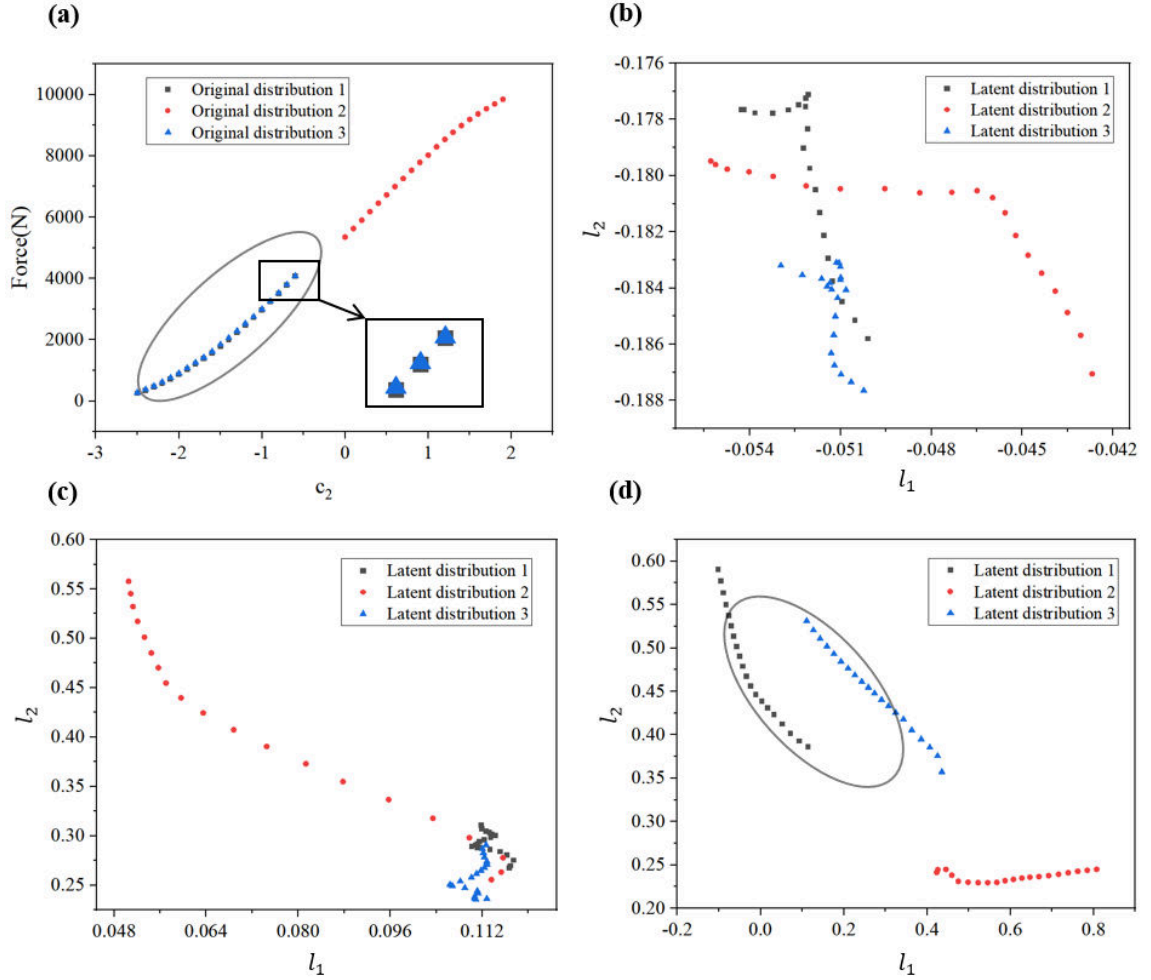


Fig.13 Three sets of data distributions selected from the original training dataset and corresponding changes in latent distribution during the training process: (a) three sets of original data distributions, (b) latent distribution after 1 epoch of training, (c) latent distribution after 3 epochs of training, and (d) latent distribution after 5 epochs of training.

The geometric structures generated by the IOA-Model under the load-displacement curve targets ① and ② are 3D printed and subjected to heat treatment. Following this, the quasi-static compression experiments are conducted to obtain the compression mechanical properties of the structures, as shown in Fig. 14. For target ①, the experimental curve in the plastic stage

exhibits a rising feature similar to the target curve (as indicated by the green dashed line), while for target ②, the experimental curve in the plastic stage exhibits a softening descent feature similar to the target curve (as indicated by the green dashed line). This indicates that the deformation patterns of the experimental curves and target curves of the structures under both mechanical property targets are well matched, as shown in Figs. 14(a)-(b). Additionally, the experimental curves for targets ① and ② are within a certain range of the target curve's load values without significant deviations.

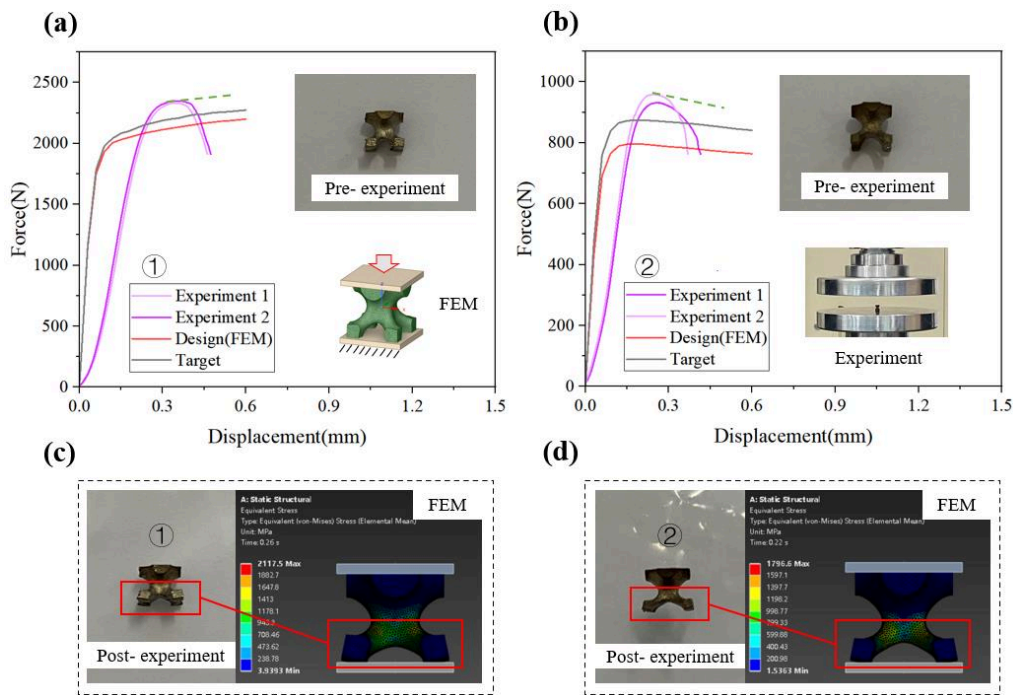


Fig.14 Pre-experiment printed structures, and experimental curves of Experiment 1 and Experiment 2 with the same structure: **(a)** under the condition of target ①, **(b)** under the condition of target ②, the experiment curves, the FEA curve and the target curve, **(c)** under the condition of target ①, and **(d)** under the condition of target ②, the comparison of the structural deformation obtained from simulations and corresponding experiments.

The discrepancies between the experimental curves and the target curves can be attributed to differences in the actual structure's quality during printing [46], differences during heat treatment, errors in the material models used in FEM simulations, and various manufacturing defects such as pores, impurities, and residual stresses generated by SLM processes [47]. The drop and absence of the posterior portion of the experimental curve is due to damage to the

structure, which is not designed with the fracture modeling of the material in mind. Furthermore, the comparison of the structural deformation obtained from numerical simulations and corresponding experiments is shown in Figs. 14(c)-(d). The ANSYS equivalent stress here is the von-Mises stress, which is applicable to plastic materials that fail in the form of yielding. It can be observed that the structural deformations from numerical simulations are in basic agreement with those from experiments, with both exhibiting outward expansion deformations in the lower part of the structure, thereby validating the effectiveness of the proposed Primitive and IWP combination structure inverse design method.

4 Conclusions

An IOA-Model framework based on BiGAN was proposed in this study, and it could take target mechanical properties as input to generate corresponding structural designs and analyze the latent data distribution of the outputs to grasp training information. Taking Primitive and IWP combined structures as objects, different types of combined TPMS structures were designed through the IOA-Model framework, obtaining different buffering and energy absorption capacities in elastic and plastic stages. The main conclusions are as follows:

(1) In the context of combined structure design under the variation of a single characteristic load value, the IOA-Model framework demonstrates excellent performance under three displacement conditions. In the training of the dataset, the R_2 values are all above 0.98, with a maximum MAPE value of only 5.92 %. When customizing target requirements for single loads of 5000 N and 8000 N, three combined structures are conducted. Following two optimizations, the design errors reduce from 9.06 % to 3.93 % and from 5.06 % to 0.26 %, achieving higher precision in structural design.

(2) The structural design of elastic modulus targets confirms that the learning capabilities of the proposed IOA-Model framework, which only employs the BiGAN network without the physical model. The generated structural parameters exhibit clear decision boundaries for

elastic modulus, and it is verified that the IOA-Model framework has the working ability for multiple classification physical models. Two sets of generated structures for high and low elastic modulus targets are distributed within their respective ideal design ranges.

(3) For combined structure design under the variation of the entire load-displacement curve demand, the IOA-Model framework achieves a minimum design error of only 2.20 % for two curve targets. Two combined structures with different characteristics in elastic and plastic stages are successfully customized. The additively manufactured structures are subjected to compression testing, and the experimental curves align well with the target curves in terms of variation trends and load value ranges, while the experimental deformations exhibit consistency with simulations.

(4) By analyzing the latent distribution generated by the Encoder of the IOA-Model framework and its corresponding original data distribution, starting from features such as data quantity, spatial distance, and continuity characteristics of the two distributions, the training process under three objectives of single characteristic load value, elastic modulus, and entire load-displacement curve is explained. This approach makes the training of the IOA-Model framework controllable, and the ultimate training outcome can better achieve the target-based structural parameter design.

Declaration of competing interest

There is no conflict of interest.

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Inverse design of cellular structures with the geometry of triply periodic minimal surfaces using generative artificial intelligence algorithms

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