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Mechanics-guided optimization of hybrid periodic architectures

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Triply periodic minimal surface (TPMS) architectures are widely investigated for lightweight mechanical applications because of their high specific performance and manufacturability. However, most studies focus on a limited number of canonical families, such as gyroid or Schwarz structures, thus restricting the accessible design space. This work proposes a mechanics-driven optimization framework to explore a broader class of hybrid TPMS architectures and identify stiffness-efficient designs beyond standard topologies.

TPMS geometries are represented through an implicit level-set formulation based on an 18-dimensional set of linearly independent periodic basis functions. This parameterization enables the continuous generation of a broad spectrum of hybrid architectures while retaining control over connectivity and volume fraction. Candidate designs are instantiated as finite 2x2x2 multi-cell specimens and mechanically evaluated through a voxel-based finite element model. The framework includes connectivity screening, endcap-based loading stabilization, and validation against analytical and internal consistency benchmarks. To efficiently explore the expensive high-dimensional design space, two Bayesian optimization strategies are considered: a baseline unconstrained formulation and a feasibility-aware formulation, in which the expected improvement acquisition function is weighted by the predicted probability of geometric feasibility.

The optimization framework successfully identified hybrid TPMS architectures with significantly improved stiffness-to-weight performance compared with canonical references. The best design obtained with the unconstrained Bayesian optimization reached an effective stiffness of approximately 217000 MPa, whereas the feasibility-aware formulation achieved 191000 MPa. Both values substantially exceeded the performance of gyroid and Schwarz P reference structures, which remained close to 100000 MPa under the same conditions. In addition, Bayesian optimization outperformed a multi-seed random-search baseline, showing an improvement of about 32.5 percent at the same evaluation budget. The optimized morphologies consistently exhibited vertically aligned and continuous load-bearing pathways, indicating that the framework captures physically meaningful structural trends rather than isolated numerical optima.

These results show that expanding the TPMS design space through a unified coefficient-based representation, combined with surrogate-assisted optimization and voxel-based mechanical evaluation, enables the discovery of high-performance architected materials beyond canonical minimal-surface families. The comparison between unconstrained and feasibility-aware formulations also highlights the trade-off between peak mechanical efficiency and robustness of the search process. Overall, the proposed framework provides a computationally efficient and mechanically interpretable strategy for the design of optimized TPMS-based metamaterials for lightweight structural applications.

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