

Elucidating Material Dynamics: Extracting Phenomena Insights through Virtual Observations

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Understanding material dynamics, encompassing phenomena such as phase transitions and chemical reactions, is imperative for interpreting material responses to fabrication conditions and advancing the development of innovative materials. Advanced microscopy techniques, such as in-situ Transmission Electron Microscopy (TEM) [1] and single-shot Coherent X-ray Diffraction Imaging (CXDI) [2], offer real-time imaging during experiments, providing avenues to explore material dynamics. However, the resultant data, presented as intricate image sequences with nuanced information, poses challenges attributed to sequential correlations and random factors. This research addresses these challenges through the innovative application of deep-learning generative models, transcending their traditional role in data synthesis [3]. Specifically, we propose a framework that integrates a generative model as a data generator for analysis using data-mining methods. The efficacy of the proposed framework is demonstrated through two distinct case studies utilizing CXDI and TEM images, each elucidating the processes of gold nanoparticle diffusion in aqueous media and the lattice transformation of gold nano-contact under deformation. Consequently, these investigations unveil intricate mechanisms governing particle diffusion and lattice transformation. Such detailed examinations underscore the considerable potential of deep-learning generative models in analyzing complex material dynamics data, thus significantly contributing to the progress in the study of material dynamics through the application of advanced instrumentation.

References

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