Generative machine learning for accelerated modelling of microstructure evolution

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Abstract

Developing sustainable pathways for metal processing is increasingly critical. While recycling can contribute to sustainability, it also introduces variability in material composition, requiring on-demand optimization of processing conditions. Traditional computational models, such as Cellular Automata and Phase-Field methods, are effective for simulating microstructural evolution under specified processing conditions but often face computational bottlenecks, limiting their application in high-throughput and on-demand process optimization. To address this, we present a conditional generative machine learning (ML) framework leveraging GPU-accelerated denoising diffusion probabilistic models (DDPMs) to accelerate microstructural evolution simulations conditioned on processing parameters. Trained on a compact dataset of process–microstructure pairs, this framework first adds noise to microstructure images and then trains a neural network to progressively remove the noise, learning the underlying statistical patterns of the microstructure. We apply this model to predict the microstructural evolution during steel processing conditioned on cooling schedules and alloying element compositions. The model accurately predicts microstructures, capturing key physical features such as phase, carbon distribution, and grain morphology, along with statistical metrics like grain size distribution, phase fraction, and interface area distribution. This approach offers a promising avenue for intelligent, adaptive material design and process optimization across diverse material classes.

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