Electronic Supplementary Material (ESI) for Materials Horizons.

Supporting information

Generative machine learning algorithm for lattice structures with superior mechanical properties

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Computational methods

The 30th-order Bézier curve with a total of 31 control points is used to consider sufficient shape variation, as shown in Fig. 1(a) in the manuscript. The Bézier curve is a parametric curve of t expressed as the following:

$$\boldsymbol{B}(t) = \sum_{i=0}^{30} \left[\binom{30}{i} (1-t)^{30-i} t^i \boldsymbol{P}_i \right], \qquad 0 \le t \le 1 \tag{1}$$

where $\boldsymbol{P}_i$ is ith control point, $\binom{n}{i}$ is the binomial coefficient, and n is the Bézier curve order. Since the elastic behavior of a lattice structure is a linear response, predicting elastic stiffness is a scale-free problem. Therefore, we normalize all lengths with a lattice constant a to get a generalized design. The x coordinates of the first and last control points are fixed at 0 and $\sqrt{3}a/2$ to fix the length of the beam element, i.e., a total of 60 independent parameters are used for modeling the geometry. Then, the curve is revolved with respect to the x-axis and a three-dimensional beam element is obtained (Fig. 1(b)). To avoid numerical errors in simulation or resolution issues in manufacturing due to excessively small cross sections, the minimum radius of the Bézier curve is set to $0.01a$.

Finite element analysis is used to predict relative Young's modulus and density, and the package COMSOL Multiphysics® is used for our simulations.[1] The relative Young's modulus is defined as E/E_0 where E and E_0 are the modulus of lattice and base material, respectively. Once the optimized relative Young's modulus is obtained, the modulus of the lattice structure can be predicted using linearity since the E is proportional to E_0. The material properties used in all simulations are E_0=1 (normalized), ν=0.33; a displacement of $0.01a$ is applied on the upper z-plane in the negative z-direction while applying roller conditions on the bottom surface. Symmetry conditions are applied on all other outer surfaces of the unit cell to mimic infinitely periodic structures. We then apply the result obtained from the FEA to homogenization method in order to predict the modulus of the lattice structure. If the unit cell is viewed as a composite with void and material phases, the macroscopic stress $(\bar{\boldsymbol{\sigma}})$ applied to the unit cell is expressed as

$$\bar{\boldsymbol{\sigma}} = (1-\bar{\rho}) \cdot \bar{\boldsymbol{\sigma}}_0 + \bar{\rho} \cdot \bar{\boldsymbol{\sigma}}_1 \tag{2}$$

where $\bar{\rho}$ and $\bar{\boldsymbol{\sigma}}_i$ refer to the relative density of lattice structure and volume-averaged stress tensor of each phase, respectively.[2] Since the stress applied to the void is zero, the macroscopic stress is expressed as

$$\bar{\boldsymbol{\sigma}} = \bar{\rho} \cdot \bar{\boldsymbol{\sigma}}_1 \tag{3}$$

According to the boundary conditions, the only non-zero macroscopic strain, $\bar{\varepsilon}_{zz}$, is -1%. The stiffness tensor of the lattice structure is then obtained by using Hill's lemma and Hooke's law.[2]

$$\bar{\boldsymbol{\sigma}} = \boldsymbol{C} : \bar{\boldsymbol{\varepsilon}} \tag{4}$$

Control points of optimized Bézier curves

In this section, the coordinates of all control points used for modeling optimized Bézier curve is listed. Since we incorporate the 30th order Bézier curve, 31 control points are used and the x coordinate of initial and last control points are fixed as 0 and $\sqrt{3}a/2$ where a is the lattice constant. All of the values are normalized by the lattice constant.

	$\bar{\rho}_0 = 0.1734$		$\bar{\rho}_0 = 0.2$		$\bar{\rho}_0 = 0.3$		$\bar{\rho}_0 = 0.4$	
	x	y	x	y	x	y	x	y
$\boldsymbol{P}_0$	0.000000	0.378009	0.000000	0.380168	0.000000	0.273431	0.000000	0.445116
$\boldsymbol{P}_1$	0.071559	0.209231	0.033166	0.453680	0.053181	0.115164	0.366581	0.062830
$\boldsymbol{P}_2$	0.094686	0.578604	0.078433	0.372448	0.361775	0.428690	0.395372	0.023525
$\boldsymbol{P}_3$	0.211459	0.337153	0.102174	0.052463	0.411909	0.107820	0.456808	0.181224
$\boldsymbol{P}_4$	0.397621	0.350283	0.153489	0.351448	0.554279	0.249273	0.607826	0.003708
$\boldsymbol{P}_5$	0.518903	0.193203	0.180915	0.886736	0.590216	0.876308	0.745650	0.124988
$\boldsymbol{P}_6$	0.531482	0.652693	0.485338	0.200795	0.603780	0.077355	0.553433	1.336076
$\boldsymbol{P}_7$	0.611161	0.268691	0.620726	0.558459	0.365877	0.642182	0.595019	0.970811
$\boldsymbol{P}_8$	0.690668	0.542536	0.708224	0.737407	0.688561	0.722237	0.596977	0.582333
$\boldsymbol{P}_9$	0.793485	0.093683	0.634059	0.295902	0.720961	1.062376	0.816350	1.268082
$\boldsymbol{P}_{10}$	0.829515	0.469715	0.692053	0.371642	0.761140	0.159635	0.860830	0.287202
$\boldsymbol{P}_{11}$	0.909111	0.149553	0.868019	0.118910	0.796970	0.324297	1.163552	0.189093
$\boldsymbol{P}_{12}$	0.977922	0.220148	0.901554	0.015462	0.816300	0.153161	1.230563	0.167541
$\boldsymbol{P}_{13}$	1.124631	0.138393	0.996383	0.171000	1.187389	0.177018	1.235472	0.373279
$\boldsymbol{P}_{14}$	1.227953	0.122571	1.294441	0.315331	1.227803	0.240293	1.292016	0.739732
$\boldsymbol{P}_{15}$	1.299038	0.341199	1.299038	0.165639	1.299038	0.846386	1.299038	0.055437
$\boldsymbol{P}_{16}$	1.370123	0.122571	1.303635	0.315331	1.370273	0.240293	1.306060	0.739732
$\boldsymbol{P}_{17}$	1.473445	0.138393	1.601694	0.171000	1.410687	0.177018	1.362605	0.373279
$\boldsymbol{P}_{18}$	1.620154	0.220148	1.696522	0.015462	1.781777	0.153161	1.367513	0.167541
$\boldsymbol{P}_{19}$	1.688966	0.149553	1.730057	0.118910	1.801106	0.324297	1.434524	0.189093
$\boldsymbol{P}_{20}$	1.768561	0.469715	1.906023	0.371642	1.836936	0.159635	1.737247	0.287202
$\boldsymbol{P}_{21}$	1.804591	0.093683	1.964017	0.295902	1.877115	1.062376	1.781726	1.268082
$\boldsymbol{P}_{22}$	1.907408	0.542536	1.889852	0.737407	1.909515	0.722237	2.001099	0.582333
$\boldsymbol{P}_{23}$	1.986915	0.268691	1.977351	0.558459	2.232199	0.642182	2.003058	0.970811
$\boldsymbol{P}_{24}$	2.066595	0.652693	2.112738	0.200795	1.994296	0.077355	2.044643	1.336076
$\boldsymbol{P}_{25}$	2.079173	0.193203	2.417161	0.886736	2.007860	0.876308	1.852426	0.124988
$\boldsymbol{P}_{26}$	2.200455	0.350283	2.444587	0.351448	2.043797	0.249273	1.990251	0.003708
$\boldsymbol{P}_{27}$	2.386617	0.337153	2.495902	0.052463	2.186167	0.107820	2.141268	0.181224
$\boldsymbol{P}_{28}$	2.503390	0.578604	2.519643	0.372448	2.236301	0.428690	2.202704	0.023525
$\boldsymbol{P}_{29}$	2.526517	0.209231	2.564910	0.453680	2.544895	0.115164	2.231495	0.062830
$\boldsymbol{P}_{30}$	2.598076	0.378009	2.598076	0.380168	2.598076	0.273431	2.598076	0.445116

	$\bar{\rho}_0 = 0.5$		$\bar{\rho}_0 = 0.6$		$\bar{\rho}_0 = 0.7$		$\bar{\rho}_0 = 0.8$	
	x	y	x	y	x	y	x	y
$\boldsymbol{P}_0$	0.000000	0.174546	0.000000	0.551494	0.000000	0.281358	0.000000	0.356075
$\boldsymbol{P}_1$	0.002543	0.498292	0.246643	0.090407	0.096550	0.467119	0.242757	0.413174
$\boldsymbol{P}_2$	0.043349	0.139439	0.243059	0.043556	0.473625	0.187607	0.257709	1.631025
$\boldsymbol{P}_3$	0.416834	0.230744	0.507226	0.067247	0.508513	0.044336	0.349411	0.802439
$\boldsymbol{P}_4$	0.575282	0.059522	0.613717	0.130576	0.508963	0.147002	0.410802	0.129183
$\boldsymbol{P}_5$	0.576070	0.157456	0.803110	0.161636	0.605391	0.148817	0.423726	1.378083
$\boldsymbol{P}_6$	0.594262	0.451154	0.496871	0.152104	0.618034	0.035124	0.533228	1.520579

$\boldsymbol{P}_7$	0.446044	0.118850	0.504711	0.214984	0.665210	1.007420	0.557760	0.387628
$\boldsymbol{P}_8$	0.540553	0.066686	0.558884	1.340347	0.674775	1.449008	0.561674	0.353197
$\boldsymbol{P}_9$	0.654357	1.490917	0.762182	0.925530	0.715108	1.137879	0.876866	0.042376
$\boldsymbol{P}_{10}$	0.748310	1.434547	0.952857	1.790664	0.899560	1.065258	0.878862	0.716019
$\boldsymbol{P}_{11}$	0.932360	0.586203	1.072028	0.364568	1.027119	0.641865	1.077843	0.343925
$\boldsymbol{P}_{12}$	1.194707	0.671131	1.237657	0.427693	1.017316	0.974648	1.172451	0.255410
$\boldsymbol{P}_{13}$	1.210228	0.624862	1.279363	0.324226	1.163447	0.635823	1.205612	1.650730
$\boldsymbol{P}_{14}$	1.283593	0.057407	1.191008	0.278732	1.186558	0.352250	1.227414	1.680231
$\boldsymbol{P}_{15}$	1.299038	0.104542	1.299038	1.662480	1.299038	0.852479	1.299038	0.602040
$\boldsymbol{P}_{16}$	1.314484	0.057407	1.407068	0.278732	1.411518	0.352250	1.370663	1.680231
$\boldsymbol{P}_{17}$	1.387848	0.624862	1.318713	0.324226	1.434629	0.635823	1.392464	1.650730
$\boldsymbol{P}_{18}$	1.403369	0.671131	1.360419	0.427693	1.580760	0.974648	1.425625	0.255410
$\boldsymbol{P}_{19}$	1.665716	0.586203	1.526048	0.364568	1.570957	0.641865	1.520233	0.343925
$\boldsymbol{P}_{20}$	1.849767	1.434547	1.645219	1.790664	1.698516	1.065258	1.719215	0.716019
$\boldsymbol{P}_{21}$	1.943720	1.490917	1.835895	0.925530	1.882969	1.137879	1.721210	0.042376
$\boldsymbol{P}_{22}$	2.057523	0.066686	2.039192	1.340347	1.923301	1.449008	2.036402	0.353197
$\boldsymbol{P}_{23}$	2.152032	0.118850	2.093365	0.214984	1.932866	1.007420	2.040316	0.387628
$\boldsymbol{P}_{24}$	2.003814	0.451154	2.101205	0.152104	1.980042	0.035124	2.064848	1.520579
$\boldsymbol{P}_{25}$	2.022006	0.157456	1.794966	0.161636	1.992685	0.148817	2.174350	1.378083
$\boldsymbol{P}_{26}$	2.022794	0.059522	1.984359	0.130576	2.089113	0.147002	2.187275	0.129183
$\boldsymbol{P}_{27}$	2.181243	0.230744	2.090850	0.067247	2.089563	0.044336	2.248665	0.802439
$\boldsymbol{P}_{28}$	2.554727	0.139439	2.355017	0.043556	2.124451	0.187607	2.340368	1.631025
$\boldsymbol{P}_{29}$	2.595533	0.498292	2.351434	0.090407	2.501527	0.467119	2.355319	0.413174
$\boldsymbol{P}_{30}$	2.598076	0.174546	2.598076	0.551494	2.598076	0.281358	2.598076	0.356075

Supporting figures

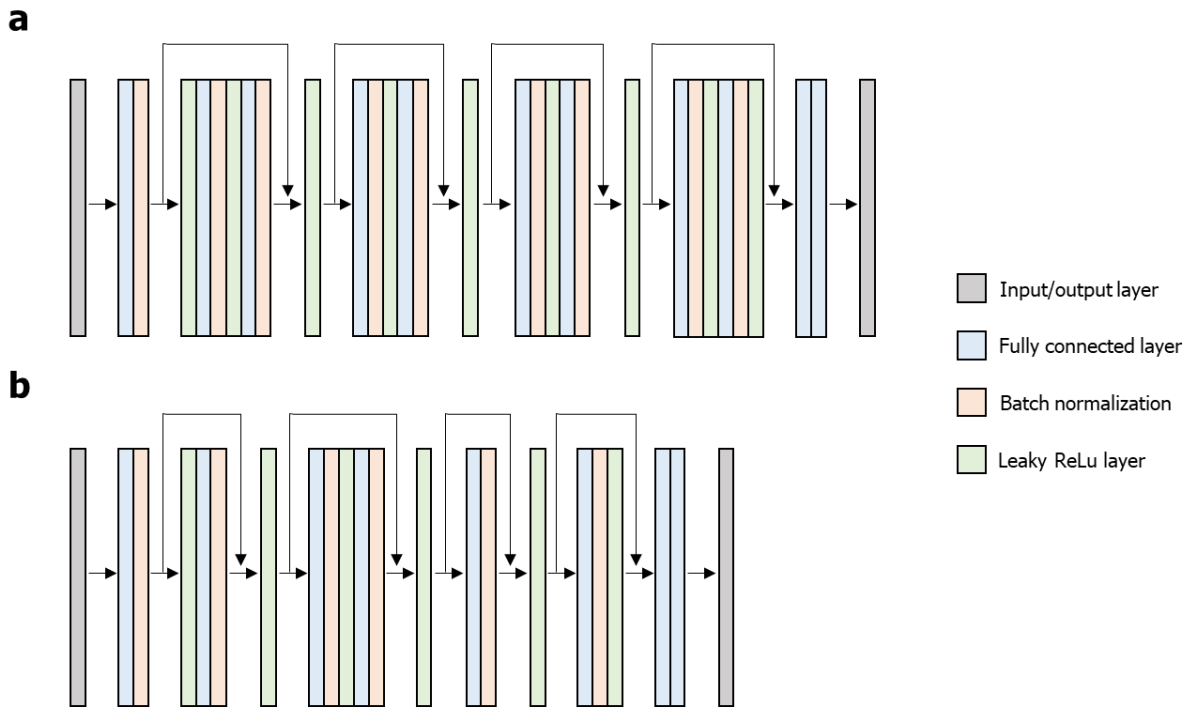

Fig. S1 The architecture of the NNs for (a) relative Young's modulus and (b) relative density of BC structure.

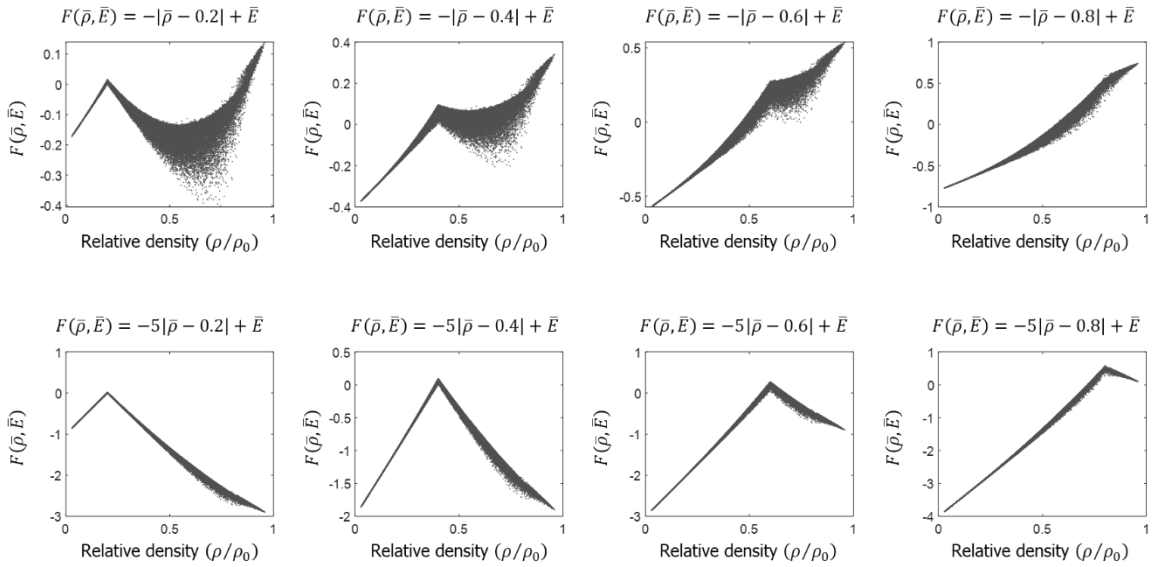

Fig. S2 The output of our objective function for different penalty coefficients.

Algorithm: Generative machine learning (GenML) algorithm

```
1:  Procedure GenML
2:      D ← Initial 20000 datasets
3:      While (maximum output is not converged) do
4:          Π1, Π2 ← Two neural networks trained using datasets D
5:          P ← Top 5000 datasets
6:          F ← Output (objective function) of P
7:          Initialization for genetic optimization {
8:              N=0: the number of new datasets
9:              Fc=F(50): top 50th output of P }
10:         // Genetic optimization loop
11:         While (N=1000) do
12:             Crossover the two datasets selected from P
13:             F0 ← Output (objective function) prediction using Π1, Π2
14:             // Greedy decision
15:             If F0 >Fc then:
16:                 N=N+1
17:             end if
18:         end while
19:         Calculate ground truth of new datasets
20:         Check for convergence
21:         D ← D + new datasets
        end while
    end procedure
```

Fig. S3. Flow of the generative machine learning algorithm used in this work. The greedy decision (line 13~15) is made during genetic optimization (line 10~16) to obtain the new datasets with high output.

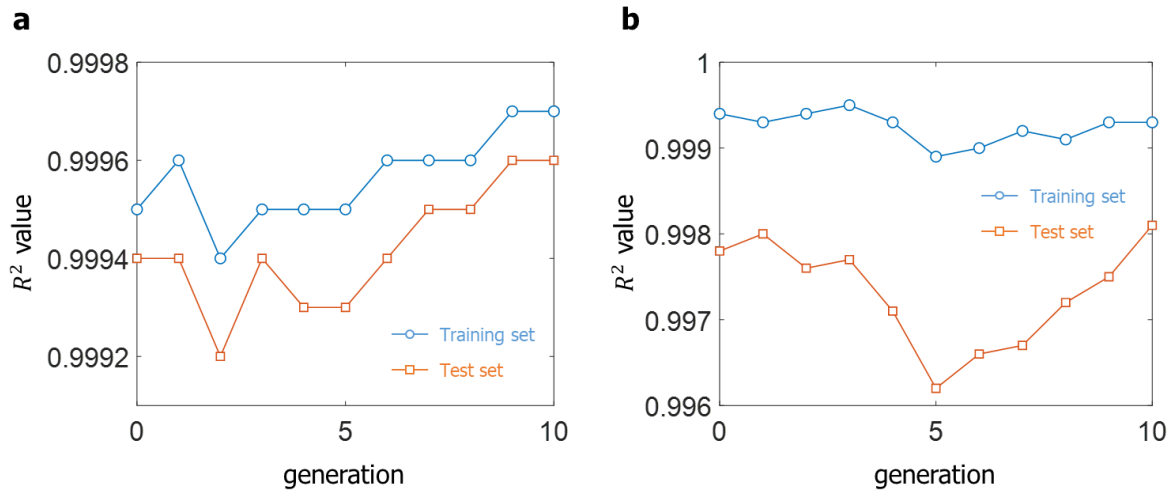

Fig. S4. R^2 values at every generation of GO: (a) The relative density and (b) Young's modulus.

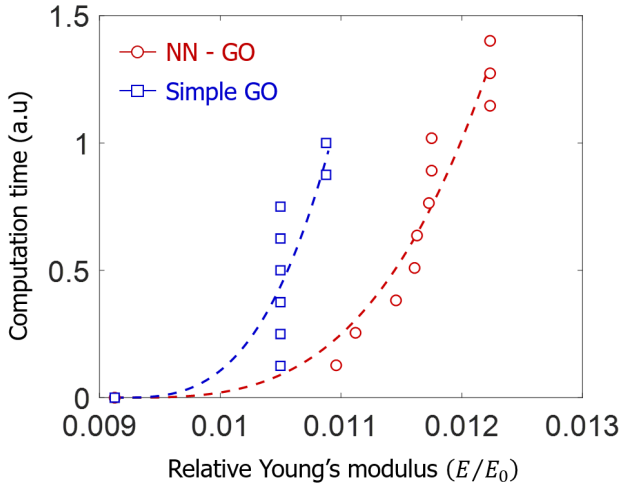

Fig. S5 Computation time of two design methods. The time is normalized by the total computation time of simple GO. The normalized computation times at every iteration are about 0.1241 (FEA), 0.00017 (NN training), 0.0029 (data generation with greedy decision), and 0.00086 (data generation without greedy decision).

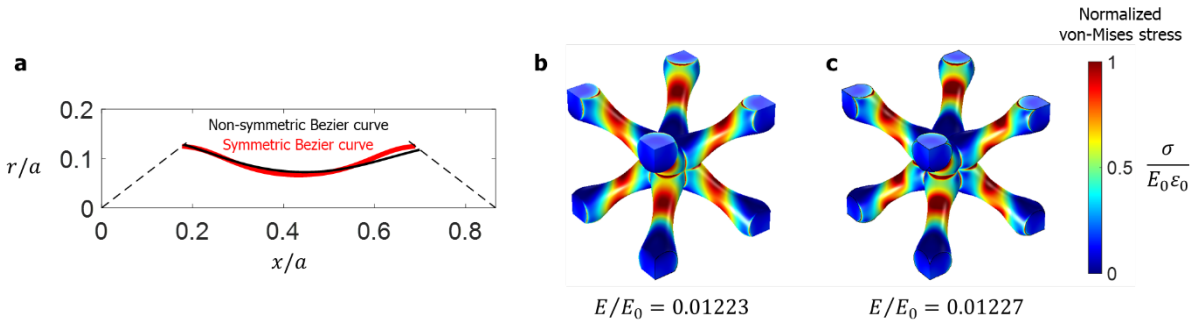

Fig. S6 (a) The two optimal Bézier curves. The normalized von Mises stress of BC structure modeled by using (b) non-symmetric and (c) symmetric Bézier curves.

References

1. S. COMSOL Multiphysics®. www.comsol.com. COMSOL AB, Sweden.
2. R. Hill, *Journal of the Mechanics and Physics of Solids*, 1963, **11**, 357-372.