Learning textures via generative machine learning on SO(3) manifold

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Abstract

Microstructure analysis in polycrystalline materials is challenging due to the high dimensionality and non-Euclidean nature of crystallographic orientations (i.e., texture) and the stochastic, multiscale interactions driving microstructural evolution. To this end, we introduce a probabilistic machine learning framework, specifically, a continuous conditional generative machine learning framework, to analyze texture data in the SO(3) manifold. The framework leverages bidirectional transformations to map simple latent distributions to complex target distributions, making them well-suited for capturing the intricacies of high-dimensional texture data. By operating on the SO(3) manifold, the proposed approach directly incorporates crystallographic symmetries and efficiently represents rotational data. Our model captures the relationships between processing parameters and resulting microstructures by embedding them into a low-dimensional, orientation-aware latent space, enabling both process-structure linkage modelling and inverse design through optimization. Furthermore, the model generates microstructures with tailored textures, accurately capturing the distribution of orientations under various conditions. This framework underscores the potential of generative machine learning to advance materials design and microstructural analysis in non-Euclidean domains.

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