AFM-SPARK (Sparse Patch Assisted Reconstruction Kernel)

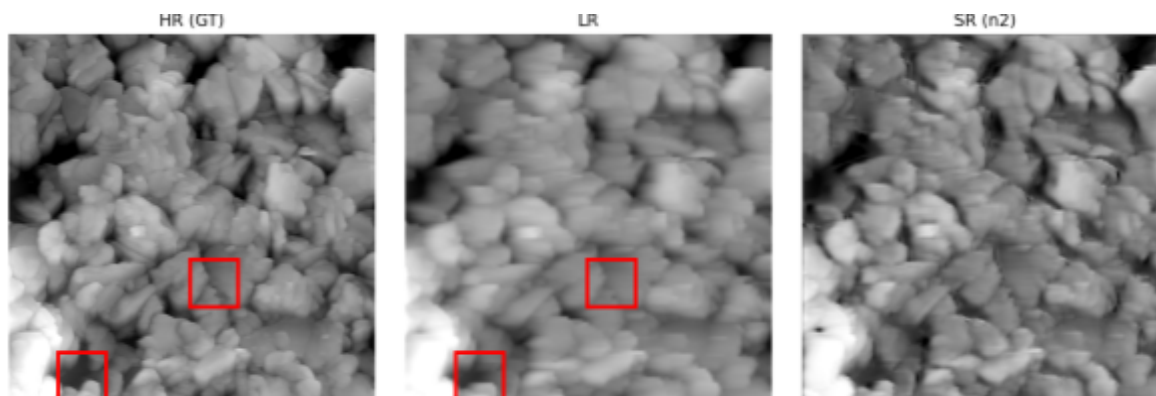Youngwoo Choi, Seunghwan Ryu, Junho Yang, Jihui Won, Sanggil Park, Chaeyul Kang

Background and Introduction

Atomic force microscopy (AFM) enables quantitative surface analysis with nanometer-scale resolution, but obtaining high-resolution (HR) imaging is impractical due to its point-by-point raster scanning. While faster tip motions allow rapid imaging over wide areas, the resulting low-resolution (LR) scans often miss critical nanoscale details. Recent AFM Super-Resolution (SR) studies formulate reconstruction as a supervised single-image LR-to-HR mapping learned with CNN (Convolutional Neural Network) or Transformer-based model. For example, Xun et al. introduced the More Rational Transformer (MRT), which combines attention mechanism with depth-wise convolution to improve reconstruction fidelity[1]. However, when LR inputs are generated solely by down-sampling HR AFM images, the resulting training pairs may fail to capture acquisition-specific features and artifacts that emerge in real high-speed AFM scans.

In this work, we propose a AFM high-resolution imaging framework based on experimental intuition. Physics-based simulations of the AFM imaging process are used to generate precisely aligned LR and HR image pairs for training a flow matching model. The DTM constructs train datasets by degrading high-resolution AFM images into low-resolution counterparts via controlled scan-rate modulation.[2] Moreover, train dataset includes corresponding partial high-resolution regions. During inference, a global LR image and a limited number of HR measurements selected by a rule-based algorithm are used to reconstruct a global HR AFM image, reducing experimental acquisition time while preserving image fidelity. The key novelty of this work is that it explicitly treats each upscaling problem as system specific tasks. By reconstructing the image through the exact image content, we offer a path that realizes measurement and materials specific features, ultimately proving the model's capability of one AFM image instance regime.

Results

Methods

Image Preparation:
Graphite: 80 × 80 μm HeightRetrace image was acquired at 512 ×512 pixels using an AFM MFP-3D (Assylum Research), and was used as ground-truth.

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[1] ACS Appl. Nano Mater. 2024, 7, 22, 25470–25479

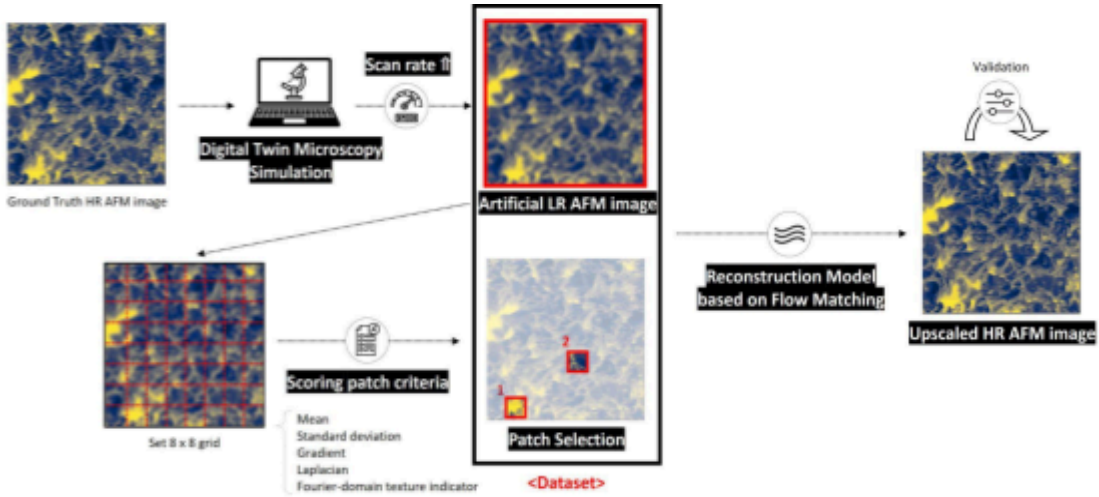[2] https://github.com/pycroscopy/DTMicroscope.git

Workflow

Figure 2. The schematic of AFM-SPARKS. During data preprocessing, the ground-truth (GT) and Low-resolution (LR) images were loaded. LR image was divided in to a 8 × 8 grid, resulting in 64 × 64 pixels patch. For each patch, 5 indicators were used to compute a patch score, then information-rich patches were selected using a farthest-first strategy while partially weighting the gradient (slope) and laplacian indicator (curvature). After the rescaling of LR image sizes, image pairs (global LR and partial HR patches) at identical coordinates were chosen as training data.

In real experiments, LR-HR pairs can become misaligned due to drift during repeated scans; therefore, DTM-based simulation was used to maintain consistent measurement conditions when constructing the dataset. Detailed process is described in Figure 2.

Model Training:
The model was trained using a flow-based super-resolution approach. For each training step, an intermediate state between a low-resolution patch and its high-resolution ground truth was generated using a randomly sampled time variable. The model learned to predict the transformation direction that moves the intermediate state toward the high-resolution target. Training was guided by a velocity matching loss, with additional gradient and edge losses to preserve structural details in microscopy images. A subset of patches was used for training, and the remaining patches were used for validation.

Conclusions
We performed three key tasks to enable super-resolution reconstruction of AFM image from sparse high-resolution observations and enlarger low-resolution frame: selecting informative measurement patches from the global low-resolution scan, constructing aligned and consistently normalized LR–HR training pairs based on the selected regions, and training a conditional flow-matching model that learns the LR-to-HR transport dynamics for faithful image recovery.

Future Works
We suggest two directions for future work based on the current project. First, our current patch selection is still rule-based. So future work should define an elaborate selection criterion that targets HR regions that most improve the final SR reconstruction. Second, we only created LR images by changing scan speed, but real AFM images can be low quality for many other reasons, such as tip shape changes, PID noise, drift, and line artifacts. Providing the degradation parameters as conditioning inputs would build a robust framework when applying to real experimental measurements.