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Inverse design of shell-based architected materials via algebraic language models

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Abstract

Generative machine learning models have revolutionized material discovery by capturing complex structure-property relationships, yet extending these approaches to the inverse design of three-dimensional architected materials remains limited by computational complexity and underexplored design spaces due to the lack of expressive representations. Here, we present a new generative framework integrating diffusion transformers with a novel algebraic language representation, encoding 3D geometries as mathematical sentences. This compact, unified parameterization spans diverse topologies while enabling direct application of transformers to structural design. We leverage diffusion models to generate novel shell structures with precisely targeted stress-strain responses under large deformations, accounting for buckling and contact while addressing the inherent one-to-many mapping by producing diverse solutions. Uniquely, our approach enables simultaneous control over multiple mechanical objectives, including linear and nonlinear responses beyond training domains. Experimental validation of fabricated structures further confirms the validity of our approach for accelerated design of architected materials and structures with tailored properties.

Keywords:

architected material metamaterial design machine learning shell buckling