AtomDiffuser: Time-Aware Degradation Modeling for Drift and Beam Damage in STEM Imaging

CLEMSON UNIVERSITY

UCI University of California, Irvine

Hao Wang[1], Hongkui Zheng[2], Kai He[2], and Abolfazl Razi[1]

[1]Clemson University

[2]University of California, Irvine

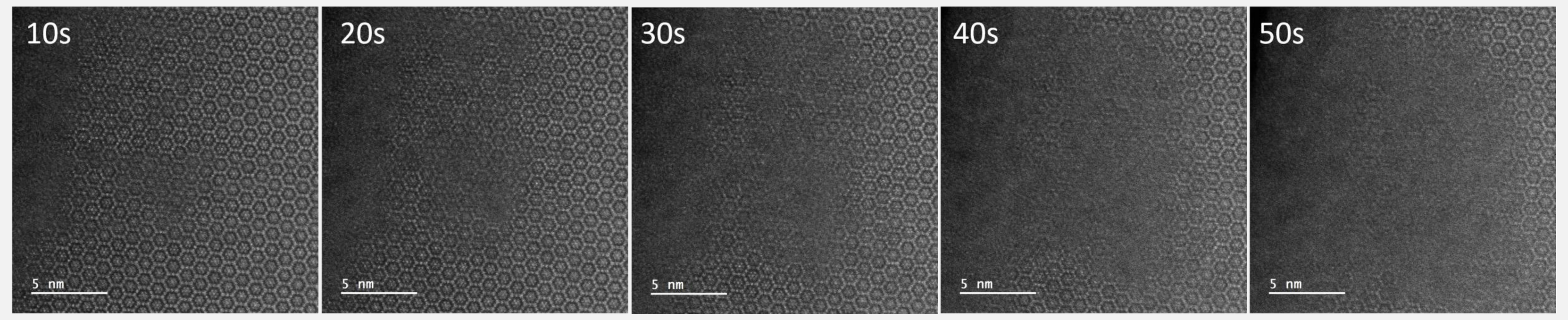
ICCV HONOLULU HAWAII OCT 19-23, 2025

Introduction

Scanning transmission electron microscopy (**STEM**) plays a critical role in modern materials science, enabling direct imaging of atomic structures and their evolution under external interferences. However, interpreting time-resolved STEM data remains challenging due to two entangled degradation effects: spatial drift caused by mechanical and thermal instabilities, and beam-induced signal loss resulting from radiation damage. These factors distort both geometry and intensity in complex, temporally correlated ways, making it difficult for existing methods to explicitly separate their effects or model material dynamics at atomic resolution. In this work, we present **AtomDiffuser**, a time-aware **degradation modeling** framework that disentangles sample drift and radiometric attenuation by predicting an affine transformation and a spatially varying decay map between any two STEM frames. Unlike traditional denoising pipelines, our method leverages degradation as a physically heuristic, temporally conditioned process, enabling interpretable structural evolutions across time. Trained on synthetic degradation processes, **AtomDiffuser** also generalizes well to real-world **cryo-STEM data**. It further supports high-resolution degradation inference and drift alignment, offering tools for visualizing and quantifying degradation patterns that correlate with radiation-induced atomic instabilities.

Background

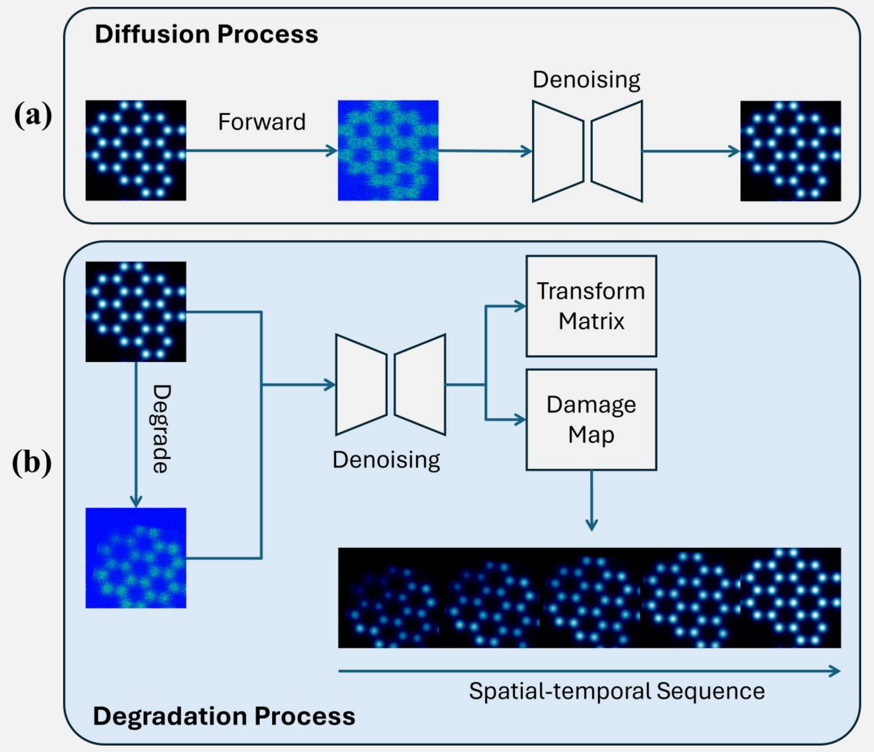
Scanning transmission electron microscopy (STEM), transmission electron microscopy (TEM), and cryogenic variants (cryo-STEM/TEM) enable visualization of individual atomic columns and structural changes under controlled environments.



For instance, the garnet-type solid **$Li_7La_3Zr_2O_{12}$ (LLZO)** is a promising candidate for solid-state lithium batteries. However, its crystal lattice is prone to beam-induced degradation even under cryogenic temperatures, and tools for quantitatively analyzing such degradation pathways remain limited due to its current way of imaging.

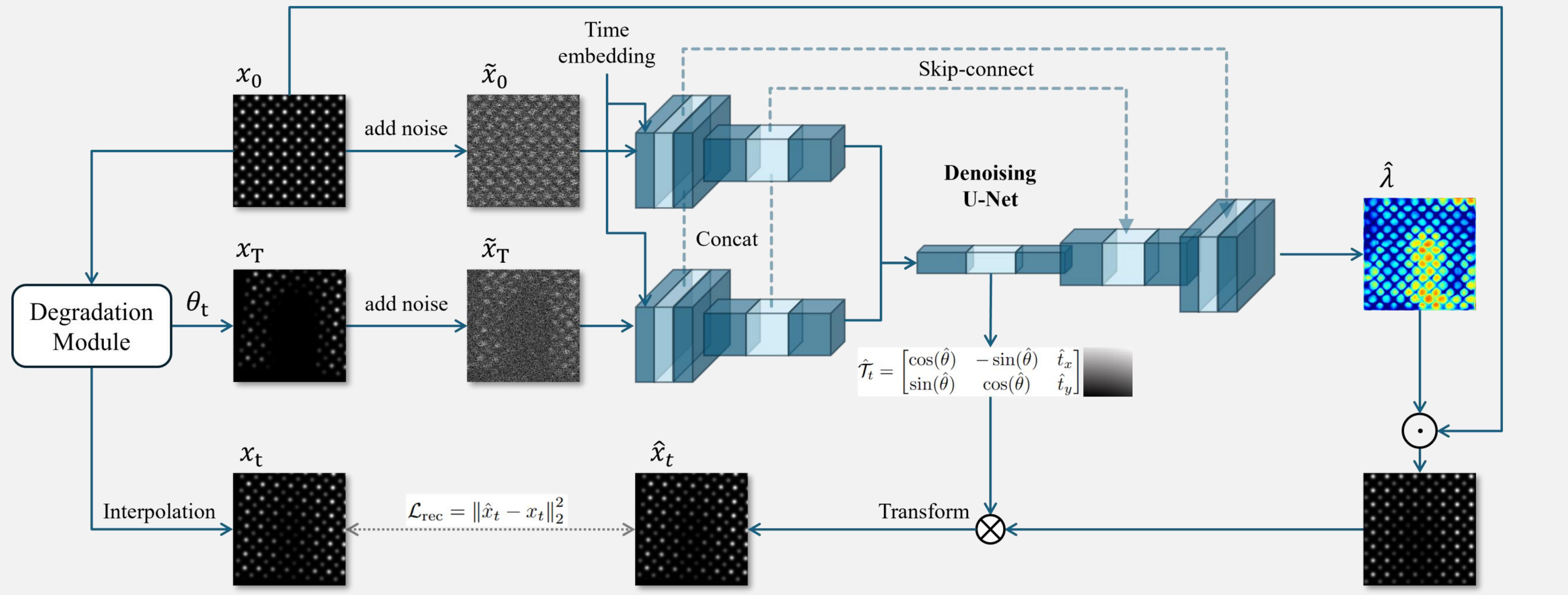
During atomic-resolution STEM imaging, two degradation mechanisms: **atomic drift** and **beam-induced damage**, intertwined, pose challenges to accurate structural interpretation. Disentangling these two mechanisms is essential for reliable interpretation of material behavior.

To address these challenges, we present **AtomDiffuser**, a diffusion-variant spatiotemporal degradation model that disentangles atomic drift and beam-induced damage from sequential STEM image pairs.



Methods

End-to-end prediction of atomic changes in STEM sequences, such as directly regressing x_t from x_0, is often unreliable due to the presence of noise, sparsity, and large-scale rigid motion. To address this, we adopt a degradation modeling approach inspired by diffusion models, enabling continuous and physically interpretable modeling of structural evolution. While classical diffusion models have shown strong performance in generative and denoising tasks by learning to reverse a stochastic corruption process, they are less suited for modeling physically driven phenomena such as drift or beam damage.



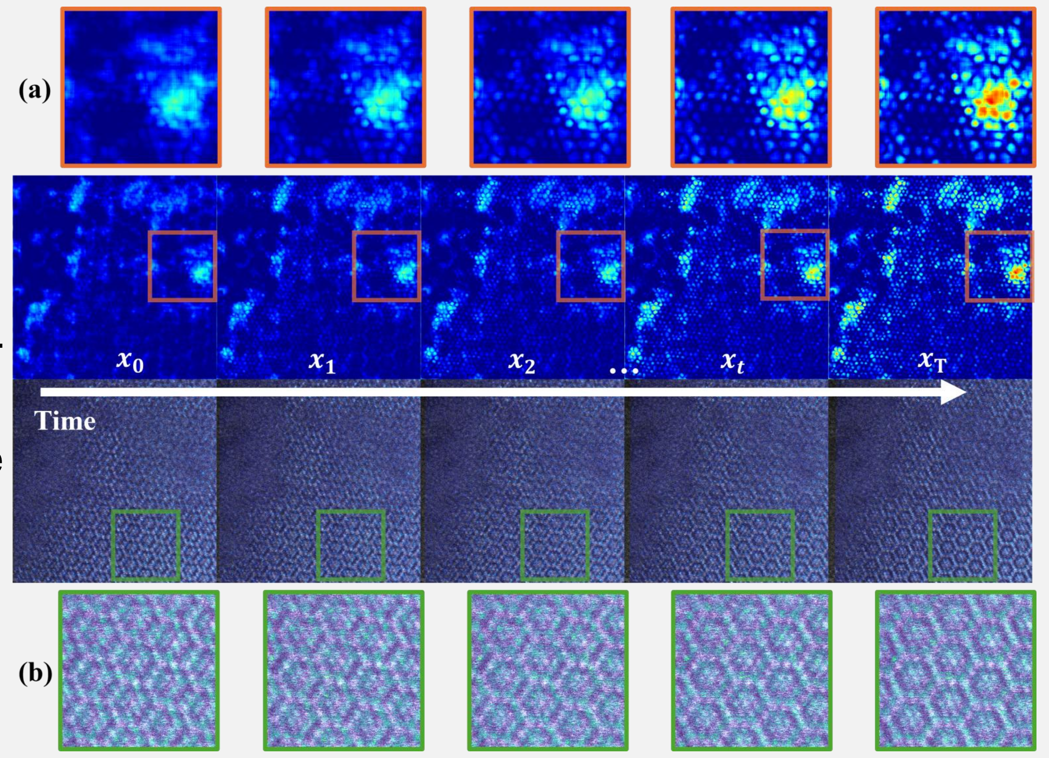
In contrast, deterministic degradation models, such as ***Cold Diffusion***, replace the stochastic noise process with a physically interpretable degradation process.

This preserves temporal consistency and structural semantics while aligning more naturally with real-world degradation patterns, allowing the degraded state x_t to be computed directly from any time step t, which is consistent with the classical DDPM.

Experiments

To demonstrate the full potential of **AtomDiffuser**—the ability to continuously infer between frames and explore material characteristics by observing beam damage progression without the interference of sample drifting, we apply the model to two consecutive frames selected from a high-resolution **cryo-STEM** dataset of the garnet-type solid electrolyte **LLZO.**

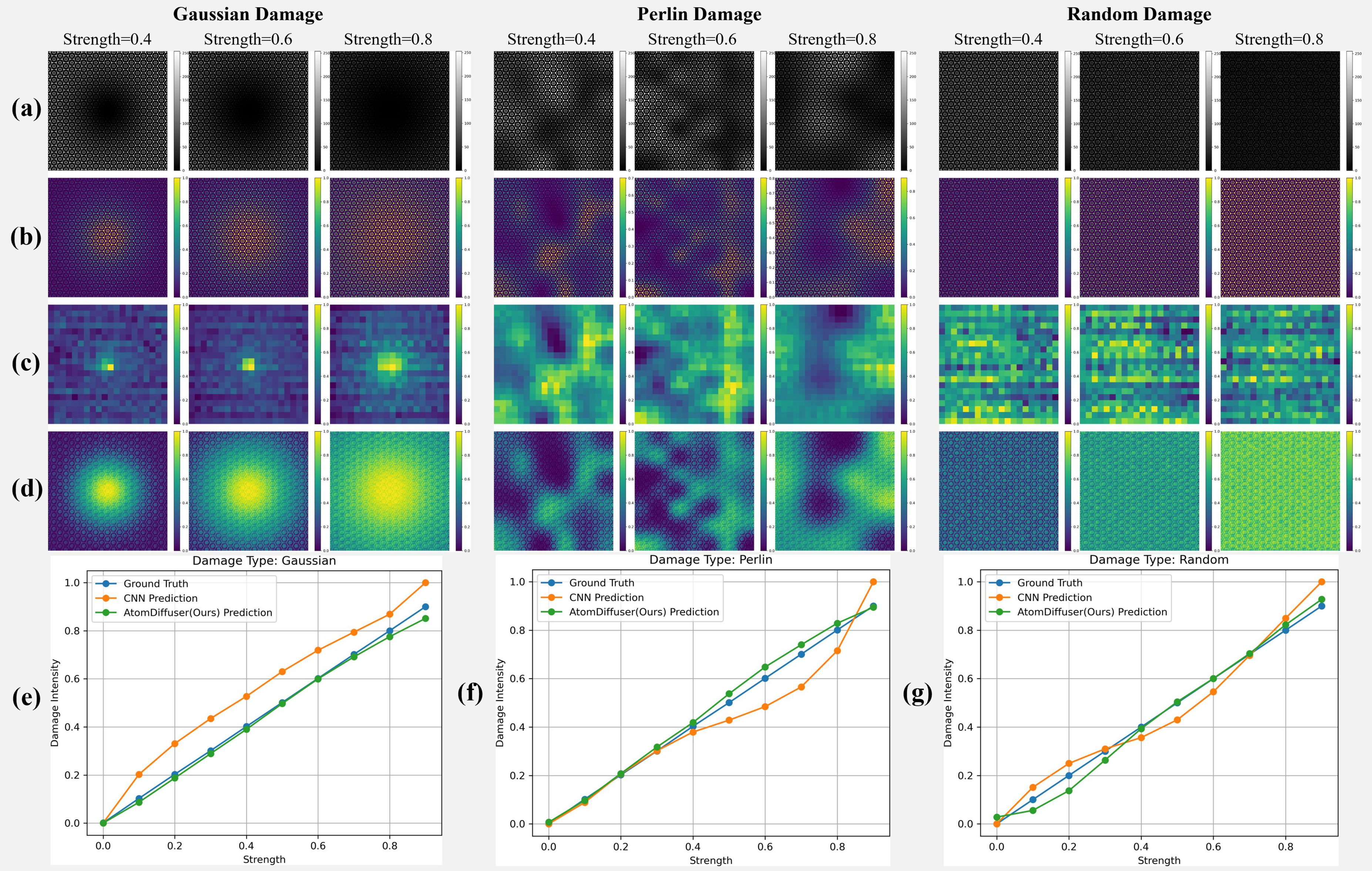
Specifically, given two frames x_0 and x_T, the model generates intermediate degradation states, including motion T and decay factor **lambda**, by varying the time input. Notably, the target frame x_T exhibits both atomic drift and beam-induced damage relative to x_0, indicating the two frames are both misaligned and structurally dissimilar.



Results

To evaluate the model's ability to estimate beam-induced signal degradation independently of spatial drift, we perform a controlled experiment using a fixed synthetic atomic image. We generate degradation-only sequences by applying progressive attenuation while introducing one of three noise types: (1) **Gaussian** noise with structured black hole artifacts, (2) Low-frequency **Perlin** noise, (3) **Random** noise mimicking scan jitter and long-range distortions.

Each sequence consists of ten frames with linearly increasing damage intensity, ranging from **0** (undamaged) to **0.9** (severely degraded), and no geometric transformation is applied. This setting isolates the signal decay process, allowing us to assess the model's capacity to infer spatially varying attenuation under different degradation conditions.



To assess the spatial quality of the predicted decay maps, we conduct side-by-side comparisons with a **CNN-based** baseline. While the CNN performs well under the Perlin setting, our model produces full-resolution predictions aligned with the input image dimensions, enabling fine-grained localization of damage regions.

Acknowledgments

NSF Award #2239598,

UCI Materials Research Institute,

UCI Center for Complex & Active Materials (DMR-2011967)

Special thanks to organizers of the Computer Vision for Materials Science (**CV4MS**) workshop

Please check our paper & code below:

AIS Clemson

Paper

Code