Controllable inverse designing of auxetic metamaterials

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WHAT IS AN AUXETIC METAMATERIAL ?

- Auxetic metamaterials are mechanical metamaterials with negative Poisson's ratios that exhibit counterintuitive deformation behavior. Under uniaxial compressive loading, auxetic metamaterials contract in the orthogonal directions rather than expanding.
- Such distinctive behaviors make auxetic metamaterials promising candidates for developing impact absorbers, strain sensors, and actuators, as well as for applications in biomedicine and electrochemical energy storage and conversion.

Auxetic metamaterials vs other materials:

Under uniaxial compressive loading, auxetic metamaterials contract in the orthogonal directions rather than expanding; this behavior is in contrast to that of natural and synthetic materials, which have positive Poisson's ratios.

Under bending loading, an auxetic metamaterial plate deforms into a convex shape, in contrast to the saddle shape usually seen for common materials.

Compared with conventional materials, auxetic metamaterials have higher shear resistance, fracture resistance, indentation resistance, impact resistance, and energy absorption.

Building a deep learning framework

Data acquisition

A large dataset composed of tens of thousands of geometric patterns and were derived from Voronoi tessellation, and their mechanical properties were calculated using a homogenization algorithm. The randomly created patterns scattered in the material property space form a nearly triangular shape, with $2.1 \text{ kPa} < E < 13.7 \text{ kPa}$ and $-0.28 < \nu < 0.38$.

Training

The dataset was then used to train a conditional generative adversarial network (CGAN) which consists of a solver (linear regression module), a generator and discriminator. The CGAN uses a solver to predict the properties of patterns from the generator. The discriminator was trained to push the generator to produce realistic patterns, and the solver was trained to push the generator to yield patterns with user-defined properties.

Generation and testing

After the CGAN had been well trained, it could rapidly generate new patterns with user-defined properties and could generate auxetic metamaterials with constantly negative Poisson's ratios during large deformations. Finally, the auxetic behaviors of the generated metamaterials were verified by FEM simulations and uniaxial compression tests.

ALGORITHMS USED

Voronoi tessellation algorithm

- It is a robust method that is capable of creating various porous materials. In this method, a seed consisting of 64 coordinate points was initially created according to Mitchell's best candidate algorithm. Then, a 2D Voronoi diagram was created based on the seed by merging two adjacent polygons to mimic the nature of actual auxetic foams, which have both convex and concave cells. Finally, a new pattern was formed after smoothing the edges of the polygons using Chaikin's algorithm. The relative density of the patterns was approximately 0.154. By repeating this process, an infinite number of different two-dimensional (2D) topology patterns can be created to facilitate big-data-driven material design.

Homogenization algorithm

- The elastic moduli (Young's modulus and Poisson's ratio) were calculated according to the theory of homogenization, which has been used extensively to probe the equivalent linear elasticity of periodic composites. In this work, each pattern was first converted into a 256×256 element matrix consisting of 0 (void regions) and 1 (solid regions). Subsequently, trial strain fields were applied to the element matrix to determine the reaction forces and stored elastic energy. Then, a homogenized elasticity tensor was obtained after the homogenization calculation. Finally, the effective elastic moduli of the patterns were calculated according to the elasticity tensor. The material model used in the homogenization was a linear elastic material with Young's modulus of 0.6615 MPa and a Poisson's ratio of 0.49; these values were chosen to fit the equivalent elastic moduli of an incompressible neo-Hookean solid under a small deformation.

Tests conducted

Uniaxial compression tests

The auxetic behaviors of the generated metamaterials were first investigated using a set of 3D-printed samples. The mechanical properties of the 3D-printed specimens were investigated by performing static compression tests using a motorized test stand (EMX-500 N, IMADA, Japan). A constant displacement rate of 10 mm/min was set during the tests, in which the samples were uniaxially compressed between two plates. The deformation process was captured using a high-speed camera, and the stress–strain curves were plotted using the recorded load–displacement data. The Young's modulus E_l for the longitudinal (compression) direction was calculated by linear fitting of the initial linear portions of the stress–strain curves. Least-squares approach was used to find the suitable value of E_l.

Finite element method simulations

The mechanical properties of the proposed patterns were further validated using a FEM simulation platform. A 2D plane strain model was utilized under periodic boundary conditions. To mimic the properties of the 3D-printed material, the material model in the simulations was defined as an incompressible neo-Hookean model with Young's modulus of 0.6615 MPa that was fitted from the compression tests. All the model geometries were meshed using approximately 2.5×105 second-order triangular solid elements. A contact condition based on an augmented Lagrangian method was set in the finite element model. For the large deformation, a parametric sweep of the longitudinal displacement was used with a stop condition of $\varepsilon l=0.2$. The Poisson's ratios and Young's moduli in the simulation results were calculated using the same method that was employed to obtain the experimental results.

Results and discussion

After the CGAN had been well trained using appropriate parameters, it could invert the design of auxetic metamaterials: a label (Young's modulus and Poisson's ratio) was input, and the CGAN generated a batch of geometrical patterns with the corresponding Young's modulus and Poisson's ratio. We tested the performance of our CGAN model during each epoch by generating 1024 patterns with labels that were randomly sampled from the available E–ν space. The performance was evaluated in terms of the mean squared error (MSE) of the sum of E (Poisson's ratio) and ν (Young's modulus). A smaller MSE indicates better performance. The low MSE indicates that our CGAN is capable of generating patterns with a user-defined Young's modulus and Poisson's ratio.

In addition, the line plots for the loss of the generator and discriminator were plotted. The plots represent typical loss–epoch graphs of a stable GAN training process: the losses of the generator and discriminator begin erratically and gradually converge to a stable equilibrium. This finding further demonstrates the stability of our CGAN.

The comparison between the CGAN-generated patterns and randomly created patterns shows that it is easy to generate auxetic metamaterials with very low negative Poisson's ratios using the CGAN, in contrast to the random generation method. Although among the structures randomly generated with the Voronoi tessellation algorithm, only 3% had a negative Poisson's ratio, the proposed approach can almost certainly generate the intended disordered structures having negative Poisson's ratios. More importantly, this inverse design method does not require a delicate arrangement of the shapes, distributions, and combinations of geometrical elements. This method is independent of prior knowledge about the design of auxetic metamaterials.

Conclusion

The experimental and simulation results show a consistent deformation tendency wherein the metamaterial gradually contracts when compressed uniaxially along with the shrinkage of its interior holes. The overall shrinkage phenomenon proves that the metamaterial is an auxetic metamaterial with a negative Poisson’s ratio. The progressively deformed shapes of other patterns with Poisson’s ratios range from -0.2 to 0.3 whereas the patterns with a positive Poisson’s ratio expand laterally when compressed uniaxially. The experimental and simulation results demonstrate that the negative Poisson’s ratio can maintain a wide range of compressive strain (ε=0.2). Furthermore, some patterns that initially have positive Poisson’s ratios exhibit auxetic behavior during further compression, which is caused by the shrinking of interior concave pores.

We also analyzed the stresses of the auxetic metamaterials during deformation which showed that the auxetic behavior of the designed metamaterials is a result not of buckling, but rather of ligament bending. The trained CGAN can facilitate the mass generation of 2D auxetic metamaterials with user-desired elastic moduli. The proposed method can be easily extended to the inverse design of 3D auxetic metamaterials in combination with Voronoi tessellation.

Details of CGAN

The CGAN used in this study was composed of three neural network structures: a generator, discriminator, and solver. The generator was trained to produce patterns of auxetic metamaterials from latent variables (multivariate normal distribution) and user-defined labels (Young’s modulus and Poisson’s ratio) and simultaneously aimed to deceive the discriminator and solver. The discriminator was trained to distinguish between the patterns produced by the generator and those from the real dataset. The solver was trained to predict the Young’s modulus and Poisson’s ratio of a given pattern.

Deep learning calculations were performed using TensorFlow. An Adam optimizer with a learning rate of 0.0001 and $\beta 1$ of 0.5 was used to train the model. The batch size for the training was set to 32. The detailed network structures used in this study. In short, the layers used included a 2D convolutional layer, a 2D transposed convolutional layer, 2D max pooling, a fully connected layer, batch normalization, and dropout, and the activation functions used included Leaky ReLU and tanh. The circular padding used in the 2D convolutional layer and 2D transposed convolutional layer to maintain and identify the periodicity of the patterns can more effectively help the output tensor retain its periodicity as compared to the commonly used zero padding. Because the solver is independent of the generator and discriminator, we first trained the solver with supervised learning. Each dataset was split as follows: 80% was used as the training set and 20% was used as the testing set. To prevent the solver from overfitting, early stopping was performed. The linear relationship of the solver-predicted results was better than that of the CGAN-generated results.

Thank You