Simulation-Informed Models for Amorphous Metal Additive Manufacturing

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Abstract

To enable design of additively manufactured amorphous metal parts with desired mechanical properties, including strength and toughness, we are pursuing simulation-informed modeling as an integral component of a simultaneous design approach. This work involves development of two machine learning frameworks. The first utilizes a variational autoencoder to build connections between experimental nanodiffraction data and atomistic structural glass models. The second develops a data-centric stochastic constitutive formulation of metallic glass plastic constitutive response. Through the interrogation of an 3D atomistic representative volume element of a binary glass, we harvest simulation data that quantifies plastic constitutive response. The resulting data quantifies the stress drops characteristic of metallic glass mechanical response in terms of state variables related to the stress and the structural state of the glass. This data informs a stochastic finite state automata model that can reproduce aspects of the mechanical response and the associated evolution of the material's structural state. This serves as a lower-scale constitutive model for a continuum model capable of achieving predictions of mechanical response on significantly larger length scales. Validation of the continuum model is undertaken in comparison with large scale atomistic simulations. This work is supported by the US National Science Foundation under Grant Nos. DMR-2323718/DMR-2323719/DMR-2323720.

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