

Supplementary Materials for Data-driven Inverse Design of Multifunctional Bicontinuous Multiscale Structures

This Supplementary Information includes:

- Section 1 provides the calculation of mechanical properties.
- Section 2 details the boundary mask construction.
- Section 3 describes initial dataset construction and statistics.
- Section 4 explains the active learning strategy.
- Section 5 presents the final dataset statistics.
- Section 6 showcases the multifunctional bicontinuous multiscale design.
- Section 7 provides a simplified theoretical understanding of the structural parameters governing permeability.
- Section 8 shows 3D printing visualization.

Additional Supplementary Files:

- Movie 1: Representative microstructures of the first dataset.
- Movie 2: Representative microstructures of the second dataset.
- Movie 3: Representative microstructures of the third dataset.
- Movie 4: Representative microstructures of the fourth dataset.
- Movie 5: Experiment on the liquid permeability of six structures.
- Source data file containing Figures 2–7, all supplementary figures and tables, and the four datasets.

1 Mechanical properties evaluation

1.1 Elastic modulus calculation

Homogenization theory [1] simplifies the analysis of macroscopic material properties by reducing complex microstructures to equivalent homogeneous materials. This method employs the Representative Volume Element (RVE) of the microstructure to capture microscopic variations and predict overall mechanical behavior.

We consider RVEs with cubic symmetry, meaning these microstructures remain invariant under the symmetry operations of the cubic crystal system. This symmetry implies that the material possesses identical physical properties along the three mutually perpendicular axes. For materials with cubic symmetry, the elasticity tensor $\mathbf{C}$ can be expressed as follows:

$$\mathbf{C} = \begin{pmatrix} C_{1111} & C_{1122} & C_{1122} & 0 & 0 & 0 \\ C_{1122} & C_{1111} & C_{1122} & 0 & 0 & 0 \\ C_{1122} & C_{1122} & C_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{1212} \end{pmatrix}. \quad (1)$$

Here C_{1111} , C_{1122} , and C_{1212} are the elastic constants of the material.

The bulk modulus K and shear modulus G of cubic symmetric materials can be calculated from the elastic tensor components C_{1111} , C_{1122} , and C_{1212} :

$$K = \frac{1}{3}(C_{1111} + 2C_{1122}), \quad (2)$$

$$G = C_{1212}. \quad (3)$$

Young's modulus E and Poisson's ratio ν are determined using the following equations:

$$E = \frac{(C_{1111} - C_{1122})(C_{1111} + 2C_{1122})}{C_{1111} + C_{1122}}, \quad (4)$$

$$\nu = \frac{C_{1122}}{C_{1111} + C_{1122}}. \quad (5)$$

The Zener ratio Z , which characterizes the anisotropy of the material, is defined as:

$$Z = \frac{2C_{1212}}{C_{1111} - C_{1122}}. \quad (6)$$

When Z approaches 1, the material exhibits higher isotropy; deviations from 1 correspond to increased anisotropy.

1.2 Voigt upper bound

For composite materials composed of multiple constituents, each constituent material possesses unique mechanical properties, such as Young's modulus and Poisson's ratio. The Voigt upper bound [2] estimates the upper limit of the overall mechanical properties of the composite materials by assuming a state where all component materials are perfectly uniform and free of stress concentrations. The Voigt upper bounds for the bulk modulus, shear modulus, and Young's modulus with specified volume fraction V are:

$$K_V = \frac{V E_s}{3(1 - 2v_s)}, \quad (7)$$

$$G_V = \frac{V E_s}{2(1 + v_s)}, \quad (8)$$

$$E_V = V E_s. \quad (9)$$

where E_s and v_s are the Young's modulus and Poisson's ratio of the solid material, respectively.

1.3 Hashin-Shtrikman upper bound

For isotropic composite materials, the Hashin-Shtrikman upper bounds provide estimates of the theoretical upper limits for their modulus. Here are the specific equations for bulk modulus, shear modulus, and Young's modulus [3]:

$$K_{HS} = \frac{4G_s K_V}{4G_s + 3K_s(1 - V)}, \quad (10)$$

$$G_{HS} = \frac{(9K_s + 8G_s)G_V}{20G_s + 15K_s - 6(K_s + 2G_s)V}, \quad (11)$$

$$E_{HS} = \frac{9G_{HS}K_{HS}}{3K_{HS} + G_{HS}}, \quad (12)$$

where $K_s = E_s/3(1 - 2v_s)$ and $G_s = E_s/2(1 + v_s)$ are the bulk modulus and shear modulus of the constituent solid material, respectively. The K_V and G_V are given by Equations (7) and (8), respectively.

2 Boundary mask construction

We construct the four types of microstructure boundary masks through the following workflow: first, collecting extensive boundary data from diverse sources, then performing clustering-based deduplication, and finally conducting generation tests based on the streamlined data to finalize the four mask types.

2.1 Multi-source boundary mask design and feasibility analysis

The boundary mask data primarily are obtained from three sources: the 3D microstructure dataset [4], the 2D microstructure dataset [5], and user-designed masks, as shown in Figure S1a.

For the 3D microstructure dataset, we extract the masks of each structure as mask data. Since 2D microstructure patterns exhibit high similarity to the masks of 3D microstructures, 2D microstructure images are also utilized as mask data. Additionally, to enrich the mask data, we collected some user-specified masks.

The selection of masks significantly influences the potential property range of the ultimately generated bicontinuous open-cell dataset. Therefore, it is necessary to test microstructure generation with different masks. However, given the substantial scale of the mask data, it is impractical to perform generation tests for each mask. To address this, we employ clustering methods to streamline the mask data.

2.2 Cluster analysis and candidate mask extraction

We perform cluster analysis on the mask data obtained in the previous step using K-means clustering. Focusing on microstructures with a low volume fraction (0.1–0.4), we extract 15 representative cluster centers as candidate mask patterns for 3D microstructure generation.

2.3 Screening and evaluation according to quality metrics

Building on the above explorations, we refer to existing 3D boundary design schemes [6, 7, 8] and select approximately 30 boundary masks for further testing (Figure S1b). For the microstructures generated from these candidate masks, we perform a systematic evaluation based on two key metrics:

- **Proportion of bicontinuous open-cell structures:** To ensure that the generated 3D microstructures possess the requisite connectivity, we employed a connected component labeling algorithm to verify whether these structures are bicontinuous open-cell architectures and then calculated their proportion.

The connected component labeling algorithm is used to assess independently the number of connected components in both the solid and void regions of a microstructure. A microstructure is considered bicontinuous if and only if both its solid and void parts exhibit exactly one connected component each; otherwise, it is deemed non-bicontinuous. Details of the connected component labeling algorithm are provided below:

(1) First scan

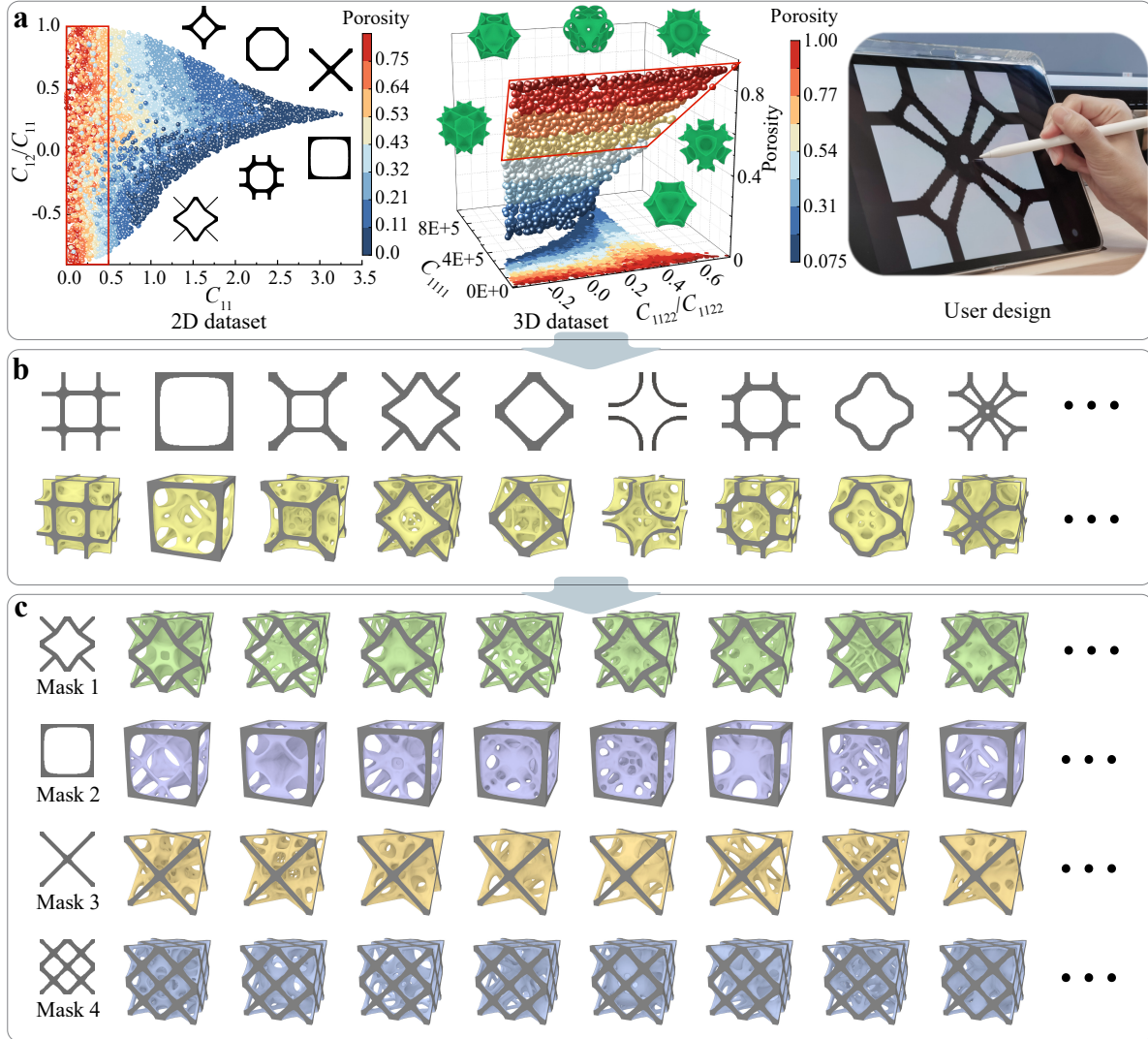


Figure S1: **Boundary mask construction.** **a** The left and middle panels show the relationships between elastic tensor components (C_{12}/C_{11} and C_{11} for the 2D dataset, and C_{1111} and C_{1122}/C_{1111} for the 3D dataset) together with porosity information. The red boxes in both datasets indicate the candidate boundary regions, while the right panel illustrates user-specified mask generation. The right panel illustrates user-specified masks. **b** Representative masks and their corresponding example microstructures. **c** The four finally selected masks (Masks 1–4) and their associated example microstructures.

For each element p at coordinate (i, j, k) , assign a label $L(i, j, k)$ to the output through the following procedure:

$$L(i, j, k) = \begin{cases} \text{a new label,} & \text{if neighboring elements } N(p) \text{ are unlabeled;} \\ \min(N(p)), & \text{if neighboring elements } N(p) \text{ are labeled;} \end{cases} \quad (13)$$

where $N(p)$ denotes the neighboring elements of p . When multiple labels exist in $N(p)$, select the minimum label and record these labels as equivalence relationships;

(2) Second scan

Traverse each element p again and update labels to unify all equivalent labels into a single label:

$$L(i, j, k) = \text{find}(L(i, j, k)), \quad (14)$$

where the find function retrieves the minimum equivalent label associated with $L(i, j, k)$, thereby achieving label consolidation.

- **Poisson’s ratio coverage:** We calculate and compare the Poisson’s ratios ranges of structures generated from different masks to assess the diversity of their mechanical properties. Specifically, this process involves performing mechanical analysis on each microstructure generated from the candidate masks to determine their Poisson’s ratio values. The goal is to identify masks that could produce a wide range of Poisson’s ratios, indicating their suitability for designing materials with diverse mechanical responses.

Based on the evaluation results from these two key metrics, we conduct multiple rounds of testing and screening and ultimately identify four optimal fixed masks, as shown in Figure S1c. The four boundary configurations not only demonstrate excellent coverage of Poisson’s ratios but also achieve a high proportion of bicontinuous open-cell architectures, thereby facilitating the subsequent generation of high-quality datasets.

3 Initial dataset construction and statistics

3.1 Isotropic optimization models

Topology optimization is a class of engineering methods that seek the optimal material distribution within a given design space, commonly used for microstructure generation [9]. Using the Solid Isotropic Material with Penalization (SIMP) model [10, 11, 12], the setup for a topology optimization problem aiming to maximize the bulk modulus, while incorporating isotropic constraints and specified boundary conditions, is as follows:

$$\begin{aligned}
\min_{\boldsymbol{\rho}} \quad & f(\mathbf{C}(\boldsymbol{\rho})) = -\frac{1}{3}(C_{1111} + 2C_{1122}) \\
\text{s.t.} \quad & \mathbf{K}(\boldsymbol{\rho})\mathbf{U} = \mathbf{F}, \\
& \frac{\sum_{e=1}^M v_e \rho_e}{|\Omega|} \leq V, \\
& \phi(b_1 - b_2) < \epsilon_1, \\
& (Z - 1)^2 < \epsilon_2, \\
& 0 \leq \rho_e \leq 1, \forall e = 1, \dots, M.
\end{aligned} \tag{15}$$

Here, $\boldsymbol{\rho}$ represents the design variable, which corresponds to the material density in the SIMP method. The objective function $f(\mathbf{C}(\boldsymbol{\rho}))$ is the negative value of the bulk modulus. $\mathbf{U}$ denotes the displacement field within the microstructure design domain, and $\mathbf{F}$ represents the applied external force. $\mathbf{K}(\boldsymbol{\rho})$ is the global stiffness matrix. The equilibrium constraint is given by $\mathbf{K}(\boldsymbol{\rho})\mathbf{U} = \mathbf{F}$. The base solid material is defined with a Young's modulus of $E_0 = 1 \times 10^6$ and a Poisson's ratio of $\nu = 0.3$.

The design domain is discretized into M elements, where ρ_e represents the density of the e -th element and v_e denotes its volume. Thus, $\sum_{e=1}^M v_e \rho_e$ represents the material volume. $|\Omega|$ is the volume of the microstructure design domain, and V represents the prescribed volume fraction. The volume fraction constraint ensures that the ratio of the material volume to the design domain volume does not exceed V . b_1 denotes the material boundary, b_2 denotes the specified boundary, and ϵ_1 and ϵ_2 denote the permissible convergence errors. During the optimization process, the boundary constraint $\phi(b_1 - b_2) < \epsilon_1$ ensures that the material boundary b_1 closely matches the specified boundary b_2 . The isotropy constraint $(Z - 1)^2 < \epsilon_2$ ensures that Z remains sufficiently close to 1, with deviations bounded by ϵ_2 . The density variable constraint $0 \leq \rho_e \leq 1 (\forall e = 1, \dots, M)$ ensures that the density ρ_e of each element is bounded between 0 and 1, where $\rho_e = 0$ indicates void material and $\rho_e = 1$ indicates solid material.

The optimization problem above is solved using the Moving Asymptotes Method (MMA) [13] to determine the optimal property distribution $\boldsymbol{\rho}$. Figure S2 illustrates the optimization process for maximizing the bulk modulus under isotropic and specified boundary conditions. The leftmost figure shows the result at step 10, with subsequent figures showing results at steps 20, 30, and so on, until the final result at step 2000. Table S1 details the mechanical parameters corresponding to Figure S2. From the numerical results, porosity stabilizes starting at step 20 as the microstructure begins to form. As the number of iterations increases, the surface-to-volume ratio (S/V) decreases, the Poisson's ratio

remains stable, Z approaches 1, and both stiffness and rigidity increase. Ultimately, we achieved an isotropic microstructure with a specified boundary, porosity of 0.84, S/V of 0.31, Poisson’s ratio of 0.30, K/K_{HS} of 53.34%, G/G_{HS} of 39.49%, and E/E_{HS} of 41.15%.

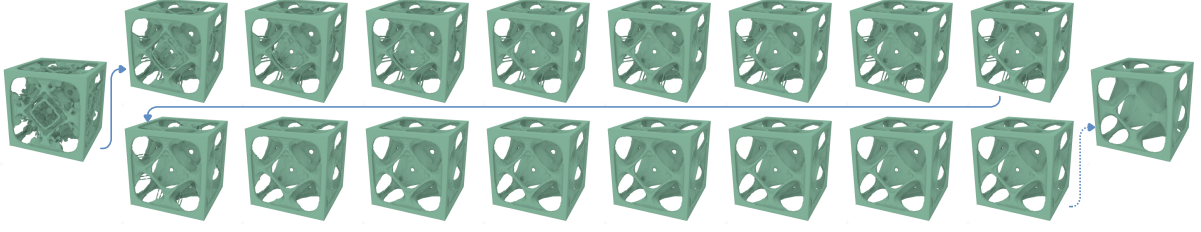


Figure S2: Intermediate results of the optimization process.

Table S1: Statistical properties of intermediate results during the optimization process. Listed parameters include elastic tensor components (C_{1111} , C_{1122} , C_{1212}), porosity ($1 - V$), surface-to-volume ratio (S/V), Poisson’s ratio (ν), and Zener ratio (Z). Normalized moduli K/K_{HS} , G/G_{HS} , and E/E_{HS} represent the bulk, shear, and Young’s moduli with respect to the Hashin–Shtrikman upper bound, respectively. Source data are provided as a Source Data file.

Iter	C_{1111}	C_{1122}	C_{1212}	$1 - V$	S/V	ν	Z	$K/K_{HS}(\%)$	$G/G_{HS}(\%)$	$E/E_{HS}(\%)$
0010	47785.27	18191.76	16243.60	0.79	0.53	0.28	1.10	35.78	33.79	31.53
0020	44574.48	17719.39	14084.58	0.84	0.48	0.28	1.05	45.74	39.06	38.46
0030	46759.90	18795.11	14444.38	0.84	0.43	0.29	1.03	48.24	40.07	40.13
0040	47606.60	19178.62	14606.28	0.84	0.41	0.29	1.03	49.22	40.57	40.86
0050	47991.83	19328.18	14574.35	0.84	0.39	0.29	1.02	49.61	40.48	41.20
0060	48300.67	19540.22	14595.74	0.84	0.38	0.29	1.01	50.05	40.56	41.38
0070	48537.41	19694.38	14632.75	0.84	0.38	0.29	1.01	50.37	40.66	41.53
0080	48692.47	19792.83	14645.20	0.84	0.38	0.29	1.01	50.50	40.65	41.57
0090	48770.22	19842.36	14653.39	0.84	0.37	0.29	1.01	50.64	40.70	41.64
0100	48827.49	19888.32	14645.25	0.84	0.37	0.29	1.01	50.74	40.68	41.68
0110	48539.99	19708.29	14576.43	0.84	0.35	0.29	1.01	50.47	40.58	41.58
0120	48832.52	19887.26	14648.16	0.84	0.35	0.29	1.01	50.74	40.69	41.68
0130	49047.05	20047.27	14650.10	0.84	0.35	0.29	1.01	50.95	40.62	41.71
0140	49125.74	20138.49	14615.12	0.84	0.35	0.29	1.01	51.17	40.58	41.77
0150	49117.80	20175.05	14582.31	0.84	0.34	0.29	1.01	51.25	40.52	41.75
0160	49183.18	20253.11	14578.38	0.84	0.34	0.29	1.01	51.36	40.50	41.74
...										
2000	49925.15	21624.19	14219.07	0.84	0.31	0.30	1.00	53.34	39.49	41.15

To generate an initial microstructure dataset with rich properties, we employ optimization models with three objectives: maximizing K , G , and E . The optimization objectives for maximizing G and E are formulated as follows, with their constraint settings being identical to those used for maximizing K :

$$f(\mathbf{C}(\boldsymbol{\rho})) = -C_{1212}, \quad (16)$$

$$f(\mathbf{C}(\boldsymbol{\rho})) = -\frac{(C_{1111} - C_{1122})(C_{1111} + 2C_{1122})}{C_{1111} + C_{1122}}. \quad (17)$$

Additionally, to broaden the Poisson's ratio coverage in the initial dataset, we develop two additional objective functions. First, for generating microstructures with specified Poisson's ratios, the following Poisson's ratio constraint is incorporated into the optimization problem. For isotropic microstructures, the upper limit of Poisson's ratio is 0.5 [14]. In experiments, this optimization successfully produces isotropic microstructures with specified Poisson's ratios, except for pentamode structures [15, 16, 17] approaching the Poisson's ratio upper limit.

$$\begin{aligned}
\min_{\boldsymbol{\rho}} \quad & f(\mathbf{C}(\boldsymbol{\rho})) = -\frac{1}{3}(C_{1111} + 2C_{1122}) \\
\text{s.t.} \quad & \mathbf{K}(\boldsymbol{\rho})\mathbf{U} = \mathbf{F}, \\
& \frac{\sum_{e=1}^M v_e \rho_e}{|\Omega|} \leq V, \\
& \phi(b_1 - b_2) < \epsilon, \\
& (Z - 1)^2 < \epsilon, \\
& \left(\frac{C_{1122}}{C_{1111} + C_{1122}} - v_0\right)^2 < \epsilon, \\
& 0 \leq \rho_e \leq 1, \forall e = 1, \dots, M,
\end{aligned} \tag{18}$$

where v_0 represents the specified Poisson's ratio.

To address challenges in the aforementioned optimization models, the following objective function is proposed to generate pentamode structures approaching the near-0.5 Poisson's ratio. The denominator term 0.05 is introduced to prevent singularity.

$$f(\mathbf{C}(\boldsymbol{\rho})) = -K + \frac{G - 0.8G_0}{K(0.5\frac{G_0}{K_0}) + 0.05}, \tag{19}$$

where K and G are defined in Equations (2) and (3), respectively. K_0 and G_0 denote their initial values, determined from the initial random simulations.

3.2 Anisotropic optimization models

Anisotropic microstructures have garnered significant attention due to their unique physical properties, such as negative Poisson's ratio, and ultra-high elastic modulus. These properties are not only of great importance in fundamental scientific research but also show immense potential for practical applications in engineering. To further expand and augment our dataset, we design a series of optimization models for generating anisotropic microstructures. The optimization model for K maximization is as follows:

$$\begin{aligned}
\min_{\boldsymbol{\rho}} \quad & f(\mathbf{C}(\boldsymbol{\rho})) = -\frac{1}{3}(C_{1111} + 2C_{1122}) \\
\text{s.t.} \quad & \mathbf{K}(\boldsymbol{\rho})\mathbf{U} = \mathbf{F}, \\
& \frac{\sum_{e=1}^M v_e \rho_e}{|\Omega|} \leq V, \\
& \phi(b_1 - b_2) < \epsilon, \\
& 0 \leq \rho_e \leq 1, \forall e = 1, \dots, M.
\end{aligned} \tag{20}$$

For the optimization objectives of maximizing G and E and generating pentamode structures, Equations (14), (15), and (17) are employed as the respective objective functions.

The optimization model for specifying Poisson's ratio is defined as follows,

$$\begin{aligned}
\min_{\boldsymbol{\rho}} \quad & f(\mathbf{C}(\boldsymbol{\rho})) = -\frac{1}{3}(C_{1111} + 2C_{1122}) \\
\text{s.t.} \quad & \mathbf{K}(\boldsymbol{\rho})\mathbf{U} = \mathbf{F}, \\
& \frac{\sum_{e=1}^M v_e \rho_e}{|\Omega|} \leq V, \\
& \phi(b_1 - b_2) < \epsilon, \\
& \left(\frac{C_{1122}}{C_{1111} + C_{1122}} - v_0 \right)^2 < \epsilon, \\
& 0 \leq \rho_e \leq 1, \forall e = 1, \dots, M.
\end{aligned} \tag{21}$$

Figure S3 shows the optimized microstructures from the four datasets, including those maximizing bulk (orange), shear (green), and Young's modulus (purple), as well as structures with near-pentamode behavior (yellow) and negative Poisson's ratio (blue). Supplementary Table S2 lists the corresponding mechanical parameters for all 20 microstructures.

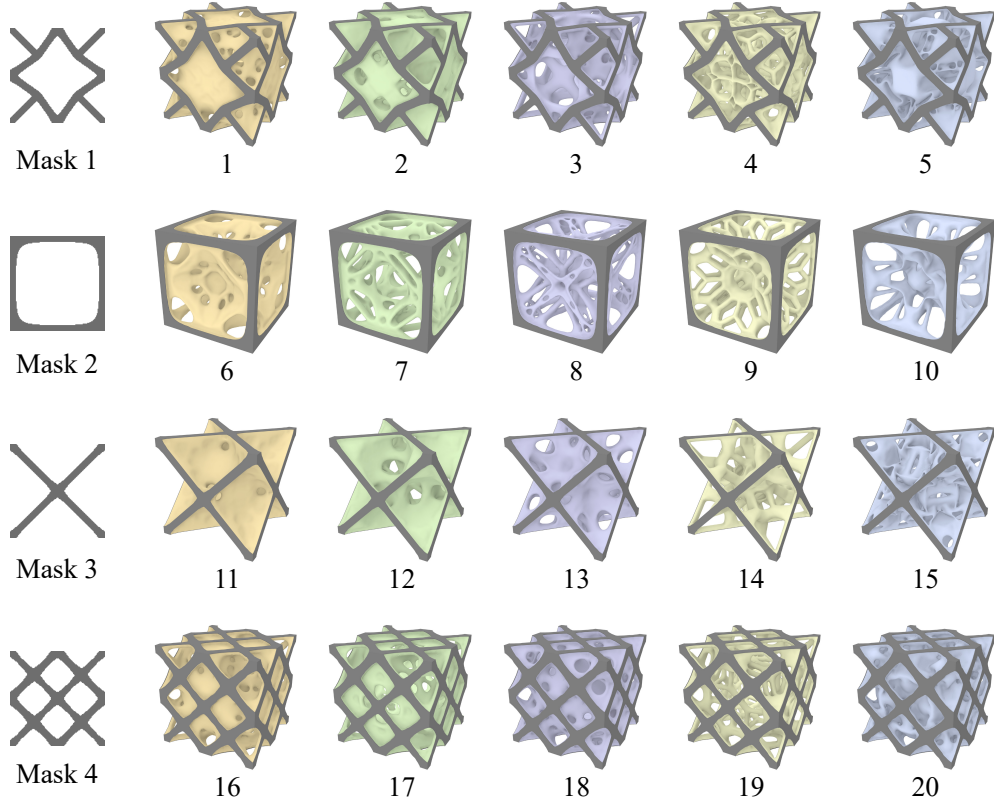


Figure S3: Partial optimization results corresponding to the four masks.

Table S2: Properties of the 20 microstructures shown in Figure S3. Source data are provided as a Source Data file.

No	C_{1111}	C_{1122}	C_{1212}	$1 - V$	S/V	v	Z	K/K_{HS} (%)	G/G_{HS} (%)	E/E_{HS} (%)	K/K_v (%)	G/G_v (%)	E/E_v (%)
1	156443	57291	47451	0.71	0.29	0.27	0.96	81.75	71.02	75.37	37.85	43.08	43.90
2	147516	52451	47403	0.71	0.29	0.26	1.00	73.58	68.68	69.62	34.28	41.85	40.74
3	78063	32435	22375	0.79	0.36	0.29	0.98	61.66	47.21	50.00	27.03	27.50	27.90
4	59431	29757	12710	0.78	0.42	0.33	0.86	49.91	26.11	32.63	21.96	15.25	18.26
5	37270	-2180	18790	0.78	0.62	-0.06	0.95	13.32	37.28	29.46	5.89	21.85	16.55
6	117403	42822	37872	0.71	0.26	0.27	1.02	59.59	55.23	55.19	27.73	33.62	32.27
7	81130	27739	27477	0.77	0.31	0.25	1.03	54.10	53.39	52.24	23.99	31.37	29.42
8	61748	24494	18546	0.80	0.40	0.28	1.00	51.68	42.23	43.75	22.43	24.42	24.22
9	57453	30755	11786	0.79	0.36	0.35	0.88	51.87	25.13	30.82	22.71	14.62	17.18
10	51428	10690	20554	0.79	0.28	0.17	1.01	32.19	44.42	41.43	14.07	25.81	23.06
11	135060	56549	39097	0.75	0.23	0.30	1.00	90.06	69.85	72.85	40.45	41.43	41.44
12	117500	42656	38889	0.75	0.27	0.27	1.04	71.96	67.99	66.44	32.44	40.43	37.89
13	114553	43379	35487	0.74	0.28	0.27	1.00	68.96	59.98	61.48	31.26	35.81	35.21
14	40242	21678	8218	0.84	0.31	0.35	0.89	48.92	23.32	28.59	20.71	13.23	15.52
15	41013	1822	18464	0.81	0.65	0.04	0.94	21.46	43.25	38.44	9.28	24.94	21.22
16	129549	48185	40307	0.73	0.38	0.27	0.99	72.65	64.13	65.93	33.27	38.58	38.07
17	99681	35802	32291	0.76	0.29	0.26	1.01	64.27	59.56	59.76	28.72	35.20	33.86
18	115904	46428	33564	0.75	0.43	0.29	0.97	75.65	59.88	63.93	33.99	35.52	36.37
19	46962	22905	10842	0.83	0.43	0.33	0.90	51.77	29.37	34.78	22.02	16.73	18.95
20	90283	16882	35213	0.72	0.45	0.16	0.96	38.71	54.45	52.63	17.82	32.88	30.51

4 Active learning strategy

4.1 Diffusion model

We begin by reviewing the diffusion model proposed by Ho et al. [18]. The diffusion model consists of two phases: the forward diffusion process and the reverse denoising process. Suppose we have a real data distribution $q(\mathbf{x}_0)$. The forward diffusion process gradually adds noise to $\mathbf{x}_0$ over T steps through the following equation: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_{t-1} + \sqrt{1 - \bar{\alpha}_t}\epsilon_{t-1}$, where ϵ_{t-1} is noise sampled from a standard Gaussian distribution, and $\bar{\alpha}_t = \prod_{s=1}^t (1 - \beta_s)$, where β_t is a set of an adjustable parameter that controls the intensity of the noise. After T steps of adding noise, we obtain a data point $\mathbf{x}_T$ that is nearly pure noise. The reverse process starts from $\mathbf{x}_T$ and progressively removes the noise through T steps of denoising to recover the original data $\mathbf{x}_0$, typically using a neural network for noise prediction. Rather than directly predicting the noise, we indirectly retrieve it by predicting $\mathbf{x}_0$, thereby restoring $\mathbf{x}_{t-1}$. The reverse process is formulated as $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\bar{\alpha}_t}}\mathbf{x}_t + \sqrt{1 - \bar{\alpha}_t}\mathbf{x}_\theta(\mathbf{x}_t, t)$, where $\mathbf{x}_\theta$ is the network’s prediction of $\mathbf{x}_0$ given $\mathbf{x}_t$, and θ represents the network parameters, typically using a U-Net architecture.

To train the network that predicts $\mathbf{x}_0$, we use the following loss function:

$$\mathcal{L}_{\mathbf{x}_0} = \mathcal{E}_{t \sim [1, T], \mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(0, I)} \|\mathbf{x}_0 - \mathbf{x}_\theta(\mathbf{x}_t, t)\|_2^2. \quad (22)$$

By minimizing the difference between the network’s predicted data and the original data, we obtain a network that can be used for denoising.

During the generation phase, we sample noise from a standard Gaussian distribution and use the trained network to perform denoising to generate a sample close to the true data distribution. Figure S5 illustrates the complete process of obtaining target data from Gaussian noise through 50 steps of DDPM sampling.

4.2 Microstructure representation

We represent all microstructures using voxels; that is, each microstructure is represented as an $n \times n \times n$ binary matrix. Considering that our microstructures exhibit cubic symmetry, during network training, we only consider the top-left $\frac{1}{8}$ of the structure as input, as shown in Figure S4. Furthermore, due to the symmetry of the structures, we utilize cubic symmetric noise in both the forward and reverse diffusion processes.

4.3 Conditions

The generative process of unconditional diffusion models is inherently uncontrollable, resulting in microstructures with highly stochastic properties. This randomness prevents fine-grained manipulation of microstructural attributes during generation and hinders the effective expansion of dataset property coverage. To address this limitation, we propose a conditional diffusion model conditioned on elastic tensors, which achieves precise control over the generation of microstructures with specified attributes, thereby significantly enhancing the efficiency of dataset synthesis. Additionally, to ensure that the net-

work adheres to specified boundary masks during generation, we also incorporate the microstructure’s masks as one of the conditions.

Elastic tensor conditions Since we are only considering microstructures with cubic symmetry, the elastic tensor $\mathbf{C}$ for these structures can be fully defined by three independent components: C_{1111} , C_{1122} , and C_{1212} . Therefore, during the specified elastic tensor generation, we only need to use these three components as conditions. We use Learnable Sinusoidal Embedding (LSE) [19] to encode elastic tensor conditions and employ classifier-free guidance [20] to incorporate these conditions into the network.

Our implementation of LSE is as follows:

$$PE_{(pos, 2i)} = \sin(pos \cdot w_i \cdot 2\pi), PE_{(pos, 2i+1)} = \cos(pos \cdot w_i \cdot 2\pi), \quad (23)$$

where w_i is a learnable parameter initialized as:

$$w_i = \frac{1}{10000^{2i/d}}. \quad (24)$$

We normalize the C_{1111} , C_{1122} , and C_{1212} components before embedding, encode them separately using LSE, and sum the three encodings as the final elastic tensor representation. The encoded elastic

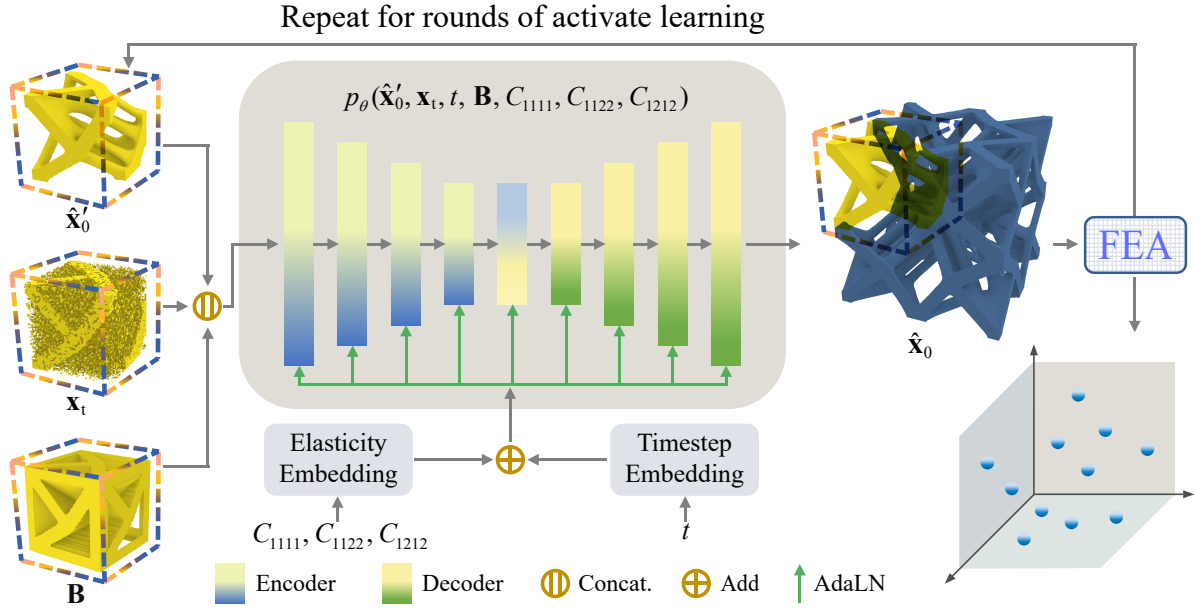


Figure S4: **Network architecture and workflow of the active learning process.** The active learning (AL) framework integrates a denoising U-Net (U-shaped convolutional neural network) with finite-element analysis (FEA) for microstructure generation and evaluation. Due to cubic symmetry, all microstructures are represented by their top-left 1/8 subdomain. The network incorporates elasticity embeddings (based on independent components C_{1111} , C_{1122} , C_{1212} of the elasticity tensor $\mathbf{C}$) and timestep embedding for the diffusion step t , fused via concatenation, addition, and adaptive layer normalization (AdaLN). The encoder-decoder architecture maps the noisy input $\mathbf{x}_t$ to the current denoised prediction $\hat{\mathbf{x}}_0$, while $\hat{\mathbf{x}}'_0$ denotes the denoised prediction from the previous iteration. Boundary conditions are denoted by $\mathbf{B}$. FEA evaluates mechanical responses, and the model is iteratively refined through multiple rounds of active learning. The blue-yellow-green gradient illustrates the encoder-to-decoder transition from noisy input to reconstructed output.

tensor is then added to the encoding of time, and finally, adaptive layer normalization (AdaLN) [21] is applied to incorporate this encoding into every layer of the network, as shown in Figure S4.

Boundary conditions We first encode the boundary conditions and then append them as a new channel to the input matrix. The specific encoding method is as follows: assuming the boundary input is B , we project and stretch the image at each face of the boundary in the direction perpendicular to that face. For example, for the boundary on the x-y plane, we project the boundary pattern along the z-axis. After performing this operation for all three faces, we obtain the boundary encoding $\mathbf{B}$, as shown in Figure S4.

4.4 Self-conditioning

Self-conditioning [22] is a method to enhance the generation quality of diffusion models. The main idea is to use the content generated by the network in the previous steps as a condition for subsequent generation. This practice leverages the model’s conditional generation capability, enabling it to produce outputs that more closely match the target. To implement self-conditioning, during the sampling process, we use a slightly modified denoising function $\mathbf{x}_\theta(\mathbf{x}_t, \hat{\mathbf{x}}'_0, t)$, where $\hat{\mathbf{x}}'_0$ is the result from the previous denoising step.

According to [22], during training, we set $\hat{\mathbf{x}}'_0$ to zero with a 50% probability, and to $\mathbf{x}_\theta(\mathbf{x}_t, 0, t)$ with a 50% probability.

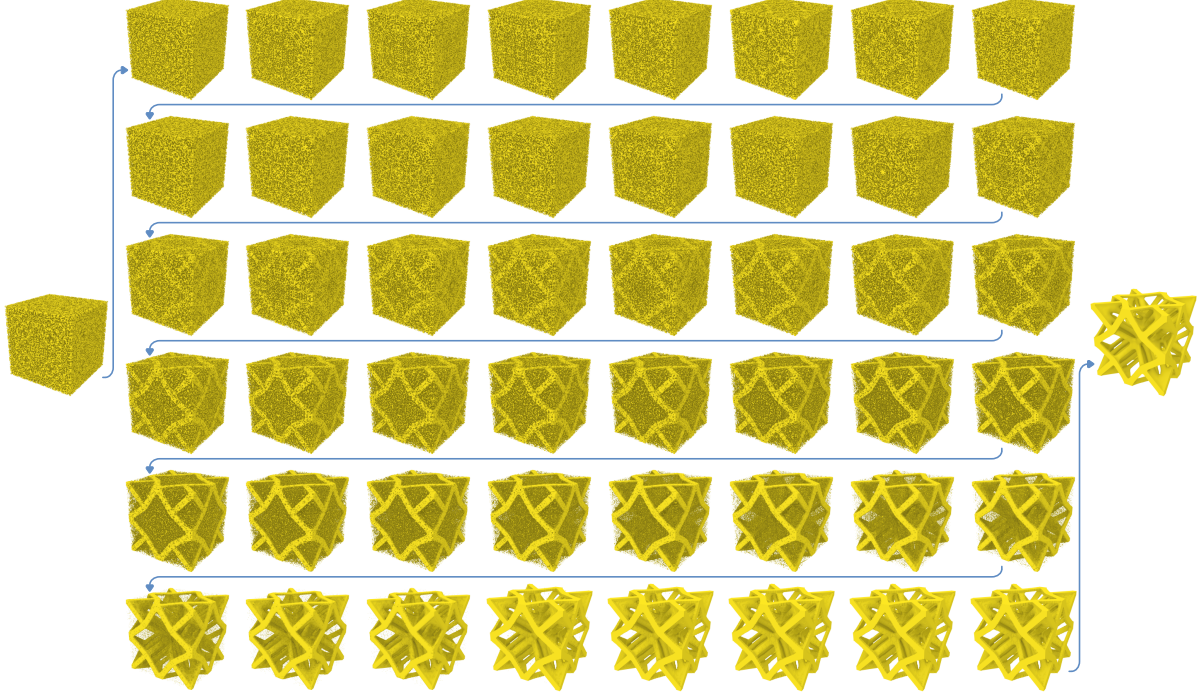


Figure S5: Complete process for generating microstructures from noise using 50-step DDPM sampling.

4.5 Network architecture

The U-Net architecture [23] consists of an encoder and a decoder, each comprising five stages with each stage constructed as a ResBlock. We have incorporated an attention mechanism within the ResBlocks to enhance the network’s capabilities, setting the feature map’s attention resolution to 4 and 8 (Figure S4). During training, we use a total of 1000 diffusion steps and adopt a linear noise schedule. During the sampling phase, we employ 50 steps of DDPM sampling (Figure S5).

4.6 Training details

Incorporating all the conditions mentioned above, we define the denoising function as $\mathbf{x}_\theta(\mathbf{x}_t, \hat{\mathbf{x}}'_0, t, \mathbf{B}, C_{1111}, C_{1122}, C_{1212})$ and train it using the following loss function:

$$\mathcal{L}_{\mathbf{x}_0} = \mathbb{E}_{t \sim [1, T], \mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(0, I)} \|\mathbf{x}_0 - \mathbf{x}_\theta(\mathbf{x}_t, \hat{\mathbf{x}}'_0, t, \mathbf{B}, C_{1111}, C_{1122}, C_{1212})\|_2^2. \quad (25)$$

The training and sampling algorithms we ultimately used are shown in Algorithms 1 and 2. We utilize the AdamW optimizer [24] to update network parameters. For all networks used in this study, we set the hyperparameters as follows: a learning rate of 10^{-4} , a batch size of 120, and a training duration of 510 epochs.

Algorithm 1 Diffusion model training with prediction of x_0

Require: Initial data distribution $q(\mathbf{x}_0)$; number of diffusion steps T ; noise schedule β_t for $t = 1, 2, \dots, T$;

Ensure: Trained model parameters θ ;

- 1: Initialize the model parameters θ randomly;
- 2: **repeat**
- 3: Sample $\mathbf{x}_0 \sim q(\mathbf{x}_0)$, initial data point with elastic tensor $C_{1111}, C_{1122}, C_{1212}$;
- 4: Sample $\epsilon \sim \mathcal{N}(0, I)$, cubic symmetric noise from the standard normal distribution;
- 5: Sample $t \sim \text{uniform}(\{1, \dots, T\})$;
- 6: Calculate the boundary condition encoding $\mathbf{B}$ based on $\mathbf{x}_0$;
- 7: # Unconditional training
- 8: **if** $\text{uniform}(0, 1) > 0.8$ **then**
- 9: $C_{1111} = -1, C_{1122} = -1, C_{1212} = -1$;
- 10: **end if**
- 11: # Self-conditioning
- 12: $\hat{\mathbf{x}}'_0 = 0$;
- 13: **if** $\text{uniform}(0, 1) > 0.5$ **then**
- 14: $\hat{\mathbf{x}}'_0 = \mathbf{x}_\theta(\mathbf{x}_t, 0, t, \mathbf{B}, C_{1111}, C_{1122}, C_{1212})$;
- 15: **end if**
- 16: Compute $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon$, where $\bar{\alpha}_t = \prod_{s=1}^t (1 - \beta_s)$;
- 17: Compute $\hat{\mathbf{x}}_0 = \mathbf{x}_\theta(\mathbf{x}_t, \hat{\mathbf{x}}'_0, t, \mathbf{B}, C_{1111}, C_{1122}, C_{1212})$, the model’s prediction of the original data $\mathbf{x}_0$;
- 18: Update the model parameters θ using the loss function:
- 19:
$$\mathcal{L}_{\mathbf{x}_0} = \mathbb{E}_{t \sim [1, T], \mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(0, I)} \|\mathbf{x}_0 - \hat{\mathbf{x}}_0\|_2^2;$$

20: **until** converged

21: **return** Trained model parameters θ ;

Algorithm 2 Diffusion model inference with prediction of x_0

Require: Trained model parameters θ ; number of diffusion steps T ; noise schedule β_t for $t = 1, 2, \dots, T$; boundary condition encoding $\mathbf{B}$; target elastic tensor C_{1111} , C_{1122} , C_{1212} ; guidance scale w ;

Ensure: Generated sample $\mathbf{x}'_0$;

- 1: Initialize $\mathbf{x}_T \sim \mathcal{N}(0, I)$, starting from pure cubic symmetric noise;
 - 2: $\hat{\mathbf{x}}'_0 = 0$, initialize the $\mathbf{x}_0$ from the previous step prediction required for self-conditioning to 0;
 - 3: **for** $t = T$ down to 1 **do**
 - 4: Compute $\mathbf{x}_0^{start} = \mathbf{x}_\theta(\mathbf{x}_t, \hat{\mathbf{x}}'_0, t, \mathbf{B}, C_{1111}, C_{1122}, C_{1212})$, the $\mathbf{x}_0$ predicted by the model under the specified elastic tensor conditions C_{1111} , C_{1122} , C_{1212} ;
 - 5: Compute $\mathbf{x}_0^{null} = \mathbf{x}_\theta(\mathbf{x}_t, \hat{\mathbf{x}}'_0, t, \mathbf{B}, -1, -1, -1)$, the $\mathbf{x}_0$ predicted by the model under null elastic tensor conditions, which means all three conditions are set to -1;
 - 6: Compute $\hat{\mathbf{x}}_0 = (1 + w) \cdot \mathbf{x}_0^{start} - w \cdot \mathbf{x}_0^{null}$, the linear weighted estimate of $\mathbf{x}_0$ in classifier-free guidance;
 - 7: $\hat{\mathbf{x}}'_0 = \hat{\mathbf{x}}_0$, update $\hat{\mathbf{x}}'_0$ with the $\mathbf{x}_0$ predicted in the current step;
 - 8: Compute $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \mathbf{x}_t + \sqrt{1 - \bar{\alpha}_t} \hat{\mathbf{x}}_0 + \sigma_t \epsilon$, where $\bar{\alpha}_t = \prod_{s=1}^t (1 - \beta_s)$ and $\epsilon \sim \mathcal{N}(0, I)$;
 - 9: **end for**
 - 10: **return** $\mathbf{x}'_0 = \mathbf{x}_{t=0}$ as the generated sample;
-

4.7 Active learning

To enhance the capabilities of our network to meet the demands of constructing a large-scale microstructure dataset, we employ an active learning strategy for iterative network enhancement. The core steps involve using the trained original network to perform large-scale conditional generation, producing a substantial amount of data. This generated data is then processed and added to the training set, and a new network is trained. The newly trained network maintains the generative capability of the original while typically surpassing it in the initial rounds of iteration. The entire active learning process is shown in Algorithm 3.

Algorithm 3 Active learning for iterative network enhancement

Require: Initial trained network net_0 ; initial training dataset D_0 ; number of iterations I ; batch size BS ;

Ensure: Enhanced network net_I ;

- 1: Initialize the current network $net \leftarrow net_0$ and training dataset $D \leftarrow D_0$;
 - 2: **for** $i = 1$ to I **do**
 - 3: Use net to generate microstructures under specified elastic tensors and boundary masks, producing a batch of new data D_{new} of size BS ;
 - 4: Process D_{new} to ensure quality and consistency;
 - 5: Augment the training dataset: $D \leftarrow D \cup D_{new}$;
 - 6: Train a new network net' on the augmented dataset D ;
 - 7: Update the current network: $net \leftarrow net'$;
 - 8: **end for**
 - 9: **return** The final enhanced network net_I ;
-

In the active learning framework, to sample microstructures from the network in a diverse manner, we leverage the Signed Distance Function (SDF) to obtain target elasticity tensors for sampling.

4.7.1 Signed Distance Function

The SDF is a common tool for processing point clouds and is typically used to represent the “external boundary surface” of a point cloud. For a point $\mathbf{p}$ within the point cloud, its SDF value is denoted as

$\text{SDF}(\mathbf{p}) = d(\mathbf{p}, P)$, where $d(\mathbf{p}, P)$ is the shortest Euclidean distance from point $\mathbf{p}$ to the surface P of the point cloud. The SDF is defined as follows:

$$\begin{cases} \text{SDF}(\mathbf{p}) < 0, & \text{(Inside)} \\ \text{SDF}(\mathbf{p}) = 0, & \text{(Boundary)} \\ \text{SDF}(\mathbf{p}) > 0, & \text{(Outside)} \end{cases} \quad (26)$$

The terms “inside” and “outside” are defined relative to the surface of the point cloud, which is assumed to be a closed surface. We define the side containing the point cloud as the interior of the surface, and the opposite side as the exterior. According to this definition, regions where the SDF value is negative correspond to the interior of the point cloud surface (referred to as the interior of the SDF), regions with positive SDF values correspond to the exterior, and points with zero SDF lie exactly on the surface.

We utilize the SDF to conveniently delineate the range of the elastic tensor space covered by the dataset. This enables efficient and structured sampling across the elastic tensor space.

4.7.2 Microstructure Generation Process

Given a dataset and the corresponding trained network, we first compute SDF values at each node of a Cartesian grid that spans the property space of the training dataset. Next, we set the SDF values to negative in a small neighborhood around all nodes where the original SDF is already less than zero. This expansion ensures that the sampling region is not strictly confined to the coverage of the original training data, thereby promoting diversity. Finally, we perform sampling exclusively in regions where the modified SDF is negative to obtain the target elastic tensors required for generation.

These sampled elastic tensors, together with the encoding of the target boundary condition, are provided as conditional inputs to the network. Microstructures are then generated using 50-step DDPM sampling.

4.7.3 Post-processing of Generated Data

For the microstructures generated during the active learning loop, we apply the connected component labeling algorithm described in Section 2.3 to filter out any structures that are not bicontinuous. Additionally, we compute the physical properties for each valid microstructure. The resulting dataset—comprising the filtered microstructures and their corresponding physical properties—is then merged with the current training set to form the updated training dataset for the next iteration of model training.

5 Final dataset statistics

Detailed results corresponding to Figure 3 are summarized in Supplementary Tables S3–S5.

Table S3: Statistics on the properties of microstructures in the four datasets. Microstructural parameters are abbreviated as MSPs. Max, min, and avg represent the maximum value, minimal value, and average value, respectively. V is the volume fraction, ν represents Poisson’s ratio, and S/V represents surface-to-volume ratio. Source data are provided as a Source Data file.

MSPs	Mask 1 (106445)			Mask 2 (142980)			Mask 3 (75350)			Mask 4 (79580)		
	max	min	avg	max	min	avg	max	min	avg	max	min	avg
C_{1111}	660176	7046	230188	461504	17077	223097	554552	7547	242794	692873	18470	322667
C_{1122}	198040	-15558	50570	166562	-4551	31618	146217	-2473	72059	231532	3145	98445
C_{1212}	183038	4563	33009	172420	280	33456	162684	3452	65598	180703	7130	76277
$1 - V$	0.94	0.17	0.55	0.96	0.19	0.56	0.96	0.14	0.56	0.93	0.21	0.50
ν	0.45	-0.20	0.18	0.41	-0.05	0.24	0.44	-0.04	0.24	0.40	0.04	0.24
S/V	0.93	0.05	0.30	0.84	0.06	0.23	1.00	0.05	0.22	0.78	0.08	0.23

Table S4: Counts and percentages of anisotropic microstructures grouped by the ratios K/K_V , G/G_V and E/E_V (relative to the Voigt upper bounds) across the four datasets. Source data are provided as a Source Data file.

MSPs	Mask 1 (93456)			Mask 2 (133420)			Mask 3 (67250)			Mask 4 (74006)		
	< 20%	20%–40%	> 40%	< 20%	20%–40%	> 40%	< 20%	20%–40%	> 40%	< 20%	20%–40%	> 40%
K/K_V	33959	33024	26473	12772	114531	6117	4329	51395	11526	3363	34831	35812
	36.3%	35.4%	28.3%	9.6%	85.8%	4.6%	6.4%	76.5%	17.1%	4.5%	47.1%	48.4%
G/G_V	9112	49604	34740	34833	50963	47624	11589	24283	31378	7530	33733	32743
	9.8%	53.0%	37.2%	26.1%	38.2%	35.7%	17.2%	36.1%	46.7%	10.2%	45.6%	44.2%
E/E_V	14480	38519	40457	9145	58486	65789	5370	16065	45815	3588	15015	55403
	15.5%	41.2%	43.3%	6.9%	43.8%	49.3%	8.00%	23.9%	68.1%	4.9%	20.2%	74.9%

Table S5: Counts and percentages of isotropic microstructures grouped by K/K_{HS} , G/G_{HS} , E/E_{HS} (relative to the Hashin–Shtrikman upper bounds) across the four datasets. Source data are provided as a Source Data file.

MSPs	Mask 1 (12989)			Mask 2 (9560)			Mask 3 (8100)			Mask 4 (5574)		
	< 40%	20%–40%	> 70%	< 40%	20%–40%	> 70%	< 40%	20%–40%	> 70%	< 40%	20%–40%	> 70%
K/K_{HS}	6936	2671	3382	981	7536	1043	600	3620	3880	288	3147	2139
	53.4%	20.6%	26.0%	10.3%	78.8%	10.9%	7.4%	44.7%	47.9%	5.2%	56.4%	38.4%
G/G_{HS}	947	10352	1690	648	8156	756	609	3617	3874	244	4152	1178
	7.3%	79.7%	13.0%	6.8%	85.3%	7.9%	7.5%	44.7%	47.8%	4.4%	74.5%	21.1%
E/E_{HS}	1814	9287	1888	749	8043	768	575	3654	3871	168	4179	1227
	14.0%	71.5%	14.5%	7.8%	84.2%	8.0%	7.1%	45.1%	47.8%	3.0%	75.0%	22.0%

6 Multifunctional bicontinuous multiscale design

6.1 Femoral implants and lumbar interbody fusion cage design

Effective Young’s modulus To ensure mechanical compatibility between the implant and host bone, we define the effective Young’s modulus E_{eff} of a microstructured macro-cube (compact bone implant: $1 \text{ cm} \times 1 \text{ cm} \times 3 \text{ cm}$, cancellous bone implant: $2 \text{ cm} \times 2.8 \text{ cm} \times 1.6 \text{ cm}$) under uniaxial loading. Specifically, consider a rectangular domain Ω subjected to a uniformly distributed surface traction F on its top surface Γ_{top} , while the bottom surface is fixed. Let u_z be the vertical displacement field and L be the height of the domain. The effective Young’s modulus is defined as

$$E_{\text{eff}} = \frac{FL}{\bar{u}_z}, \quad (27)$$

where $\bar{u}_z = \frac{1}{|\Gamma_{\text{top}}|} \int_{\Gamma_{\text{top}}} u_z(\mathbf{x}) dS$. In the finite element discretization, assuming a unit total force $F = 1$ equally distributed over the N nodes on Γ_{top} , this becomes

$$E_{\text{eff}} = \frac{L}{\frac{1}{N} \sum_{i=1}^N U_i}, \quad (28)$$

where U_i denotes the vertical displacement at the i -th node on the loading surface.

Multiscale optimization is currently divided into two parts: the first phase screens the data that meets the requirements, and the second phase performs gradient optimization on this dataset.

Data filtering We first filter the data from the third dataset that satisfies the following criteria from all the data sets: $d_{\min} - d_e \leq 0$ and $p_{\min} \leq p_e \leq p_{\max}$. $d_{\min}$ represents the minimum required pore size of the implant, and d_e denotes the porosity of the e -th unit cell. $p_{\max}$ and $p_{\min}$ refer to the maximum and minimum porosity thresholds, respectively, and p_e is the porosity of the e -th unit cell. To promote cell growth and material exchange, we select microstructural units from the database with an average pore size exceeding $26 \mu\text{m}$ (specifically calculated as $1 \text{ cm} \div 3 \div 128 \approx 0.0026 \text{ cm} = 26 \mu\text{m}$, where 1 cm represents the macroscopic size of the compact bone implant and 128 represents the microstructure resolution) and a porosity ranging from 0.2 to 0.85 during the design process.

Gradient-based optimization The optimization model for femoral implants and lumbar interbody fusion cages is formulated as follows:

$$\begin{aligned} \min_{\mathbf{C}} \quad & f(\mathbf{C}) = \frac{|E_{\text{eff}}(\mathbf{C}) - E_{\text{target}}|}{E_{\text{target}}} \\ \text{s.t.} \quad & \mathbf{K}(\mathbf{C})\mathbf{U} = \mathbf{F}, \\ & \text{SDF}(\mathbf{C}_e) \leq 0. \end{aligned} \quad (29)$$

Here, $\mathbf{C} = \{\mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_N\}$ is the elastic tensor of macroelement. The total number of macroelements are denoted as N . E_{target} denotes the target Young's modulus of bone tissue. $\mathbf{K}(\mathbf{C})$ is the stiffness derived from the assembly from the elastic tensor of the macroelement. $\mathbf{U}$ and $\mathbf{F}$ are the displacement and the external force, respectively. The inequality constraint $\text{SDF}(\mathbf{C}_e \leq 0)$ [25, 4] is used to ensure that $\mathbf{C}_e$ is within the feasible range of the dataset.

In the multiscale design of rabbit femoral implants, titanium is selected as the base material, with the objective of minimizing the relative stiffness mismatch between the implant and the target bone to achieve mechanical compatibility. This study focuses on compact bone implants for the femoral shaft and cancellous bone implants for the femoral head. In the compact bone design domain, the structure consists of $3 \times 3 \times 9$ units, with a target Young's modulus of 5000 MPa and a Poisson's ratio of 0.3. The cancellous bone design domain consists of $5 \times 7 \times 4$ units, with a Young's modulus of approximately 2500 MPa and a Poisson's ratio of 0.3. The optimization problem is solved using MMA, as mentioned in section 3.1. The optimization process terminates when the number of iterations reaches 50 or when the design variable change between two consecutive iterations is less than 0.001.

Then, the closest matching microstructure is identified by calculating the distance to the predefined dataset, thereby determining the final microstructure for each design unit. Based on these matching indices, the corresponding microstructures are retrieved and assembled into the complete structure. Finally, the designed implant structure is intersected with the femoral implantation region to generate the final multiscale implant.

The optimization objective of the lumbar interbody fusion cage is similar to that of the femoral implant. However, we select microstructures with negative Poisson's ratios for the fusion cage design. The design domain is divided into $11 \times 8 \times 3$ units. The total computation time for the entire multiscale design process does not exceed 50 seconds.

6.2 Femoral implants designed using BCC truss, IWP, and spinodal microstructures

Due to the limited property coverage of the BCC truss, IWP, and spinodal structures, we adopt a bottom-up optimization approach [26, 27], with the optimization problem defined as follows:

$$\begin{aligned} \min_{\mathbf{C}} \quad & f(E_{\text{eff}}(\mathbf{C})) = \frac{|E_{\text{eff}}(\mathbf{C}) - E_{\text{target}}|}{E_{\text{target}}} \\ \text{s.t.} \quad & \mathbf{K}(\mathbf{C})\mathbf{U} = \mathbf{F}. \end{aligned} \tag{30}$$

In these three sets of optimization experiments, we employ the same boundary conditions and objectives as outlined in Section 7.1. The total computation time is divided into five components: optimization, matching, assembly, boundary connectivity processing, and solid intersection handling (Supplementary Table S6). To improve connectivity between adjacent units during multiscale structure assembly, we adopt an interpolation algorithm [28]. Notably, resolving connectivity issues accounted for over two-thirds of the total computation time. However, our design intrinsically avoids such issues from the outset, reducing the time for this step to zero.

The experimental results are shown in Figure S6a-c, from which it can be observed that the op-

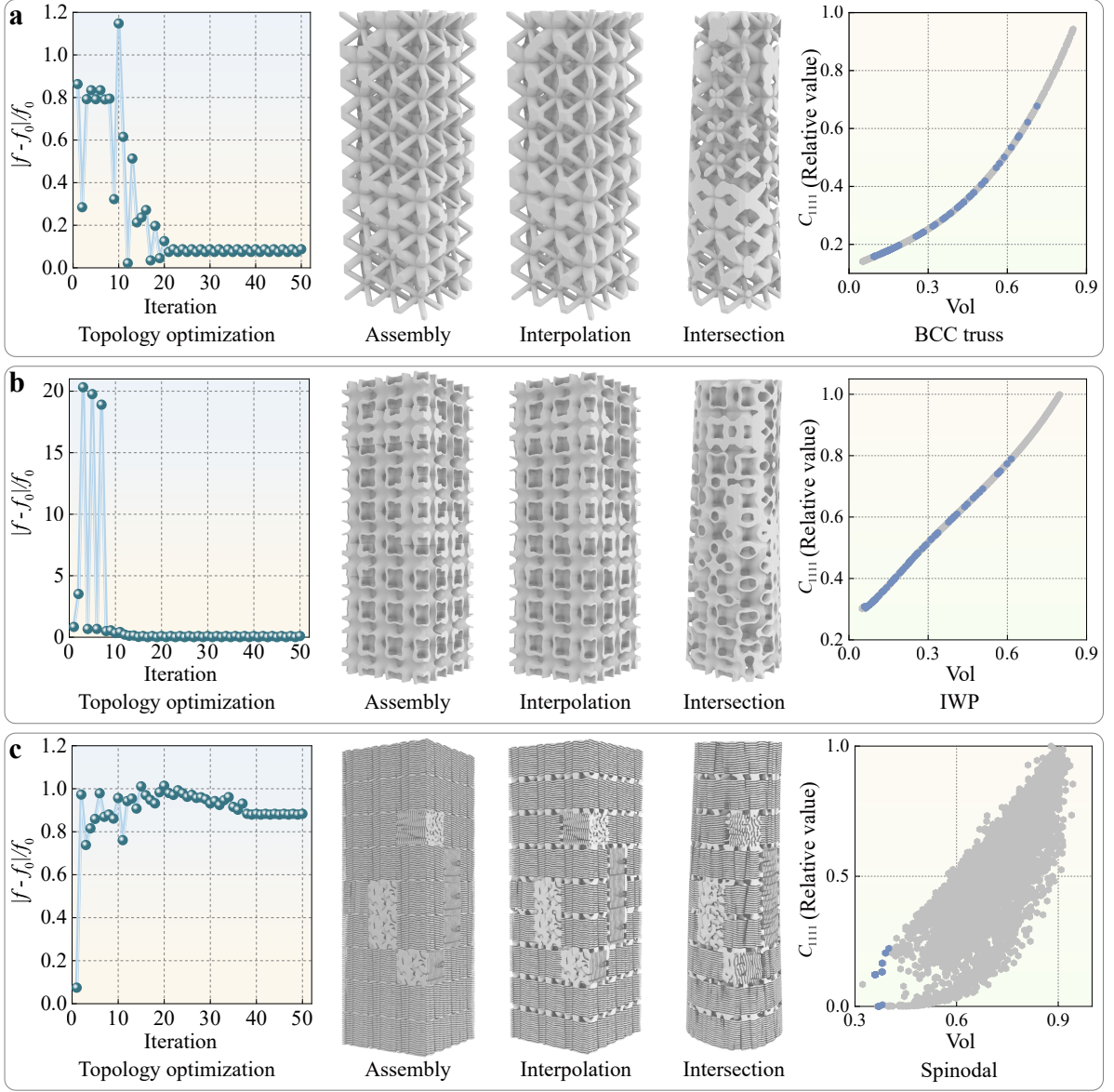


Figure S6: Multiscale optimization results for BCC truss, IWP, and spinodal structures, including iteration curves, assembled structures, interpolation results, intersection results, and the selected microstructure distribution in each dataset. Source data are provided as a Source Data file.

timization processes of the BCC truss and IWP structures gradually stabilized. However, due to the limited range of the spinodal dataset [29], particularly the lack of structures with low volume fractions, oscillations occurred during the optimization process, and the final optimization results exhibit poor matching with Young’s modulus of cancellous bone (Table S7).

Additionally, analysis of volume and S/V reveals that our optimized structure is lighter than the IWP and spinodal structures, with a higher S/V compared to the BCC truss and spinodal structures, demonstrating superior structural characteristics, as shown in Table S7.

Furthermore, in our design, the average pore sizes (APS) of the compact bone structure is 286.64 μm , which falls within the optimal range of 200–400 μm [30, 31]. In contrast, the APS of the other three structures lie outside this ideal range. It is noteworthy that the APS of the designed cancellous bone structure is 299.31 μm , which also falls within the ideal range. In contrast, the other three structures exhibit more significant deviations from this range, resulting in larger discrepancies.

For compact bone, our method favors plate-like structures, while for cancellous bone, it produces truss-like forms that better mimic real bone. Although the optimization depends on initial conditions, our dataset makes the results less sensitive compared to IWP, BCC truss, and spinodal structures.

6.3 Chair design

The optimization model for the chair is as follows:

$$\begin{aligned} \min_{\mathbf{C}} \quad & f_c(\mathbf{C}) = \mathbf{U}^T \mathbf{K}(\mathbf{C}) \mathbf{U} \\ \text{s.t.} \quad & \mathbf{K}(\mathbf{C}) \mathbf{U} = \mathbf{F}, \\ & SDF(\mathbf{C}_e) \leq 0. \end{aligned} \tag{31}$$

Using a multiscale design process analogous to that employed for the femoral implant, we obtained a final chair design with a volume fraction of 0.38. The entire multiscale design process was completed in approximately 1 minute (Table S8).

6.4 Mechanical cloaks

The invisibility cloak is a structure designed to conceal objects in its inside environment [25]. Using the second dataset, we designed a three-dimensional mechanical invisibility cloak within a design space composed of $20 \times 20 \times 20$ units. The cloak consists of concentric rings with an outer radius of 7 units and an inner radius of 3 units, featuring a void in the center (Figure S7 left). Taking the displacement as the design target, the optimization model for mechanical cloaks is as follows:

$$\begin{aligned} \min_{\mathbf{C}} \quad & f_m(\mathbf{U}) = \|(\mathbf{U} - \mathbf{U}_0)\|_2^2 / \|\mathbf{U}_0\|_2^2 \\ \text{s.t.} \quad & \mathbf{K}(\mathbf{C}) \mathbf{U} = \mathbf{F}, \\ & SDF(\mathbf{C}_e) \leq 0. \end{aligned} \tag{32}$$

Here, $\mathbf{U}_0$ denotes the reference displacement field. The objective function represents the displacement distortion, which is quantified as the deviation of the actual displacement field $\mathbf{U}$ from the desired

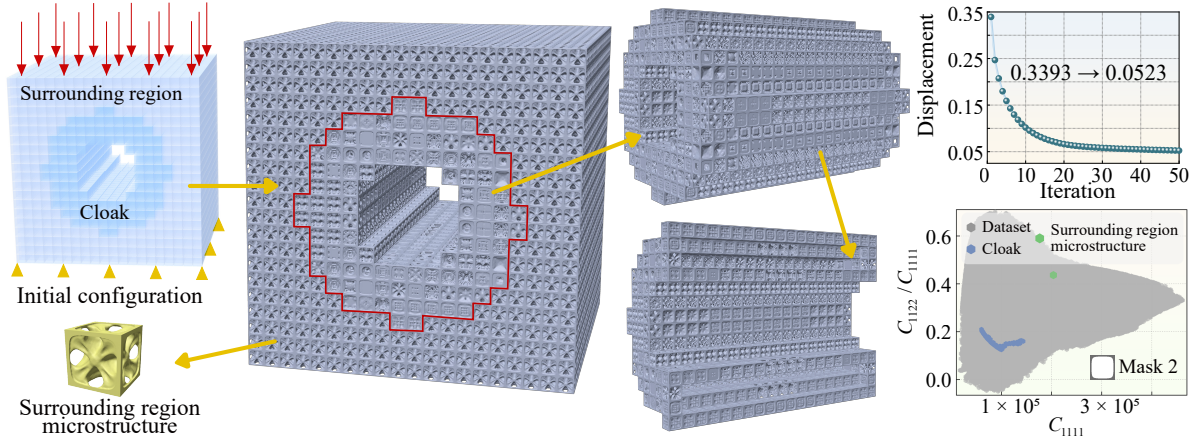


Figure S7: Problem setup and final results of the mechanical cloak ($20 \times 20 \times 20$ units). The right side shows the iteration curve of the optimization process and the property distribution of the microstructures used to fill the cloak. Source data are provided as a Source Data file.

reference field U_0 , normalized by the reference field.

Through the optimized design of the invisibility cloak, we successfully reduce the displacement distortion from 33.13% to 4.85%. During this process, we determine the cloak's property distribution and select matching microstructures from the second dataset. Figure S7 (middle) presents an enlarged view of the assembled cloak structure and its internal layout, while Figure S7 (right) illustrates the optimization process and highlights the locations and property distributions of the selected microstructures within the dataset.

Through the above optimization model, we obtain the multiscale design results for the mechanical invisibility cloak, where the displacement distortion is optimized from 0.3313 to 0.0485. The total duration of the entire multiscale design process does not exceed 5 minutes (Table S6), which is significantly less than the time spent by Yang et al. [4] on their multiscale design of the mechanical invisibility cloak, which takes 37,014.26 seconds, exceeding 10 hours. This remarkable reduction in time highlights the computational efficiency advantages of our optimization method (Table S6).

6.5 Surfing shoes

Surfing shoes, a key piece of equipment for surfing extreme sports, need to exhibit excellent water permeability to minimize the impact of waves. The bicontinuous structures offer a natural advantage in addressing this challenge, as they feature interconnected solid and void channels, promoting efficient water flow inside. In addition, surfing shoes need to provide superior comfort to protect the feet, enhance stability, and prevent fatigue failure during prolonged standing or high-intensity activity. Inspired by the analysis of foot pressure distribution [32, 33, 34] and existing surfing shoe designs [35], this paper proposes a customizable surfing shoe design based on foot pressure distribution by adopting bicontinuous open-cell datasets. By embedding microstructures with different elastic modulus in areas of varying pressure, the design effectively reduces the stress on the metatarsal region for greater comfort.

The whole pipeline and final optimized results are shown in Figure S8. After determining the

initial configuration (Figure S8a), the stress distribution within the sole is obtained from Abaqus simulations (Figure S8b left). By analyzing the displacement-stress relationship, the distribution of the sole's elastic constants is determined. To enhance the comfort and softness of the sole, we select the second dataset, characterized by lower maximum stiffness and a smaller stiffness range, and screen the microstructures based on their property distribution, which significantly reduces the design cycle (Figure S8b right). The final results and computation times are shown in Figure S8c and Table S8.

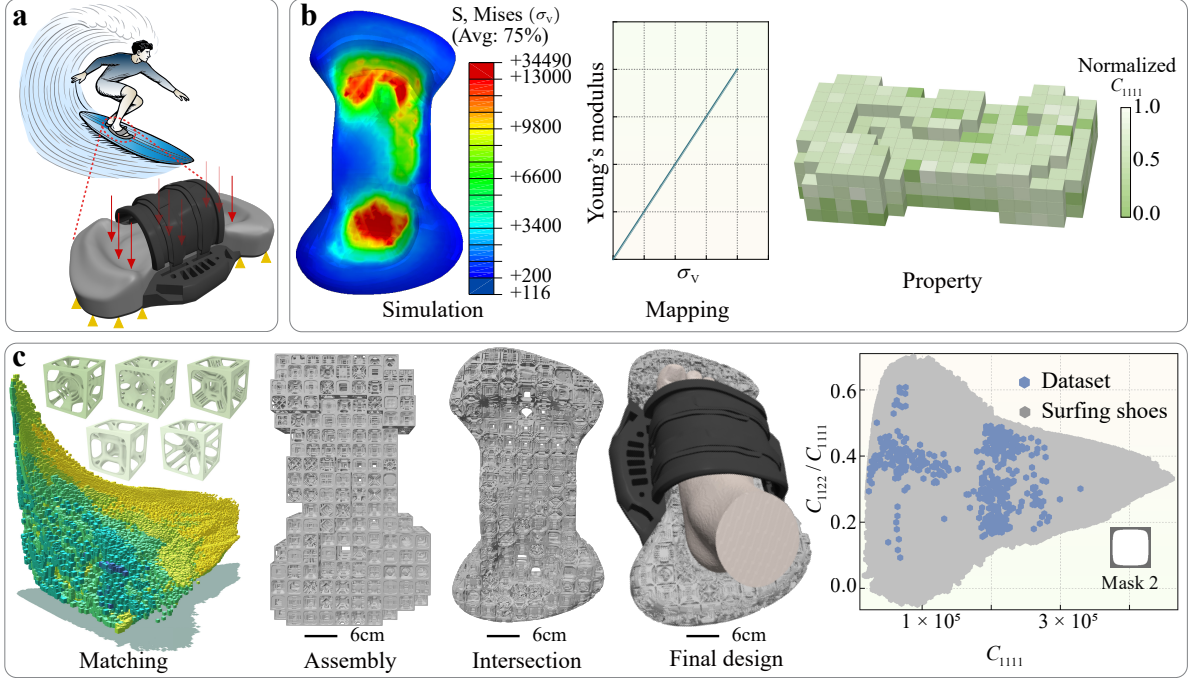


Figure S8: **Surfing shoes multiscale design.** **a** The surfing shoe sole template ($18 \times 10 \times 4$ units) along with applied loads and boundary conditions. **b** The corresponding microstructures are determined in the second dataset through the mapping of equivalent stress distribution and its relationship to Young's modulus. **c** Results of surfing shoe design, examples of microstructures used in the design, and the property distribution of microstructures in the original dataset used for filling multiscale structures. Source data are provided as a Source Data file.

6.6 Broad permeability design

This section presents the results of our investigation into the design of structures with enhanced permeability. The study is conducted in three stages: computational analysis, simulation validation, and experimental testing to evaluate the permeability performance of the multiscale designs.

6.6.1 Computational analysis

In the computational analysis stage, we perform detailed calculations for the permeability and S/V of four datasets (Source Data file with masks 1 to 4) and triply periodic minimal surface (TPMS) structures [36, 37]. The second dataset is selected. The results indicate that, compared to TPMS structures, our designed multiscale structures exhibit a broader range of variations in both permeability and S/V ratio (Figures S9-S12).

Table S6: Time consumption statistics for implant design and mechanical cloak design in the multiscale design process. Here, Opt. denotes optimization, Match. denotes matching, Assem. denotes assembly, Interp. denotes interpolation, and Intersec. denotes intersection. Source data are provided as a Source Data file.

Multiscale design		Unit cell count	Opt. (s)	Match. (s)	Assem. (s)	Interp. (s)	Intersec. (s)	Total (s)	Total (min)
Cancellous bone	Mask 3	$3 \times 3 \times 9 \times 128^3$	2.89	0.11	2.20	—	3.34	8.54	0.14
	IWP		2.56	0.09	2.57	22.97	3.39	31.58	0.53
	BCC truss		2.71	0.09	2.36	23.32	3.31	31.79	0.53
	Spinodal		3.51	1.49	4.39	23.21	3.37	35.97	0.60
Cancellous bone	Mask 3	$5 \times 7 \times 4 \times 128^3$	3.34	0.13	5.18	—	11.46	20.11	0.34
	IWP		3.06	0.10	5.06	55.34	11.85	75.41	1.26
	BCC truss		3.11	0.11	5.52	56.16	10.23	75.13	1.25
	Spinodal		7.22	3.67	8.51	54.89	11.60	85.89	1.43
Mechanical cloak	Mask 2	$20 \times 20 \times 20 \times 128^3$	68.56	0.30	223.20	—	—	292.06	4.87
	Yang et al. [4]		67.18	0.42	235.35	—	37014.26	37317.21	621.95

Table S7: Performance comparison and analysis of compact bone, cancellous bone, and mechanical cloak. Here, APS denotes average pore sizes, Dist. denotes distance. Source data are provided as a Source Data file.

Multiscale design		Unit cell count	Porosity	V	S/V	E (MPa)	Min. Dist.	Max. Dist.	Avg. Dist.	APS (μm)	Disp.
Compact bone	Mask 3	$3 \times 3 \times 9 \times 128^3$	0.6347	0.37	0.67	4968.1	1	48.70	10.93	284.64	—
	IWP		0.6234	0.38	0.70	4624.9	3	29.90	17.81	463.81	—
	BCC truss		0.6380	0.36	0.29	4767.6	1	62.11	22.74	592.17	—
	Spinodal		0.5770	0.42	0.59	5835.8	1	15.65	1.58	41.25	—
Cancellous bone	Mask 3	$5 \times 7 \times 4 \times 128^3$	0.7781	0.22	0.67	2511.3	1	41.12	9.58	299.31	—
	IWP		0.7998	0.20	0.55	2668.8	6	31.18	20.39	637.11	—
	BCC truss		0.7403	0.26	0.27	2377.6	1	61.35	27.68	865.16	—
	Spinodal		0.6773	0.32	0.68	3120.3	1	15.65	1.98	62.03	—
Mechanical cloak	Mask 2	$20 \times 20 \times 20 \times 128^3$	—	—	—	—	—	—	—	—	0.3393→ 0.0523
	Yang et al. [4]		—	—	—	—	—	—	—	—	0.3417→ 0.0581

Table S8: Time consumption statistics for each part in the multiscale design process. Source data are provided as a Source Data file.

Multiscale design	Unit cell count	Opt. (s)	Match. (s)	Assem. (s)	Intersec. (s)	Total (s)	Total (min)
Compact bone	$3 \times 3 \times 9 \times 128^3$	2.89	0.11	2.20	3.34	8.54	0.1423
Cancellous bone	$5 \times 7 \times 4 \times 128^3$	3.34	0.13	5.18	11.46	20.11	0.34
Lumbar interbody fusion cage	$11 \times 8 \times 3 \times 128^3$	7.2	0.03	12.82	26.86	46.91	0.7818
Chair (backrest)	$14 \times 6 \times 2 \times 128^3$	2.02	0.2	13.09	20.56	35.87	0.5978
Chair (seat board)	$10 \times 12 \times 1 \times 128^3$	2.1	0.16	6.9	7.88	17.04	0.2840
Mechanical cloak	$20 \times 20 \times 20 \times 128^3$	68.56	0.3	223.2	—	292.06	4.8677
Surfing shoes	$18 \times 10 \times 4 \times 128^3$	—	0.37	60.16	48.05	108.58	1.8097

6.6.2 Simulation validation

Simulation validation aims to assess the permeability performance and flow streamline distribution of the multiscale designs. The porosity of the structures is fixed at four levels: 0.5, 0.6, 0.7, and 0.8, and corresponding structures are selected from the chosen dataset for further analysis. By comparing the permeability of these structures with Gyroid, Diamond, and IWP structures, five microstructures with high S/V ratios are selected for in-depth investigation. Box plots of porosity versus S/V ratio are generated for these structures in Figures S9-S12a.

Fluid simulation experiments are conducted using COMSOL software. For each design group, the steady-state response of four structures is tested under unidirectional creeping flow conditions. Water is used as the testing fluid, with an inlet positioned at the top of a $4 \times 4 \times 1$ structure and an applied pressure of 500 Pa. The outlet is located at the outer surface of four microstructures at the bottom center, where the pressure is set to 0 Pa. The permeability of each design group is calculated using Darcy's law.

To further validate the effectiveness of the multiscale design, comparisons are made with three classical TPMS structures, Gyroid, Diamond, and IWP, which are known for their high S/V . The results of these comparative experiments are summarized in Figures S9-S12, demonstrating that our designed multiscale structures exhibit a broader range of variation in porosity and S/V ratio than TPMS structures.

6.6.3 Experimental testing

In the experimental testing stage, a specialized experimental setup is designed (Figure S13) to physically measure and validate the permeability differences among various structures. The setup evaluates the permeability performance of different structures by monitoring water flow velocity. It consists of seven key components: two buckets (one for water injection and the other for water collection), a valve for controlling water flow, a base for stability, and three shims used for sample fixation and flow regulation.

The first bucket (bucket 1) supplies water to the system, while the second bucket (bucket 2) collects the outflow. To ensure precise variable control, both buckets are marked with an 80 cm scale on their sides. The valve regulates the water flow, and the base provides structural stability. The first shim has a central square hole with a side length of 7.1 cm, fitting the 7 cm test structures while leaving a 0.1 cm gap for securing the structures with double-sided tape. This setup simulates ideal fluid boundary conditions. Additionally, double-sided tape is applied at the bottom of the test structures to ensure consistent inlet and outlet boundary conditions, creating a tight seal to prevent leakage and reduce experimental error. The second shim features a 6 cm square hole to adjust the outlet position, while the third shim includes eight 0.5 cm diameter holes to maintain pressure balance inside and outside the buckets.

The experimental procedure quantifies the permeability of different structures by measuring the time required for a predetermined volume of water to pass through the system and reach a specified height in the collection bucket. The steps are as follows:

- (1) The test structure is placed in the square hole of the first shim, and the valve is closed.

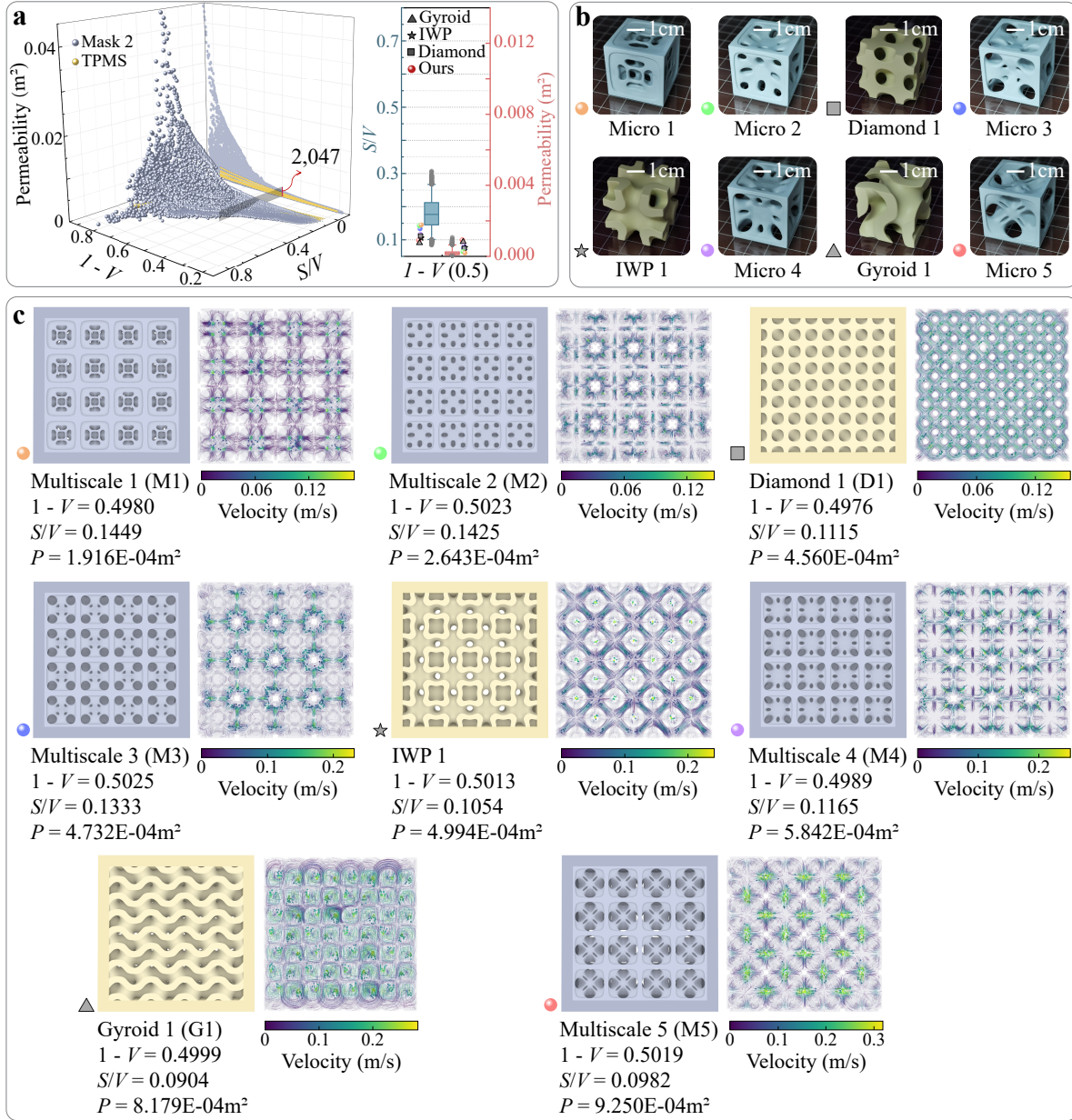


Figure S9: **Permeability test results of the structures at a porosity of 0.5.** **a** The left panel illustrates the relationships among porosity ($1 - V$), S/V , and permeability for all structures in the second dataset and the TPMS dataset. A gray plane marks the data with a porosity of 0.5, totaling 2,047 samples. In the right panel, blue box plots represent the relationship between porosity and S/V , while red box plots depict the correlation between porosity and permeability. Individual points denote test results from different datasets. **b** The 3D-printed samples of the selected microstructures, with a printing size of 3 cm. **c** Multiscale structures and their simulated velocity streamlines.

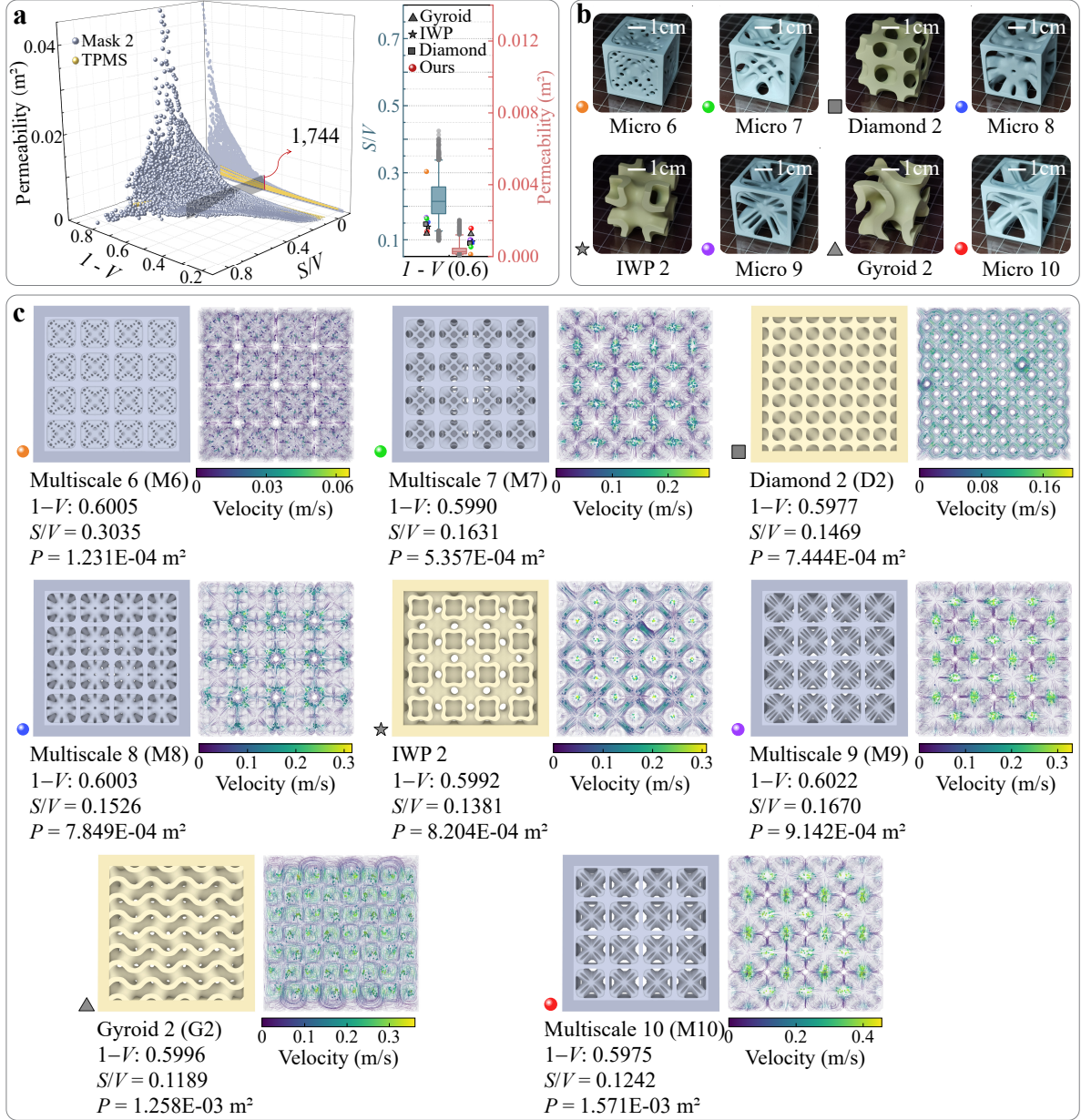


Figure S10: **Permeability test results of the structures at a porosity of 0.6.** **a** The left panel illustrates the relationships among porosity, S/V , and permeability for all structures in the second dataset and the TPMS dataset. A gray plane marks the data with a porosity of 0.6, totaling 1,744 samples. In the right panel, blue box plots represent the relationship between porosity and S/V , while red box plots depict the correlation between porosity and permeability. Individual points denote test results from different datasets. **b** The 3D-printed samples of the selected microstructures, with a printing size of 3 cm. **c** Multiscale structures and their simulated velocity streamlines.

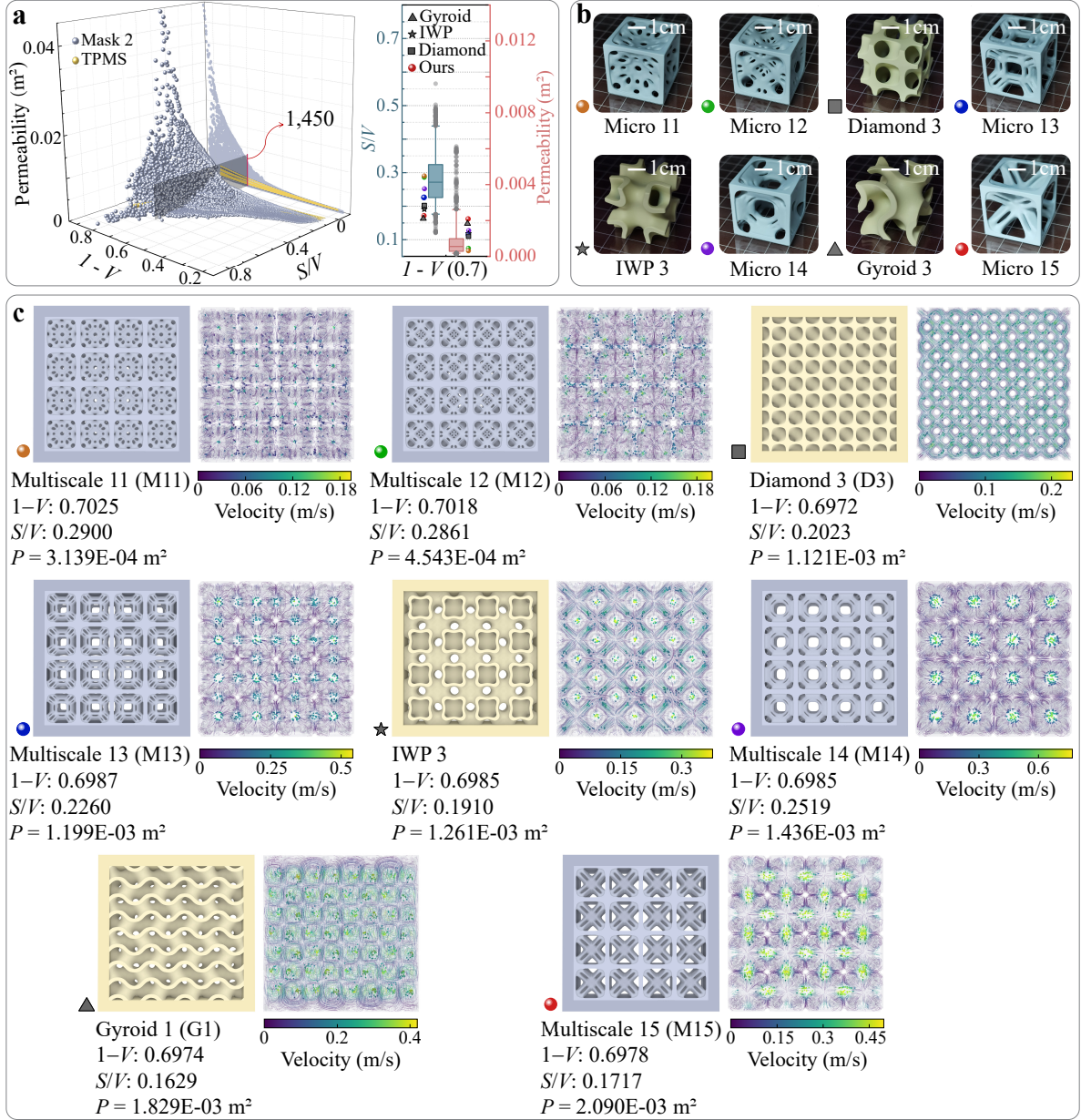


Figure S11: **Permeability test results of the structures at a porosity of 0.7.** **a** The left panel illustrates the relationships among porosity, S/V , and permeability for all structures in the second dataset and the TPMS dataset. A gray plane marks the data with a porosity of 0.7, totaling 1,450 samples. In the right panel, blue box plots represent the relationship between porosity and S/V , while red box plots depict the correlation between porosity and permeability. Individual points denote test results from different datasets. **b** The 3D-printed samples of the selected microstructures, with a printing size of 3 cm. **c** Multiscale structures and their simulated velocity streamlines.

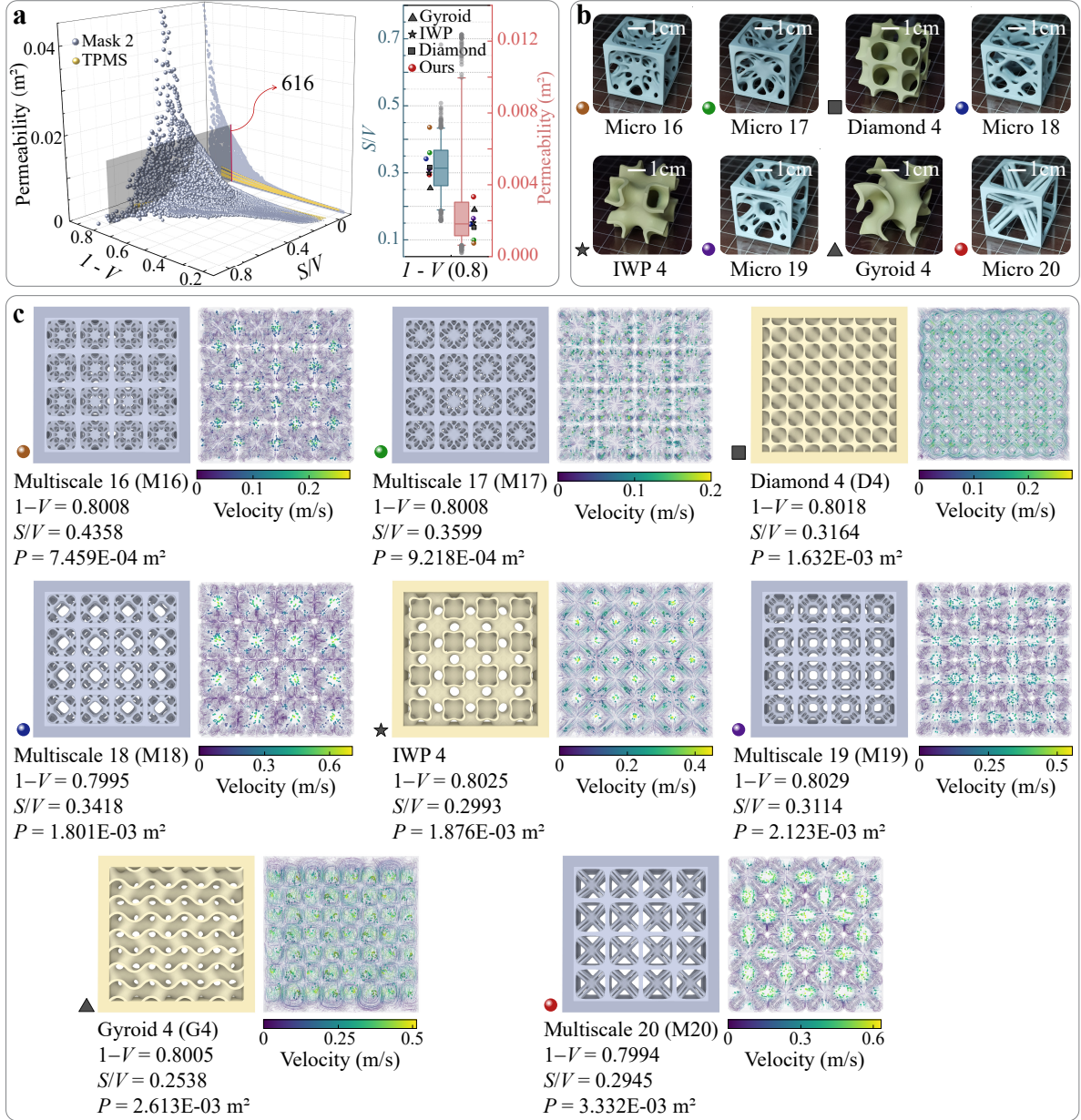


Figure S12: **Permeability test results of the structures at a porosity of 0.8.** **a** The left panel illustrates the relationships among porosity, S/V , and permeability for all structures in the second dataset and the TPMS dataset. A gray plane marks the data with a porosity of 0.8, totaling 616 samples. In the right panel, blue box plots represent the relationship between porosity and S/V , while red box plots depict the correlation between porosity and permeability. Individual points denote test results from different datasets. **b** The 3D-printed samples of the selected microstructures, with a printing size of 3 cm. **c** Multiscale structures and their simulated velocity streamlines.

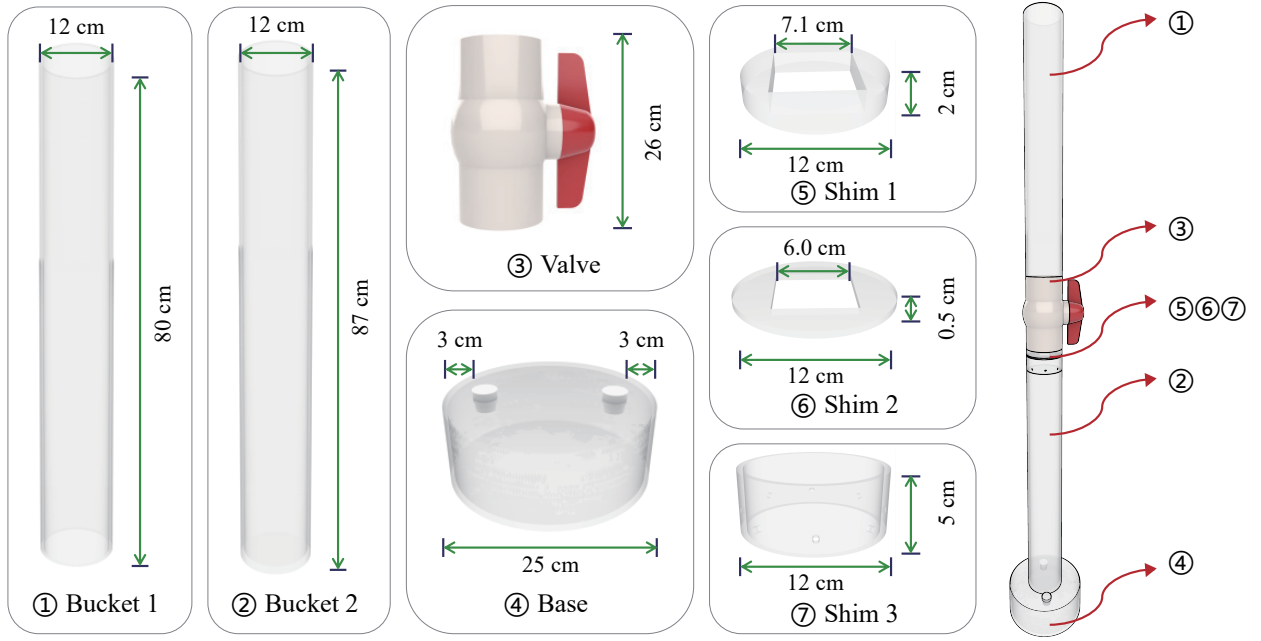


Figure S13: Design of experimental apparatus.

- (2) A fixed volume of water is added to the injection bucket.
- (3) The valve is opened, allowing water to flow through the test structure into the collection bucket.
- (4) The time required for the water level to reach the predefined height is recorded.
- (5) The permeability is calculated based on the recorded time data.

After completing the computational analysis and simulation validation, our multiscale structures demonstrate a broader permeability and S/V range than TPMS structures. To further confirm this, experimental tests are conducted on three multiscale structures with high, medium, and low permeability at a porosity of 0.8. These are compared with Gyroid, Diamond, and IWP structures. Detailed experimental procedures are presented in Video 5. The experimental results indicate a strong correlation between measured water flow velocity and simulated permeability behavior, confirming the validity of our design across different structures. Through systematic computational, simulation, and experimental validation, we effectively demonstrate that the designed multiscale structures possess a broad range of permeability characteristics.

7 Toward a Simplified Theoretical Understanding of Structural Parameters Governing Permeability

To address a theoretical understanding of how structural parameters govern permeability, we proceed in two steps:

- We examined the key influencing factors porosity, pore size, pore shape, and orientation and provided theoretical explanations for their roles. For the Kozeny–Carman (KC) framework [38, 39], it shows porosity is the dominant control, pore size is the next most significant enhancer, and pore shape/tortuosity acts as a secondary suppressor. Orientation mainly governs tensorial anisotropy.
- We model pore-scale permeability using a maximum-flow network surrogate that explicitly encodes connectivity and bottlenecks. The surrogate correlates strongly with the reference permeability (linear $R^2 = 0.801$, Spearman $\rho = 0.948$) and complements the KC framework by capturing connectivity effects that are not resolved by porosity and the surface-to-volume S/V alone.

In porous media theory, porosity is typically the dominant factor, as it defines the fraction of void space available for flow. However, porosity alone is not sufficient: materials with identical porosity can exhibit orders-of-magnitude differences in permeability due to microstructural variations [40]. Larger average pore size generally enhances permeability by creating wider flow channels, while improved connectivity reduces dead-ends and facilitates transport. Conversely, irregular **pore shapes** or unfavorable orientations increase tortuosity, thereby reducing permeability even at high porosity [41].

Thus, these quantities interact in nontrivial ways, and their combined influence on permeability cannot be easily generalized. To gain insight, we proceed under KC-type assumptions (homogenized RVE and laminar/Stokes flow) and first analyze canonical idealized geometries to decouple the effects of porosity, S/V , shape/tortuosity, and orientation, employing theoretical analysis to clarify the underlying mechanisms.

(1) A theoretical perspective

The KC framework provides a compact organizing relation linking permeability k to porosity $\phi = 1 - V$ (where V denotes the solid volume fraction), the surface-to-volume ratio S/V (interfacial area per sample volume), and tortuosity τ . The proportionality constant c (Kozeny constant) subsumes geometric details not captured explicitly.

Step 1. Starting from Poiseuille flow in capillaries and modeling a porous medium as an effective capillary bundle, with microstructures parameterized by the surface-to-volume S/V , and incorporating tortuosity τ into a proportionality constant, the KC relation reads

$$k = \frac{1}{c} \frac{\phi^3}{(1 - \phi)^2} \frac{1}{(S/V)^2} \frac{1}{\tau^2}. \quad (33)$$

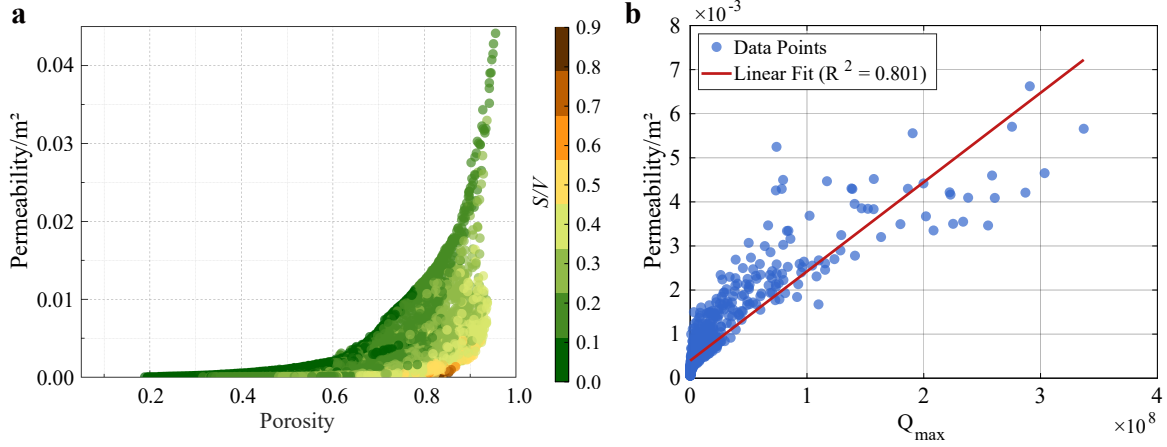


Figure S14: **a** Permeability k versus porosity ϕ ; point color encodes surface-to-volume S/V (colorbar at right). **b** Permeability k versus the graph-based maximum flow $Q_{\max}$, with a least-squares linear fit (red) yielding $R^2 = 0.801$.

Step 2. Take the logarithm of both sides of Eq. (30) simultaneously, we have

$$\ln k = (-\ln c) + 3 \ln \phi - 2 \ln(1 - \phi) - 2 \ln(S/V) - 2 \ln \tau. \quad (34)$$

Define the log-derivative $E_X \equiv \frac{\partial \ln k}{\partial \ln X}$ ($X = \phi, S/V, \tau, d$):

$$E_\phi = 3 + \frac{2\phi}{1-\phi}, \quad E_{S/V} = -2, \quad E_\tau = -2. \quad (35)$$

Using an effective pore size $d \propto 1/(S/V)$ gives $E_d = +2$. Thus, a 1% change in X produces approximately $E_X\%$ change in k . A small perturbation form is

$$\frac{\Delta k}{k} \approx \left(3 + \frac{2\phi}{1-\phi}\right) \frac{\Delta \phi}{\phi} - 2 \frac{\Delta(S/V)}{S/V} - 2 \frac{\Delta \tau}{\tau}, \quad (36)$$

Within the KC framework for scalar k , the log-derivative implies the ranking

$$|E_\phi| = 3 + \frac{2\phi}{1-\phi} > |E_d| = 2 \approx |E_\tau| = 2, \quad (37)$$

where $d \propto 1/(S/V)$. This indicates that porosity is the dominant control, pore size is the next most significant enhancer, and tortuosity acts as a secondary suppressor. Orientation does not enter explicitly in the scalar KC relation but mainly governs tensorial anisotropy. This hierarchy holds within the validity range of the KC framework, but may break down near the high-porosity limit ($\phi \rightarrow 1$).

Step 3. To test the sensitivity analysis implied by the KC framework, we plotted permeability (k) versus porosity (ϕ), with data points color-mapped by the surface-to-volume S/V (Figure S14a). This reveals several key trends:

- **Nonlinear porosity effect:** Permeability increases strongly and nonlinearly with porosity.
- **Role of S/V at fixed ϕ :** For a given porosity, the spread in permeability is modulated by S/V .

Higher S/V (more complex pore geometries with rough surfaces or narrow throats) increases flow resistance and lowers k , while lower S/V (smoother flow paths, larger hydraulic radii) yields higher k .

- **Upper envelope:** The distribution exhibits a distinct upper bound defined by low- S/V samples, representing the theoretical permeability maximum achievable for a given porosity.

To quantitatively compare the global influence of porosity and pore-size proxy on permeability, we apply a binned smoothing procedure [42]. Let $X \in \{\phi, S/V\}$. We partition the range of X into K consecutive bins $\{B_j\}_{j=1}^K$ using equal-count (quantile) edges. For each bin we compute the bin-level median permeability

$$m_j = \text{median}(k \mid X \in B_j). \quad (38)$$

We summarize the total variation in k attributable to X by the amplitude of this median trend,

$$R_X = \max_j m_j - \min_j m_j. \quad (39)$$

Side-by-side R_ϕ and $R_{S/V}$ provide a global, marginal comparison of their influences on k , with the quantitative summary from quantile-binned smoothing ($K = 25$) being:

- $R_{S/V} = 7.88 \times 10^{-4}$;
- $R_\phi = 1.11 \times 10^{-2}$.

This result confirms that porosity (ϕ) is the dominant factor controlling the global variation of permeability (k), and its influence significantly outweighs that of S/V . The negligible fluctuation range for the S/V -smoothed trend indicates that its role within the KC framework is primarily microscopic: it acts as a key modulating factor that determines the specific permeability value at a given porosity, rather than driving its macroscopic variation.

In conclusion, both theoretical and empirical analyses converge to demonstrate that: Porosity is the primary control on permeability, determining its macroscopic scaling behavior, whereas the surface-to-volume S/V acts as a secondary control, constraining the microscopic efficiency attainable within a given pore structure. This conclusion is entirely consistent with the sensitivity ranking ($|E_\phi| > |E_{S/V}|$) derived from the KC equation.

While our quantitative insight in this work is explicitly framed within the KC paradigm, prior studies e.g., Röding et al. (2020)[43] show that a model considering only porosity and specific surface is not a general predictor of permeability. Microstructures sharing ϕ and S/V may still yield widely different k . Motivated by this gap, we next introduce a connectivity-aware maximum-flow surrogate model to complement KC framework.

(2) Modeling Pore-Scale Permeability via a Maximum Flow Network

To explicitly capture connectivity and bottleneck effects that are not resolved by $\{\phi, S/V\}$ alone, we therefore introduce a graph-theoretic maximum-flow surrogate of the pore space. The core mathematical framework is as follows: Given a binarized 3D pore structure matrix $V \in \{0, 1\}^{n_x \times n_y \times n_z}$

(where 0 denotes pore space and 1 denotes solid matrix), the equivalent hydraulic radius R for each pore voxel is first calculated via the Euclidean distance transform (EDT), which assigns to each pore voxel its Euclidean distance to the nearest solid voxel:

$$R(x, y, z) = \min_{(x_0, y_0, z_0): V(x_0, y_0, z_0)=1} \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2}. \quad (40)$$

In other words, (x_0, y_0, z_0) only needs to satisfy $V(x_0, y_0, z_0) = 1$; no additional conditions are required.

Subsequently, a directed graph network $G = (V_G, E_G)$ is constructed, where V_G and E_G denote the node set and the edge set, respectively. The node set V_G comprises all pore voxels along with source and sink nodes $\{s, t\}$. The edge set E_G is defined as

$$E_G = \{(i, j) \mid i, j \text{ are face-adjacent (6-neighbor) pore voxels}\} \cup \{(s, i) \mid i \in \Gamma_{\text{in}}\} \cup \{(j, t) \mid j \in \Gamma_{\text{out}}\}, \quad (41)$$

where Γ_{in} and Γ_{out} represent the sets of pore nodes on two opposite boundary faces of the sample (chosen as inlet and outlet, respectively). The edge capacity function, based on Poiseuille's law, is defined as:

$$c(i, j) = [\min(R(i), R(j))]^4. \quad (42)$$

The prediction of permeability is ultimately transformed into solving an s - t maximum flow problem:

$$\begin{aligned} \max_{\{f_{uv}\}} \quad & Q = \sum_{(s,u) \in E_G} f_{su} \\ \text{s.t.} \quad & \sum_{(u,v) \in E_G} f_{uv} - \sum_{(w,u) \in E_G} f_{wu} = 0, \quad \forall u \in V_G \setminus \{s, t\}; \\ & 0 \leq f_{uv} \leq c(u, v), \quad \forall (u, v) \in E_G; \end{aligned} \quad (43)$$

Denote by Q_{max} the optimal objective value of the above problem, i.e., the maximum feasible net flux from s to t .

Computations on $N = 1000$ randomly selected pore structures show a strong association between the graph-based maximum flow Q_{max} and the reference permeability. A simple linear regression explains $R^2 = 0.801$; Spearman's rank correlation is $\rho = 0.948$, confirming an almost monotonic relationship (Figure S14b). The rank correlation notably exceeds the linear correlation, indicating a nearly monotonic yet mildly nonlinear relationship, consistent with interpreting Q_{max} as a bottleneck-dominated geometric surrogate rather than an exact hydraulic response under a prescribed pressure drop.

Although the surrogate captures key pore-space features through a hydraulic-radius map and global connectivity, it oversimplifies the physics of fluid transport. Permeability arises from viscous dissipation, inertial effects, tortuosity, connectivity, and anisotropy, so even small geometric variations can cause large changes under Stokes flow. Thus, while geometric proxies such as Q_{max} provide structural insight and strong discriminatory power, accurate prediction ultimately requires solving the full pressure-driven flow (e.g., hydraulic-conductance networks or Stokes/Navier-Stokes simulations). These results clarify the scope and limitations of simplified graph-based models and highlight the need

for high-fidelity simulations for quantitative accuracy.

(3) Potential future direction

A promising future direction is hybrid AI–physics approaches, which can link learned features to pore characteristics and capture subtle geometric effects that strongly influence permeability. Such methods, especially when combined with high-fidelity flow simulations, may overcome the limitations of simplified proxies and yield more accurate and interpretable predictions [44, 45]. While beyond the scope of this work, we view this as an important avenue for future research.

8 Printing visualization

To further validate the manufacturability of the designed microstructures and assess their performance at reduced scales, we fabricated a batch of complete structures with dimensions of 3 mm using a photosensitive resin using projection micro-stereolithography (P μ SL) technology on the BMF S130 3D printer. This material was selected for its excellent formability, surface finish, and ability to rapidly produce high-precision features via UV curing.

The printing outcomes are shown in Figure S15, which highlights the morphology and dimensional accuracy of the fabricated microstructures. The structures retain high shape fidelity and structural integrity, even at the reduced size of 3 mm, faithfully reproducing fine design features. These results confirm the robust printability of the microstructures across scales. Moreover, to verify bicontinuity fabrication of multiscale structures, we fabricated multiscale bone implants (Figure S16a-b).

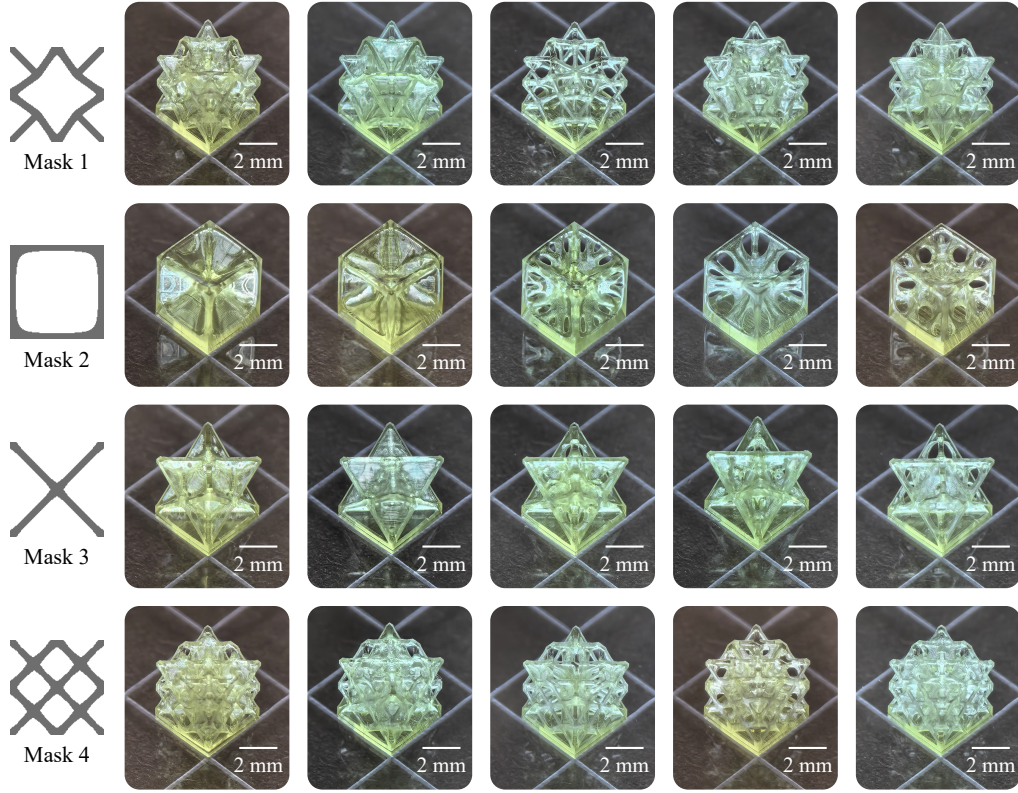


Figure S15: 3D printed samples of microstructures under the four boundary conditions.

We fabricated eight bicontinuous open-cell microstructures in dataset of Mask 2 (01-08) and randomly selected microstructures from dataset [4] (09-16) using SLA printing, and measured their weights. The results are summarized in Figure S17, with the corresponding weight data provided in Table S9. Owing to their bicontinuity, powders or resins can be readily removed from the structures, whereas randomly selected non-bicontinuous structures are substantially heavier than predicted. On average, their weight exceeds that of bicontinuous open-cell structures by more than fiftyfold.

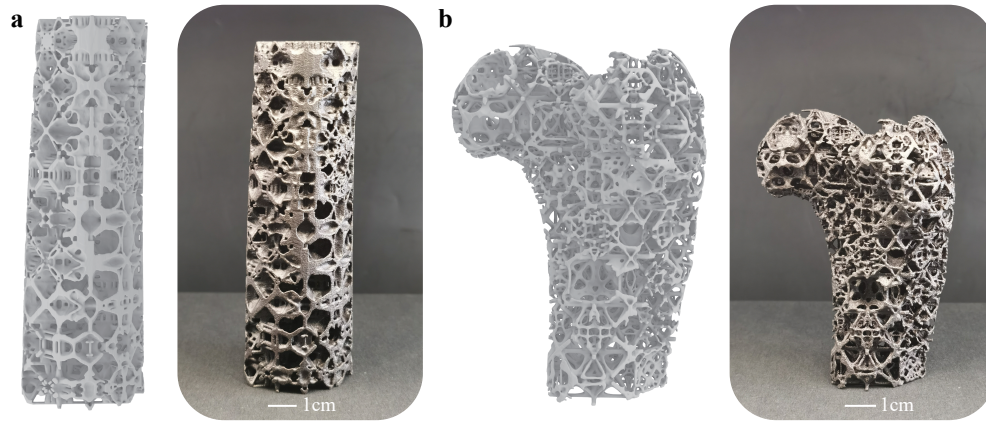


Figure S16: **Optimized results.** **a** Fabricated compact structure. **b** Cancellous bone structure.

Table S9: Calculated and measured weights of resin microstructure samples. Source data are provided as a Source Data file.

Data source	No	Vol/ mm ³	Density/ (g·mm ⁻³)	Calculated mass/g	Measured mass/g	Relative error/g	Average error/g
Mask 2	01	5324.7	1.14	6.0702	6.02	-0.0502	-0.0459
	02	5200.41	1.14	5.9285	5.82	-0.1085	
	03	5271.92	1.14	6.0100	6.11	0.1000	
	04	5273.33	1.14	6.0116	5.92	-0.0916	
	05	5305.04	1.14	6.0477	5.96	-0.0877	
	06	5346.78	1.14	6.0953	6.13	0.0347	
	07	5252.89	1.14	5.9883	5.88	-0.1083	
	08	5277.20	1.14	6.0160	5.96	-0.0560	
Yang et al.[4]	09	5418.10	1.14	6.1766	10.78	4.6034	2.9222
	10	5441.04	1.14	6.2028	8.00	1.7972	
	11	5425.41	1.14	6.1850	9.22	3.0350	
	12	5454.80	1.14	6.2185	6.98	0.7615	
	13	5455.75	1.14	6.2196	11.52	5.3004	
	14	5396.74	1.14	6.1523	6.19	0.0377	
	15	5916.36	1.14	6.7447	10.05	3.3053	
	16	5502.58	1.14	6.2729	10.81	4.5371	



Figure S17: Measured mass of the 16 3D-printed photopolymer resin samples. 01-08: bicontinuous open-cell microstructures. 09-16: randomly selectly microstructures.

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