Generative Diffusion Modeling for Predictive Digital Twins of Sustainable Nanoparticle Electronics Printing

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The distinct geometries, multi-scale material structures, and functional complexities inherent in nanoparticle-based Aerosol Jet Printing (AJP) Additive Manufacturing (AM) require a comprehensive understanding of its diverse physical phenomena to enhance sustainability. With the proliferation of big data, digital twins (DTs) augmented with sophisticated machine learning (ML) techniques improve the comprehension of AJP processes by uncovering crucial causal relationships, notably Process-Structure-Property (PSP) relationships. However, the dynamic intricacies of AJP and the vast quantities and varieties of data present a significant research gap, particularly regarding 1) the integration of causality and 2) the development of sophisticated methods for accurately inferring representations for each modality and their interactions during data fusion. To address this gap, the study presents a generative modeling methodology using a diffusion modeling-based approach, termed AMDiffusion. AMDiffusion facilitates the unprecedented prediction of PSP causal relationships using multi-modal, multi-scale AM data and the generation of newly synthesized PSP features based on learned distributions. The illustrative case study demonstrates how the AMDiffusion methodology adeptly integrates AJP process parameters and printed silver nanoparticle ink lines while capturing new, hidden causal linkage features. By leveraging AMDiffusion's predictive capabilities and focusing on the causal aspects of PSP relationships, this research provides more nuanced and comprehensive insights into nanoparticle electronic printing. Consequently, the proposed methodology has the potential to improve the simulation, prediction, and optimization of nanoparticle printing processes, thereby advancing sustainability via predictive DTs.

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