Electronic Supplementary Material (ESI) for Materials Horizons.

Supplementary Materials

Bioinspired hierarchical composite design using machine learning: Simulation, additive manufacturing, and experiment

Grace X. Gu[a,b], Chun-Teh Chen[a], Deon J. Richmond[a], and Markus J. Buehler[a*]

[a] Laboratory for Atomistic and Molecular Mechanics (LAMM), Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139, United States of America
[b] Department of Mechanical Engineering, Massachusetts Institute of Technology
77 Massachusetts Ave., Cambridge, MA 02139, United States of America
[*] Address correspondence to: mbuehler@mit.edu, +1.617.452.2750

EXPERIMENTAL SECTION

Finite element method model

FEM is used to solve for mechanical properties including toughness and strength of hierarchical composites. The FEM model and simulation method are described in more detail in our previous work[1] and also summarized in this section. A total of 100,000 hierarchical composites are randomly generated, which have an edge crack of 25% of the specimen width in the *y*-direction. The toughness of a hierarchical composite in our system is defined as the area underneath its stress-strain curve before the element at the crack tip fails; this area is proportional to the energy needed to initiate crack propagation. The definition of toughness as the area under the stress-strain curve is not flaw independent; this metric only captures the toughness of this particular configuration of edge crack and would be different for cracks of different sizes and orientations. This definition is used because we are trying to solve this condition of an edge crack problem. As a result, whenever we are comparing geometries in our finite element or machine learning model, we always compare with the same grid size and same crack size, location, and orientation. The elements used in this work are linear elastic four-node elements, with an assumption that the dominating failure mechanisms occurs in the linear elastic regime, supported by experimental evidence[2, 3]. The soft to stiff stiffness ratio is set to 0.01 and is chosen to be sufficiently low to prevent elastic stress mismatch. Displacement boundary conditions are applied along the *x*-direction to simulate a tensile test and plane stress conditions are used. The Young's modulus of the stiff material is 1 GPa with a failure strain of 10%. The toughness of the stiff and soft materials is chosen to be equal as we aim to study geometry effects rather than material effects on the composite properties. Symmetry in the geometry is assumed because the edge crack is located at the center of the composite system and the loading condition is symmetric. The strain measured at the crack tip is used to calculate the toughness and strength; once the strain reaches the failure strain of the element, the material is considered failed and the toughness and strength (maximum stress) of the composite can be determined. The modulus of a composite is defined as the effective stiffness of the sample composed of soft and stiff materials. Additional details as to calculation of the mechanical properties are discussed in our previous work[1].

Machine learning approach

The ML calculations are performed using TensorFlow[4] running on an NVIDIA Tesla K20m GPU. Specifically, convolution neural networks (CNN), a widely used deep learning method for image recognition and other imaging-related tasks, are adopted in this work, with more details in our previous work[5]. Our ML model consists of two convolutional layers which have 32 features in the first layer and 64 features in the second layer using a 3 by 3 patch. A stride of one with zero padding is used in the ML model. The weights are initialized with some randomness, added with a small bias, and passed through the ReLU activation function. 256 neurons are assigned in the fully-connected layer to balance the accuracy and computational cost, shown in more detail in Fig. S2. Note that the effects of the other hyperparameters are not investigated since searching for optimal ML architectures is beyond the scope of this work but remains for future opportunities. Specifics as to how the NRMSD value is calculated are discussed in our previous work [5]. The generation of new designs is done by using a self-learning-based sampling method. In each sampling loop, 100,000 samples with different designs are evaluated by the ML model.

These 100,000 samples include two parts. The first part is a random sampling that consists of 90,000 samples generated randomly; the second part is a self-learning sampling that consists of 10,000 samples generated based on the result of the previous sampling loop. More specifically, the probabilities of each element being U1, U2, and U3 unit cells are determined based on the occurrence of these unit cells in the top 100 samples from the previous loop. To prevent the results from readily converging to a local minimum, a noise probability is added. The probability of element *i* being a U1 unit cell in the self-learning sampling is:

$$P_{1,i} = \frac{1}{3}N_r + (1 - N_r)\bar{P}_{1,i}$$

where N_r is a noise ratio that is determined randomly from a range of 0.1 to 0.5 in each sampling loop, and $\bar{P}_{1,i}$ is the probability of element *i* being a U1 unit cell in the top 100 samples in the previous sampling loop. A similar function is applied for U2 and U3 unit cells. The random sampling part allows the ML model to explore a broader design space and the purpose of the self-learning sampling part is to find the better designs faster without the need of searching through the entire design space.

3D-printing and experiments

The samples are fabricated using a Stratasys multi-material 3D-printer with two base materials, TangoBlackPlus (soft) and VeroMagenta (stiff). The two base materials are acrylic-based photopolymers that are printed simultaneously by two print heads as liquids and cured by ultraviolet light during the printing process. The detailed material properties are discussed in the work of Gu et al.[6] and Libonati et al.[2] and a table of the material properties is in Table S1. The sample preparation and tensile testing procedures are similar to our previous work[2, 6], where aluminium grips are glued with epoxy to the specimen's end for testing. The dimensions of the samples were 76 by 76 by 2 mm in addition to 25 mm-wide buffer regions for the grips on the two opposite sides. Additionally, a notch that is 25% of the specimen width is incorporated into the design during the printing process, and then the printed notch is sharpened with a razor blade. Tensile tests on our samples are performed using an Instron 5582 universal testing machine with a 100 kN load cell (Figure S3). The displacement rate in the experiment was 2 mm/min for all samples tested (three or more for each design). Samples were sprayed with black and white paint before testing for use in digital image correlation (DIC). DIC is carried out using the VIC-2D software created by Correlated Solutions. DIC measures displacements between the black and white dots during testing and permits visualization of the strain field at each instant of time.

Supplementary figures

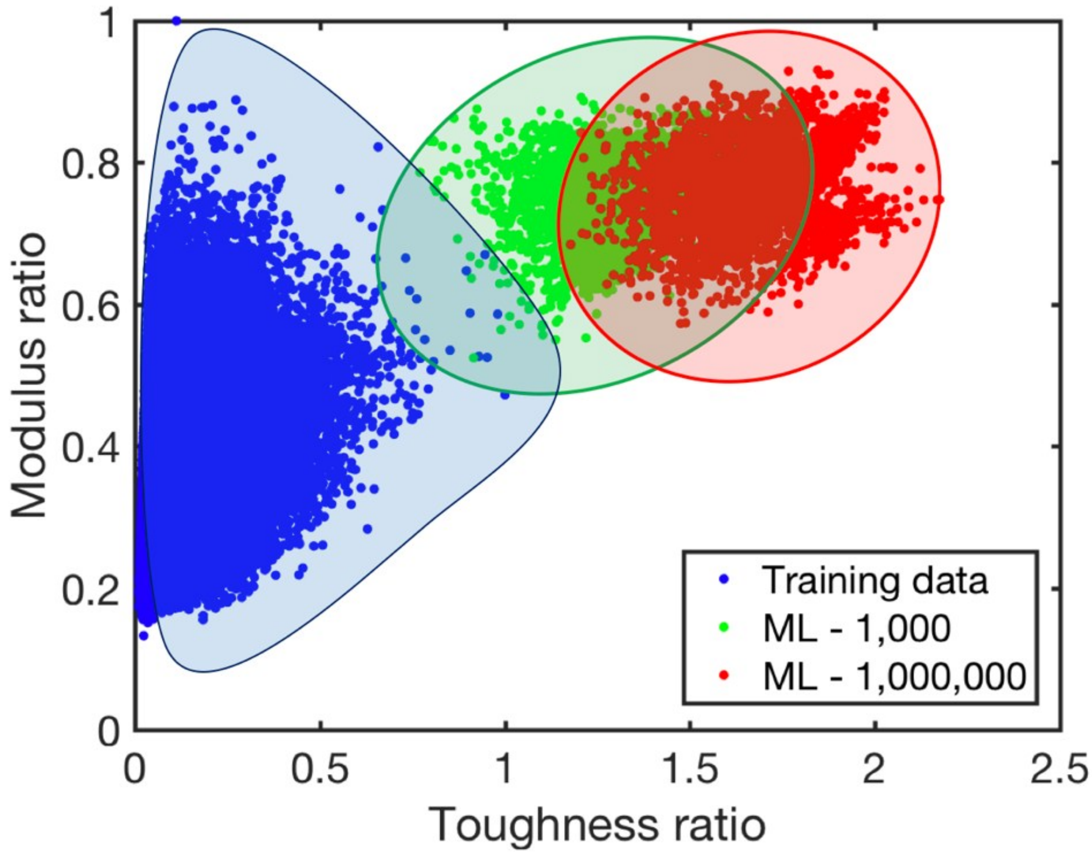

Figure S1: Performance comparison of training data and ML generated designs. Modulus ratio is the modulus normalized by the highest modulus value in the training data. Toughness ratio is the toughness normalized by the highest toughness value in the training data. The ML designs are generated using the training loops of 1,000 (shown by the green dots) and 1,000,000 (shown by the red dots). Envelopes show that mechanical properties of the ML generated designs exceed those of the training data.

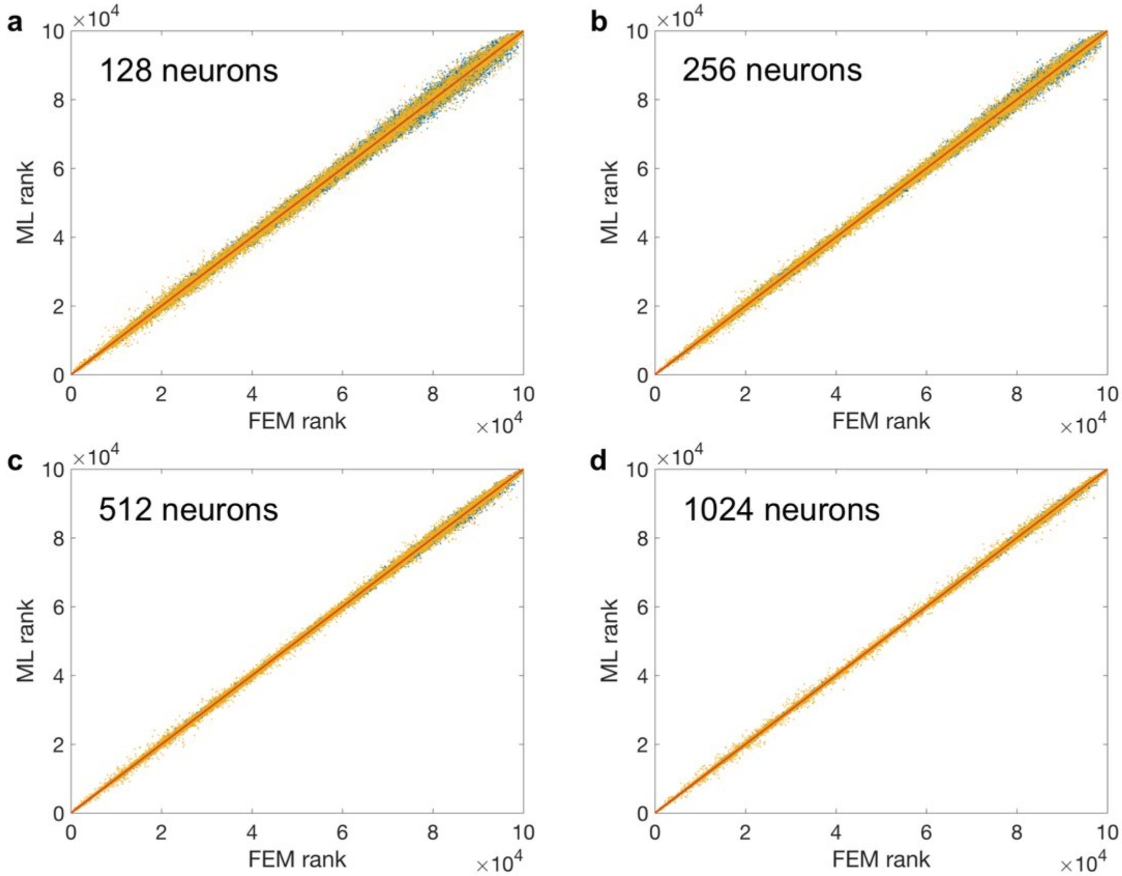

Figure S2: Training and testing results from ML models using different numbers of neurons. Blue dots represent training data, yellow dots represent testing data, and red curve represents y = x line. a) A model using 128 neurons has NRMSD = 0.4309 for training data and NRMSD = 0.6464 for testing data. b) A model using 256 neurons has NRMSD = 0.2978 for training data and NRMSD = 0.4926 for testing data. c) A model using 512 neurons has NRMSD = 0.1782 for training data and NRMSD = 0.3850 for testing data. d) A model using 1024 neurons has NRMSD = 0.1571 for training data and NRMSD = 0.3514 for testing data. The model using 256 neurons is used in this work to balance the accuracy and computational costs.

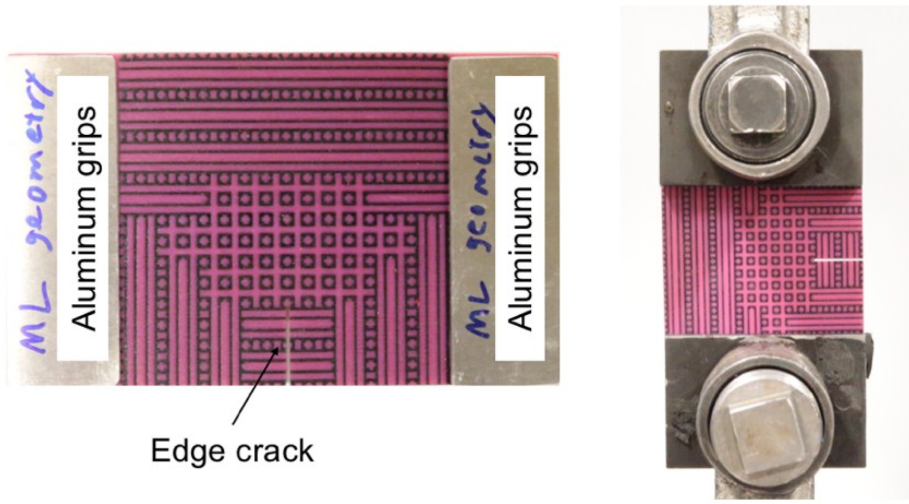

Figure S3: **Tensile testing experimental setup.** Representative sample with aluminum grips for testing (left) and tensile testing setup using Instron machine (right).

Supplementary table

	VeroMagenta	TangoBlackPlus
		
Young's modulus [MPa]	2187 ± 404	0.53 ± 0.02
Elongation at breakage [%]	9.8 ± 2.0	214 ± 12

Table S1: Material properties information for 3D-printed materials (VeroMagenta and TangoBlackPlus)[6].

References:

1. G. X. Gu, L. Dimas, Z. Qin and M. J. Buehler, *Journal of Applied Mechanics*, 2016, **83**, 071006.
2. F. Libonati, G. X. Gu, Z. Qin, L. Vergani and M. J. Buehler, *Advanced Engineering Materials*, 2016, **18**, 1354-1363.
3. L. S. Dimas, G. H. Bratzel, I. Eylon and M. J. Buehler, *Advanced Functional Materials*, 2013, **23**, 4629-4638.
4. M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G. S. Corrado, A. Davis, J. Dean and M. Devin, *arXiv preprint arXiv:1603.04467*, 2016.
5. G. X. Gu, C.-T. Chen and M. J. Buehler, *Extreme Mechanics Letters*, 2017.
6. G. X. Gu, F. Libonati, S. Wettermark and M. J. Buehler, *Journal of the Mechanical Behavior of Biomedical Materials*, 2017.