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Physics-Aware AI-directed Framework for Microstructural Design of Shocked Materials

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ABSTRACT

Advanced manufacturing technologies enabled the fabrication of complex metamaterial microstructures. However, their complex structure-property-performance (SPP) relationships require costly and laborious experiments, making it impractical to explore the large and complex design space. In this study, we propose a new design framework to discover optimal microstructure designs in an objective (data-driven), efficient, and interpretable manner using deep neural networks. The proposed framework is demonstrated on a problem of optimizing the shock sensitivity of pressed cyclotetramethylene-tetranitramine (HMX), which is an archetype of the complex materials with a strong microstructure influence on the material property and performance. In this framework, we learn micromorphology descriptors using generative adversarial networks (GAN) to depict the latent space and accelerate the estimation of material properties using Bayesian physics-aware recurrent convolutional neural networks (Bayesian-PARC) along with uncertainty in estimation. In conjunction with Bayesian-PARC, the differential evolution approach is employed to practically navigate the design space. As intermediate results, the optimal microstructure candidates with maximal expected improvement of sensitivity produced by Bayesian-PARC and differential evolution are validated against direct numerical simulations (DNS), then the Bayesian-PARC is recalibrated with updated dataset before proceeding to the next iteration. The new framework achieved a significant design improvement compared to the best performing structure in the dataset. We anticipate that the proposed framework will have a broad and significant impact on how complex materials are designed and engineered by giving insights and intuitions to material scientists.