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Customized Design of Amorphous Solids by Generative Deep Learning

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Abstract : The design of advanced amorphous solids, such as metallic glasses, with targeted properties through artificial intelligence signifies a paradigmatic shift in physical metallurgy and materials technology. Here, we developed a machine-learning architecture that facilitates the generation of metallic glasses with targeted multifunctional properties. Our architecture integrates the state-of-the-art unsupervised generative adversarial network model with supervised models, allowing the incorporation of general prior knowledge derived from thousands of data points across a vast range of alloy compositions, into the creation of data points for a specific type of composition, which overcame the common issue of data scarcity typically encountered in the design of a given type of metallic glasses. Using our generative model, we have successfully designed copper-based metallic glasses, which display exceptionally high hardness or a remarkably low modulus. Notably, our architecture can not only explore uncharted regions in the targeted compositional space but also permits self-improvement after experimentally validated data points are added to the initial dataset for subsequent cycles of data generation, hence paving the way for the customized design of amorphous solids without human intervention.

Keywords : metallic glass, artificial intelligence, mechanical property, automated generation
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