HARNESSING CONNECTIVITY FOR ELASTICALLY ISOTROPIC DISORDERED HETEROGENEOUS MATERIALS

Jehoon Moon¹, Gisoo Lee¹, Jaehee Lee¹ & Hansohl Cho^{1*}

¹Department of Aerospace Engineering, Korea Advanced Institute of Science and Technology,

Daejeon, South Korea

<u>Summary</u> To generate elastically isotropic disordered heterogeneous materials, we present a simple yet efficient design strategy on two disordered morphologies: dispersed-particle and its interpenetrating counterpart. We combine experiments and numerical simulations to examine elastic isotropy in the disordered heterogeneous materials with the two morphologies. We show the disordered heterogeneous material with interpenetrating morphology exhibits near-complete isotropy with a small number of random spatial points. Furthermore, we characterize geometric and topological features of the internal random microstructures to explore the effect of adding connectivity on elastic isotropy. Overall, the interpenetrating morphology shows great promise for the design and manufacture of heterogeneous materials with near-complete isotropy.

INTRODUCTION

Heterogeneous materials architected on various crystal lattices have been extensively explored for various engineering functionalities involving photonics, acoustics, and mechanics with the recent advances in additive manufacturing and three-dimensional (3D) printing technologies. Recently, altering the connectivity in multi-component heterogeneous materials has been found to provide new opportunities to achieve superb mechanical features in a wide variety of loading scenarios [1-3]. However, long-range order in the heterogeneous materials architected on crystal lattices often results in undesirable, intrinsic anisotropy in elasticity and inelasticity. In this work, we present a simple yet efficient design strategy to generate disordered heterogeneous materials that exhibit near-complete elastic isotropy. We combine experiments and numerical simulations to examine how the internal connectivity throughout random spatial points impacts on elastic isotropy. We show that, by simply connecting the neighbors for each of the random spatial points, near-complete elastic isotropy can be achieved in the disordered heterogeneous materials.

METHODS

We first constructed two types of disordered morphologies: dispersed-particle morphology and its interpenetrating counterpart. Representative volume element (RVE) for dispersed-particle morphology is generated by randomly placing a finite number of non-overlapping spheres in the unit cube [4]. To generate its interpenetrating counterpart, we performed a standard Voronoi tessellation on the random spatial points (centers of the spheres in dispersed-particle morphology). We then performed rod-connecting the center point and its neighboring points for each of the tessellated polyhedra in the RVE. Therefore, the RVE with interpenetrating morphology possesses randomly connected microstructures throughout the tessellated polyhedral network. For both morphologies, a constant radius of spheres and cylinders was selected to meet the desired volume fraction of the hard component (here, we consider equal fractions of hard and soft components). To examine isotropy of the RVEs with interpenetrating morphology, we fabricated prototypes using a multi-material 3D printer. A thermoplastic polymer and hyperelastic rubber were used for hard and soft components, respectively, and the ratio of initial elastic moduli ($E_{\rm soft}/E_{\rm hard}$) was taken to be $\sim 1/90$.

RESULTS AND DISCUSSION

We then examined elastic anisotropy in both morphologies (dispersed-particle vs. interpenetrating) via numerical simulations. Anisotropy was evaluated by calculating the universal anisotropy index (A^U) in each of the RVEs [5]. To systematically investigate the effect of the number of random spatial points on elastic anisotropy, we calculated the anisotropy index for both morphologies as a function of the number of random spatial points (N) from 4 to 20, as shown in Figure 1. Altering the connectivity throughout the random spatial points remarkably reduced elastic anisotropy. Furthermore, the interpenetrating morphology exhibited near-complete elastic isotropy from $N \ge 7$. To address the more isotropic behaviour observed in the RVEs with the interpenetrating morphology, we characterized the local microstructures; we computed distributions of rod lengths (between the center points and their neighbors), average connectivity, and bond-orientational order parameters [6] for each of the random spatial points. We found that there was a transition in these microstructural features between N = 6 and N = 7, where anisotropy suddenly dropped.

In addition to the numerical analysis, we conducted mechanical tests on the 3D-printed prototypes for the RVEs with N=7 along maximum and minimum elastic modulus directions predicted by the numerical simulations. As shown in Figure 2, the experimentally measured elastic modulus in its maximum direction was found to be very close to that in the minimum modulus direction in all of the five independent RVEs; furthermore, the numerically computed elastic moduli in both maximum and minimum directions matched the experimental data very nicely, supporting the

^{*} Corresponding author. E-mail: hansohl@kaist.ac.kr

near-complete elastic isotropy in these disordered heterogeneous materials with random microstructures with high connectivity as well as with a small number of random spatial points (here, N = 7).

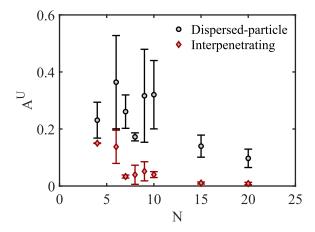


Figure 1. Anisotropy in disordered heterogeneous materials. N is the number of spatial points, and A^{U} is the universal anisotropy index.

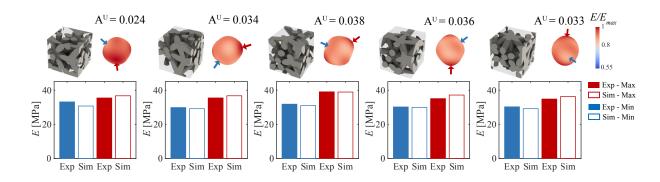


Figure 2. Experimental and numerical results of the initial stiffness along maximum and minimum modulus directions. The five realizations used in the experiments and numerical simulations are displayed along with the results on elastic moduli, and anisotropy map (here, N = 7 and $v_{\rm hard} = 50\%$); maximum modulus directions: red arrows and minimum modulus directions: blue arrows.

CONCLUSIONS

In this work, we have reported that a near-complete elastic isotropy can be achieved through interpenetrating morphology with a small number of random spatial points. Experiments and numerical simulations reveal that adding connectivity throughout dissimilar domains plays a crucial role in elastic isotropy in heterogenous disordered materials.

Acknowledgment

This work was funded by the National Research Foundation of Korea (Grant No. RS-2023-00279843).

References

- [1] S. V. Taylor, A. R. Moustafa, and Z. C. Cordero, Acta Mat., 216, 117115, 2021.
- [2] J. Bauer, M. Sala-Casanovas, M. Amiri, and L. Valdevit, Sci. Adv., 33, no. 8: 3080, 2022.
- [3] G. Lee, J. Lee, S. Lee, S. Rudykh, H. Cho, Soft Matter, 2, no. 20: 315-329, 2024.
- [4] M. Danielsson, D. M. Parks, and M. C. Boyce, J. Mech. Phys. Solids. 55, no. 3: 533-561, 2007.
- [5] S. I. Ranganathan and M. Ostoja-Starzewski, Phys. Rev. Lett. 101, no. 5: 055504, 2008.
- [6] P. J. Steinhardt, D. R. Nelson, and M. Ronchetti, *Phys. Rev. B.* 28, no 2, 784, 1983.