Solid Freeform Fabrication 2025: Proceedings of the 36th Annual International Solid Freeform Fabrication Symposium – An Additive Manufacturing Conference
Reviewed Paper

Machine-Learning-Based Inverse Design of Multi-Material Curved Lattice Structures

Xiaochen Yu*, Ajit Panesar*

* IDEA Lab, Department of Aeronautics, Imperial College London, UK

Abstract

Multi-material lattice structures offer unprecedented opportunities in designing multi-functional engineering applications. Using the heat exchanger as an example, stainless steel provides structural strength while the incorporation of copper fins enables efficient heat dissipation. In this work, we propose a machine learning (ML)-based inverse design framework to optimise multi-material, curved truss-based lattices for competing mechanical and thermal objectives. The unit cell is parameterised using a cubic spline function, enabling shape optimisation and expanding the attainable property space beyond conventional straight lattices. Material composition is treated as a categorical input to account for multi-material design. Ground truth properties are obtained via numerical homogenisation under periodic boundary conditions. The trained property predictor achieves a high prediction accuracy of $R^2 = 0.9913$ despite the mixed-type design inputs. The inverse generator employs a tandem network training strategy, capable of finding designs matching target properties ($R^2 = 0.9971$), though not necessarily reconstructing the original design. This highlights the one-to-many nature of inverse design problems and motivates future work on advanced generative models to explore the full design space.

Introduction

Multi-material structures offer significant potential in multifunctional engineering applications. By combining materials with distinct physical properties, such as the mechanical strength of stainless steel and the thermal conductivity of copper alloy, a trade-off could be realised for competing objectives in heat exchanger design [1]. Recent advancements in multi-material additive manufacturing (MMAM) [2], particularly laser powder bed fusion (LPBF) [3], have demonstrated the feasibility of fabricating such material combinations at high geometric resolution, paving the way for their integration into functional components.

In contrast to mono-scale designs, lattice structures offer additional design flexibility through control over unit cell topology, size, or shape. While extensive research has explored the effect of unit cell types [4] (e.g. truss-based, surface-based, plate-based) and applied volume fraction (VF) grading [5], comparatively less attention has been given to shape and material modulation within a unit cell. These degrees of freedom also enable property gradation and spatially varying performance. As lattice structures inherently operate across multiple length scales, numerical homogenisation [6] is typically employed to compute effective properties at the microscale, such that the computational cost during the macroscale analysis could be reduced.

Data-driven methods [7] have enabled efficient modelling and design of multi-material lattice structures by learning the complex relationships between microstructure parameters and effective properties. These approaches generally fall into two categories. In forward prediction frameworks, genetic algorithms can be used to search for optimal design parameters, with fitness evaluation assisted by predictive ML models. For example, Dong et al. [8] used a multilayer perceptron (MLP) to design curved, multi-material lattices tailored for specific lateral deformation profiles. Jiang et al. [9] applied convolutional neural networks (CNNs) to inverse design bi-material composite patterns that maximise stiffness while satisfying Poisson's ratio constraints. Conversely, direct inverse design methods aim to generate design parameters from target properties without iterative optimisation. For instance, Teawdeswan et al. [10] trained an MLP to predict the compression behaviour of PLA-TPU gyroid lattices, based on interpolated experimental data. Zeng et al. [11] proposed a pixel-based metamaterial design method that mapped mechanical properties to RGB space, enabling rapid unit cell generation via encoder-decoder networks.

This paper presents an ML-based design framework for multi-material curved lattice unit cells, with targeted values of mechanical stiffness and thermal conductivity tensors. The methodology begins with unit cell design parameterisation and property labelling via homogenisation. Subsequently, the architecture of the property predictor and inverse generator model was introduced. Model performance is evaluated in the results section, followed by a discussion on the one-to-many challenge involved in the inverse design problem. The paper concludes with a summary of key findings and future research directions.

Methodology

Unit Cell Design

The workflow of unit cell design parameterisation and obtaining ground truth properties via homogenisation is illustrated in Figure 1. In this study, a curved body-centred cubic (BCC) unit cell topology is adopted, though the methodology could be extended to any other truss-based cell types. The curvature is defined by a cubic spline function, and its geometry is determined by the spatial coordinates and tangents at two endpoints. To maintain simplicity while allowing sufficient shape variation, the tangents in the z-direction at both endpoints are selected as the two curvature control parameters. The cubic spline segment represents one-eighth of a unit cell. The full unit cell is constructed by applying symmetry operations across the three orthogonal planes. Then, it is voxelised into a 3D binary volume at a resolution of 100 voxels per side. The VF is held constant at 0.2 throughout the dataset. Two material compositions, with properties representative of stainless steel [12] and copper alloy [13], are assigned to the entire unit cell as outlined in Table 1. Intra-cell multi-material extension will remain as future work.

Table 1: Constituent material properties for homogenisation

Material	$E\ [GPa]$	ν	$\kappa\ [W/mK]$
316L stainless steel	200	0.3	15
CuCrZr	125	0.3	325

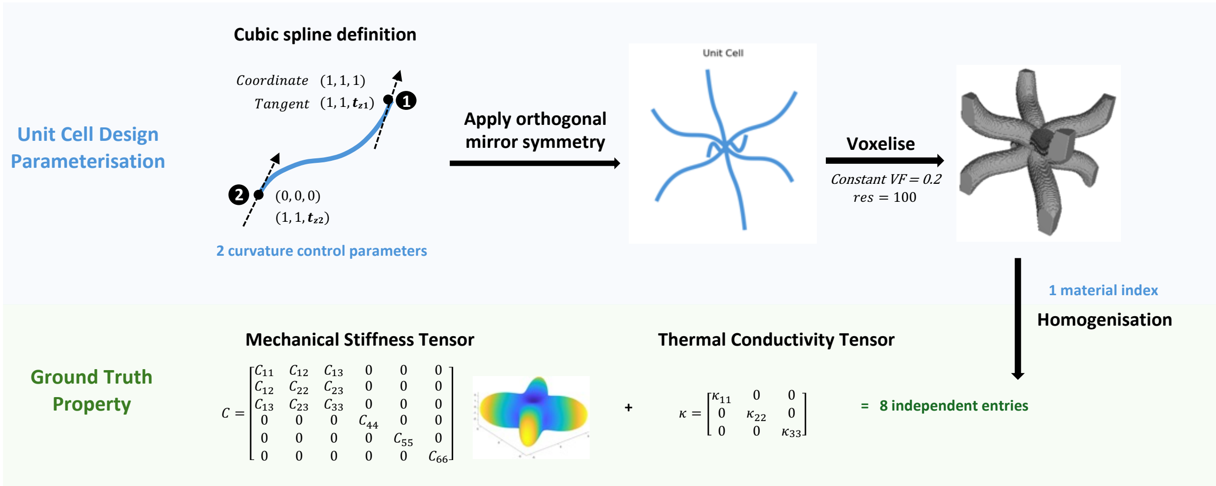


Figure 1: Unit cell design parameterisation and homogenisation for ground truth property.

To evaluate the effective mechanical and thermal properties (i.e. the homogenised response resulting from unit cell geometry and material assignment), the asymptotic homogenisation method [14] is employed, implemented using Abaqus. Periodic boundary conditions are applied to opposite faces of the unit cell. Unit mechanical loads are applied in three axial and three shear directions to construct the homogenised stiffness tensor. A similar procedure is followed for thermal homogenisation. Due to orthotropic symmetry and the fact that the curvature lies within the xy diagonal plane, the resulting stiffness and thermal conductivity tensors contain six and two independent entries, respectively. Consequently, each curved BCC unit cell is parameterised by two continuous curvature control variables, one categorical material index, and is associated with eight property features. This cubic-spline-based curvature control enables the exploration of a vast orthotropic property space not achievable with conventional straight BCC topologies [15].

To generate the dataset, the two curvature parameters are uniformly sampled in the range [0, 5] with a step size of 0.2. Combined with the two material indices, this yields 1352 unique unit cell designs. The dataset is divided into training, validation, and testing subsets using a 70:15:15 ratio. Prior to machine learning model training, MinMax normalisation is applied to all continuous variables to mitigate the effect of differing numerical scales.

Property Prediction

A property predictor was trained to map the three design parameters to eight effective properties. As illustrated in Figure 2, the model is an MLP consisting of three hidden layers each with 256 neurons. Rectified Linear Unit (ReLU) activation was applied after the fully connected layers. The model was trained using the Adam optimiser to minimise the mean squared error (MSE) between predicted and ground truth properties.

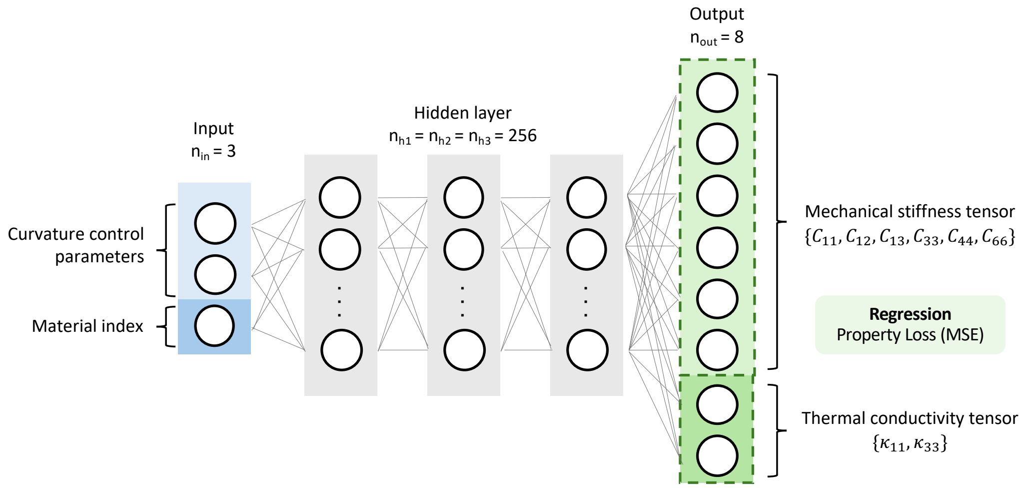


Figure 2: Property predictor ML model architecture.

Inverse Design

The inverse generator mirrors the property predictor's architecture but adopts a multi-head MLP, as shown in Figure 3. Specifically, the regression head is used to predict continuous curvature parameters while the classification head forecasts material index. Reflecting the one-to-many nature of the task, the inverse generator is trained using a tandem network strategy [16] demonstrated in Figure 4. In addition to design reconstruction, the predicted design is further evaluated by the pre-trained property predictor to assess alignment with the target properties. The overall loss function combines property loss (MSE), design reconstruction loss (MSE), and material classification loss (cross-entropy). By adjusting the weight of these terms, the model can prioritise either accurate property matching or exact design reconstruction.

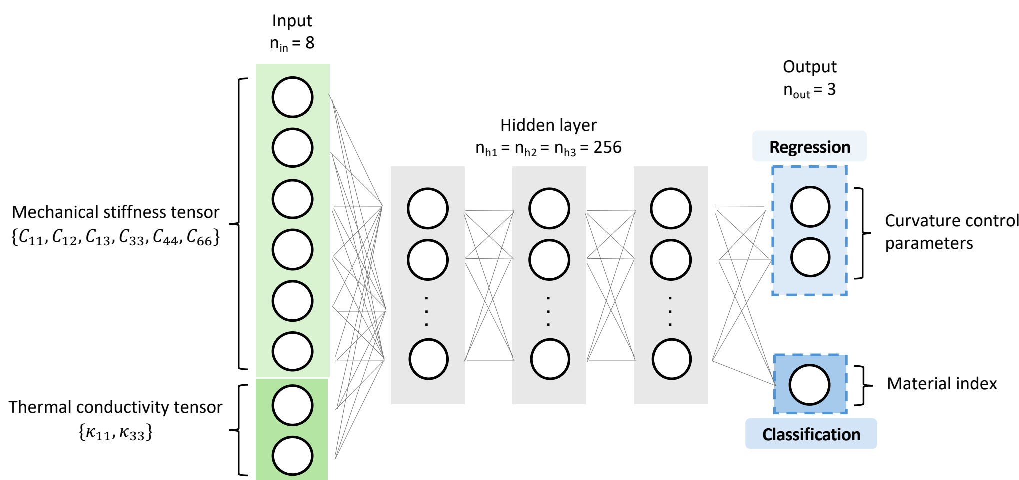


Figure 3: Inverse generator ML model architecture, consisting of a regression head and a classification head.

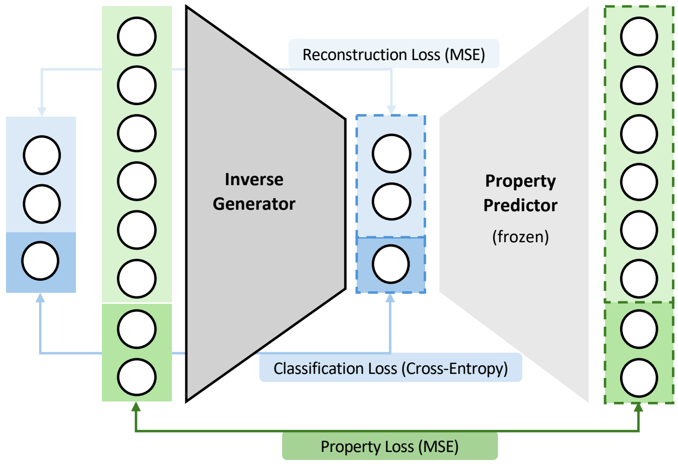


Figure 4: The tandem network architecture in training the inverse generator.

Results and Discussion

Property Prediction

The property predictor was trained with a batch size of 32, a learning rate of 1×10^{-4}, and a weight decay of 1×10^{-8}. Both the training and validation MSE loss reach convergence after 100 epochs. Model performance was evaluated on the unseen testing set, with results shown in Figure 5, where the predicted properties are plotted against the ground truth values. Predictions closely follow the $y = x$ line, implying high prediction accuracy across both mechanical and thermal features. The average R^2 score is 0.9913, confirming that the model effectively captures the mapping from mixed-type design parameters to effective properties.

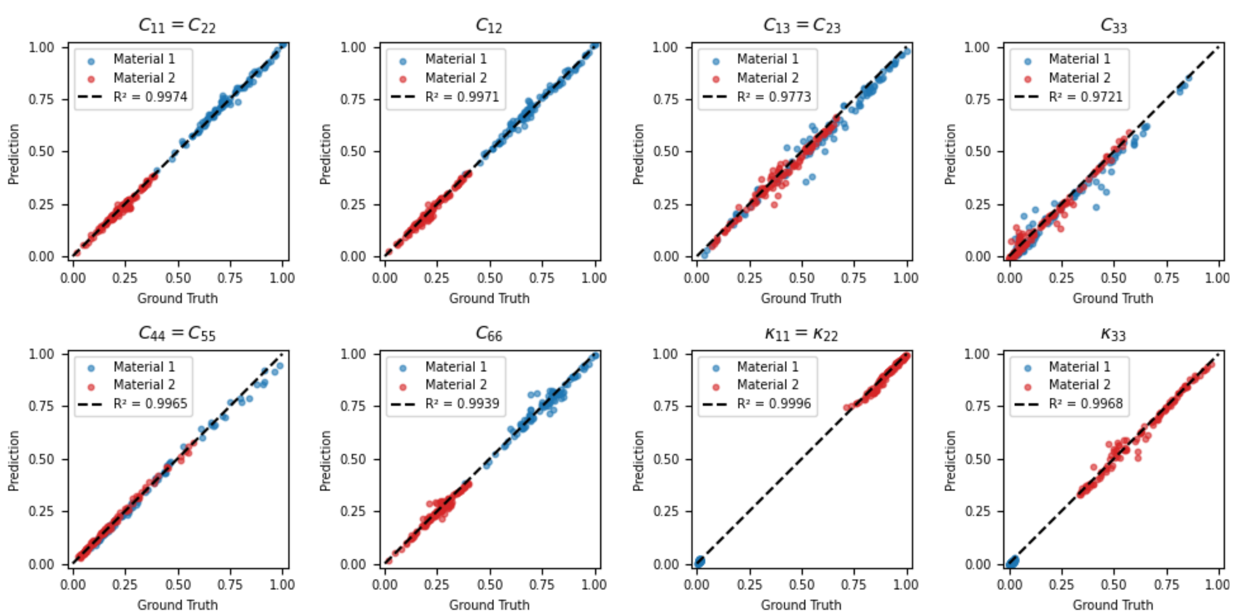


Figure 5: Performance evaluation of the property predictor on the testing dataset.

Inverse Design

The inverse generator was trained using the tandem network strategy by setting the loss weights: $W_{prop} = 1, W_{design} = 1 \times 10^{-3}, W_{material} = 1 \times 10^{-3}$. The overall loss function converges after 100 epochs. As shown in Figure 6, the model achieves perfect accuracy (100%) in reconstructing the material index on the testing set. While the curvature parameters are not always identical to the original design, the predicted properties - evaluated using the pre-trained property predictor - achieve a high average R^2 score of 0.9971. The observation suggests the one-to-many nature of the inverse design task, where multiple valid designs can yield the same target properties. However, the current model only recovers one feasible solution per target, highlighting the need for future work using more expressive ML techniques, such as conditional generative models [7] or mixture density networks [17], to capture the full inverse design space.

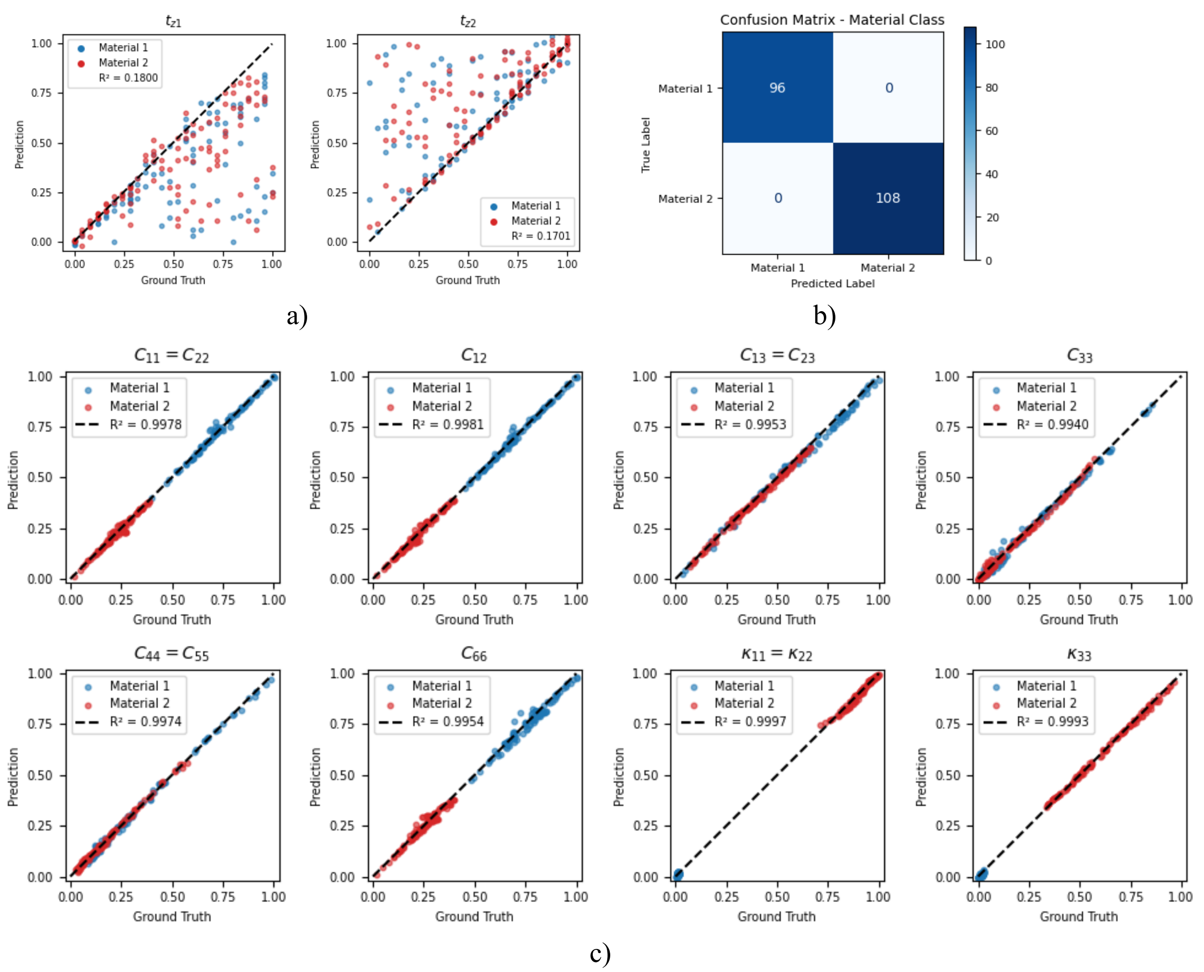
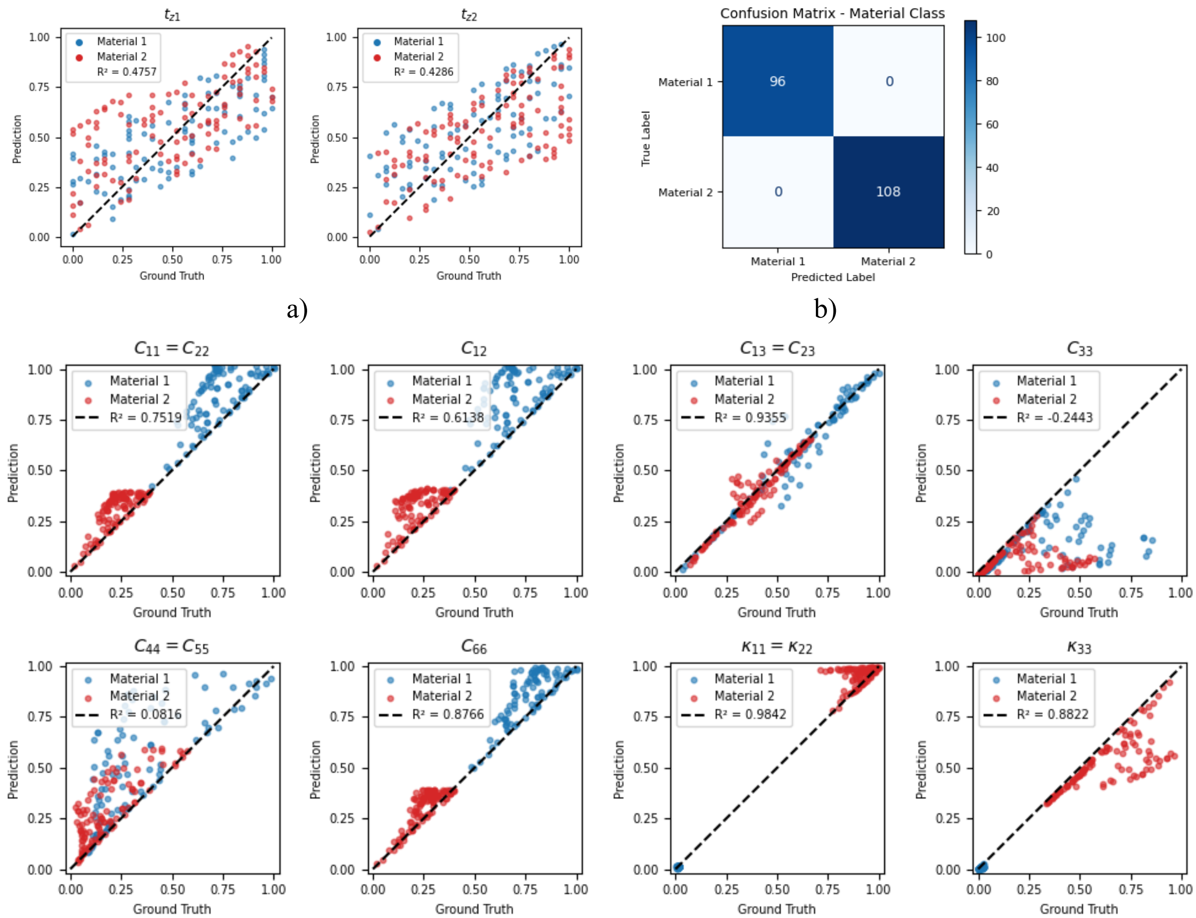


Figure 6: Performance evaluation of the inverse generator on the testing dataset, trained using the tandem network architecture. a) Design reconstruction of the two curvature control parameters. b) Material index classification accuracy demonstrated by the confusion matrix. c) Property of the inverse design compared to the target, evaluated by the pre-trained property predictor.

An investigation was also conducted by prioritising design reconstruction and material classification, effectively disabling the tandem network strategy by setting the property loss weight to zero. As illustrated in Figure 7, this approach leads to improved R^2 score for design reconstruction but still show a wide scatter along the $y = x$ line. More critically, the resulting designs fail to satisfy the target properties to an acceptable degree. These findings underscore the importance of incorporating property-based supervision in inverse design to ensure the functional validity of the generated design outputs.



c)

Figure 7: Performance evaluation of the inverse generator on the testing dataset, without incorporating property loss. a) Design reconstruction of the two curvature control parameters. b) Material index classification accuracy demonstrated by the confusion matrix. c) Property of the inverse design compared to the target, evaluated by the pre-trained property predictor.

Conclusion

This work presents an ML-based inverse design framework for multi-material, curved lattice structures targeting both mechanical and thermal performance. The unit cell is parameterised using a cubic spline function, while material composition is incorporated as a categorical input. Consequently, the proposed framework enables the exploration of a vast property space beyond the straight BCC topology. The property predictor serves as an accurate surrogate model for homogenised constitutive response ($R^2 = 0.9913$) despite the complexity introduced by the mixed-type design inputs. The inverse generator, trained via a tandem network architecture, effectively identifies one set of feasible designs that meet target properties ($R^2 = 0.9971$). Although the inverse model does not always recover the exact original design due to the one-to-many nature of the problem, it consistently produces functionally valid solutions. Ongoing work includes exploring advanced ML techniques, such as conditional generative models [7] or mixture density networks [17], to capture the full set of valid inverse designs. Overall, the proposed method paves the way for efficient design optimisation of functionally graded metamaterials with tailored mechanical and thermal performance. Future work also includes fabrication and experimental verification of the optimised multi-material designs.

References

[1] Xiaoshuang Li and Arthur Seibel, 'Case study: The development of a multi-material heat sink by Additive Manufacturing using Aerosint technology', *Metal Additive Manufacturing*, vol. 9, no. 1, pp. 183–188, Spring 2023.

[2] A. Nazir *et al.*, 'Multi-material additive manufacturing: A systematic review of design, properties, applications, challenges, and 3D printing of materials and cellular metamaterials', *Materials & Design*, vol. 226, p. 111661, Feb. 2023, doi: 10.1016/j.matdes.2023.111661.

[3] D. Wang *et al.*, 'Recent progress on additive manufacturing of multi-material structures with laser powder bed fusion', *Virtual and Physical Prototyping*, vol. 17, no. 2, Art. no. 2, Apr. 2022, doi: 10.1080/17452759.2022.2028343.

[4] C. Pan, Y. Han, and J. Lu, 'Design and Optimization of Lattice Structures: A Review', *Applied Sciences*, vol. 10, no. 18, p. 6374, Sep. 2020, doi: 10.3390/app10186374.

[5] A. Panesar, M. Abdi, D. Hickman, and I. Ashcroft, 'Strategies for functionally graded lattice structures derived using topology optimisation for Additive Manufacturing', *Additive Manufacturing*, vol. 19, pp. 81–94, Jan. 2018, doi: 10.1016/j.addma.2017.11.008.

[6] B. Hassani and E. Hinton, 'A review of homogenization and topology optimization I—homogenization theory for media with periodic structure', *Computers & Structures*, vol. 69, no. 6, pp. 707–717, Dec. 1998, doi: 10.1016/S0045-7949(98)00131-X.

[7] D. Lee, W. (Wayne) Chen, L. Wang, Y. Chan, and W. Chen, 'Data-Driven Design for Metamaterials and Multiscale Systems: A Review', *Advanced Materials*, p. 2305254, Dec. 2023, doi: 10.1002/adma.202305254.

[8] L. Dong and D. Wang, 'Optimal Design of Three-Dimensional Voxel Printed Multimaterial Lattice Metamaterials via Machine Learning and Evolutionary Algorithm', *Phys. Rev. Applied*, vol. 18, no. 5, Art. no. 5, Nov. 2022, doi: 10.1103/PhysRevApplied.18.054050.

[9] X. Jiang, F. Liu, and L. Wang, 'Machine learning-based stiffness optimization of digital composite metamaterials with desired positive or negative Poisson's ratio', *Theoretical and Applied Mechanics Letters*, vol. 13, no. 6, p. 100485, Nov. 2023, doi: 10.1016/j.taml.2023.100485.

[10] L. Teawdeswan and G. Dong, 'Inverse design of multi-material gyroid structures made by additive manufacturing', *International Journal of Mechanical Sciences*, p. 108734, Sep. 2023, doi: 10.1016/j.ijmecsci.2023.108734.

[11] Q. Zeng, Z. Zhao, H. Lei, and P. Wang, 'A deep learning approach for inverse design of gradient mechanical metamaterials', *International Journal of Mechanical Sciences*, vol. 240, p. 107920, Feb. 2023, doi: 10.1016/j.ijmecsci.2022.107920.

[12] 'Stainless Steel 316L 1.4404', thyssenkrupp. [Online]. Available: https://www.thyssenkrupp-materials.co.uk/stainless-steel-316l-14404.html
[13] 'Datasheet CuCr1Zr', METALCOR. [Online]. Available: https://www.metalcor.de/en/datenblatt/133/
[14] G. Dong, Y. Tang, and Y. F. Zhao, 'A 149 Line Homogenization Code for Three-Dimensional Cellular Materials Written in matlab', *Journal of Engineering Materials and Technology*, vol. 141, no. 1, p. 011005, Jan. 2019, doi: 10.1115/1.4040555.
[15] A. Álvarez-Trejo, E. Cuan-Urquizo, D. Bhate, and A. Roman-Flores, 'Mechanical metamaterials with topologies based on curved elements: An overview of design, additive manufacturing and mechanical properties', *Materials & Design*, vol. 233, p. 112190, Sep. 2023, doi: 10.1016/j.matdes.2023.112190.
[16] S. Kumar, S. Tan, L. Zheng, and D. M. Kochmann, 'Inverse-designed spinodoid metamaterials', *npj Comput Mater*, vol. 6, no. 1, p. 73, Jun. 2020, doi: 10.1038/s41524-020-0341-6.
[17] R. Unni, K. Yao, and Y. Zheng, 'Deep Convolutional Mixture Density Network for Inverse Design of Layered Photonic Structures', *ACS Photonics*, vol. 7, no. 10, pp. 2703–2712, Oct. 2020, doi: 10.1021/acsphotonics.0c00630.