Summary of Papers regarding: Autonomous Tip Conditioning

Contents

Conclusion

Automated Tip Conditioning for Scanning Tunneling Spectroscopy

[1] S. Wang, J. Zhu, R. Blackwell, and F. R. Fischer, "Automated Tip Conditioning for Scanning Tunneling Spectroscopy," *The Journal of Physical Chemistry A*, vol. 125, no. 6, pp. 1384–1390, Feb. 2021, doi: 10.1021/acs.jpca.0c10731.

Method Overview

Wang et al. (2021) develop a fully automated, closed-loop protocol to prepare atomically sharp scanning-tunneling-microscope (STM) tips at 4.2 K. Their routine alternates between "conditioning" (mechanical pokes) and "assessment" ($\frac{dI}{dV}$ spectroscopy + machine-learning classification) until two consecutive spectra indicate a high-quality tip, or until all candidate sites are exhausted and the scan area shifts.

Workflow Steps

1. **Image Acquisition & Flattening**
   - Capture a 100 nm × 100 nm topograph at $V_{\text{bias}} = 50$ mV, $I_t = 20$ pA.
   - Remove tilt by fitting a plane to either the entire image (uniform surfaces) or three widely separated flat regions (stepped/molecular surfaces).
2. **Surface Segmentation**
   - Build a height histogram.
   - Detect peaks and group pixels within ±0.05 nm of each peak into "terrace" labels.
3. **Site Selection**
   - Slide a 5 nm × 5 nm window across the image.
   - Select centers of uniformly labeled squares at least 15 nm apart as conditioning sites.
4. **Conditioning & Assessment Loop**
   1. Move the tip to the chosen site; perform a 2 nm "poke."
   2. Record two dI/dV spectra (lock-in frequency = 455 Hz, modulation = 10 mV).
   3. Normalize the second spectrum over −1.5...2.0 V (896 points).
   4. Classify with an AdaBoost model:

   - **Good:** mark success; two consecutive "good" → terminate.
   - **Bad:** repeat poke + spectroscopy at the same site.
5. **Scan-Area Shift**
   - If no site yields two good spectra, shift the scan window by 100 nm in X or Y and repeat from Step 1 until piezo limits are reached.

Key Findings & Recommendations

- **AdaBoost** offers the best balance of accuracy, precision, recall, and implementation simplicity.
- Deep nets require more computational overhead and careful tuning.
- The closed-loop poke, measure, classify cycle converges to a publication-quality tip in fewer than ten attempts on average.

Short Method Summary

An automated loop acquires and flattens STM images, segments flat terraces, selects conditioning sites, and iteratively "pokes" and measures dI/dV spectra at each site. A lightweight AdaBoost classifier judges tip quality; two consecutive "good" calls end conditioning. If all local sites fail, the scan region shifts and the process repeats until a sharp tip is achieved.

Autonomous In Situ Tip Conditioning via Machine Learning

[2] M. Rashidi and R. A. Wolkow, “Autonomous Scanning Probe Microscopy in Situ Tip Conditioning through Machine Learning,” *ACS Nano*, vol. 12, no. 6, pp. 5185–5189, Jun. 2018, doi: 10.1021/acsnano.8b02208.

Method Overview

Rashidi & Wolkow (2018) present an automated routine for in situ conditioning of STM tips during hydrogen-terminated Si(100) experiments. A convolutional neural network (CNN) analyzes isolated dangling-bond images to detect degraded (“double”) tips; upon detection, controlled tip indentations restore sharpness until the CNN confirms a single-atom apex.

Workflow Steps

1. **Data Acquisition & Preprocessing**
   - Collect ~3500 STM sub-images of isolated dangling bonds at $-1.8\,\mathrm{V}$, $50\,\mathrm{pA}$ ($5.6 \times 5.6\,\mathrm{nm}^2$).
   - Resize each to 28×28 px; augment by four 90° rotations and mirror (×8 total).
2. **Baseline Benchmark (Pearson Correlation)**
   - Compute Pearson’s coefficient against sharp-tip references.
   - Grid-search threshold yields 77 % classification accuracy.
3. **Model Training & Selection**
   - Evaluate KNN (k = 5), RFC (5000 trees), SVM (RBF kernel, C = 500, $\gamma = 0.5$), FCNN (18 layers × 784 nodes), and CNN.
   - Optimal CNN: conv5×5 filters (30 → 40 channels, stride 1) → max-pool 2×2 → dense 128 nodes (ReLU) → softmax output; trained with Adam (lr 10^{-4}), cross-entropy loss.
4. **Automated Tip-Conditioning Loop**
   1. Acquire full-frame STM image; detect and extract dangling-bond patches.
   2. Classify each patch via CNN; perform majority voting across N patches (>99 % reliability).
   3. If tip = “double,” perform indentation at a user-preset spot: approach 700 pm → 1 nm beyond setpoint (-1.8 V, 50 pA), incrementing by 10 pm on failure.
   4. Repeat acquisition and classification until CNN outputs “sharp.”
5. **Integration with Atomic Fabrication**
   - Demonstrated during binary atomic wire patterning: routine paused fabrication only to recondition when tip degraded, then resumed seamlessly.

Key Findings & Recommendations

- **CNN** outperforms classical and shallow ML methods, achieving 97 % raw accuracy and >99 % with voting.
- Majority voting over multiple defects significantly reduces misclassification risk.
- Framework is generalizable to any surface with recurrent atomic features (e.g., defects, adsorbates).

Short Method Summary

A loop extracts dangling-bond images, classifies tip quality with a CNN, and performs controlled indentations until tip sharpness is confirmed, enabling uninterrupted, autonomous atomic-scale fabrication.

Scanbot: An STM Automation Bot

[3] J. Ceddia, J. Hellerstedt, B. Lowe, and A. Schiffrin, "Scanbot: An STM Automation Bot," *Journal of Open Source Software*, vol. 9, no. 99, p. 6028, Jul. 2024, doi: 10.21105/joss.06028.

Method Overview

Ceddia et al. (2024) introduce Scanbot, a Python-based "robot" that fully automates key STM tasks—tip conditioning, sample surveying, and data acquisition—by coordinating piezoceramic scanners with a real-time camera feed and requiring **Nanonis V5** control software for STM integration.

Workflow Steps

1. **DSH Calibration & Tip Tracking**
   - Initialize camera feed to locate and track the STM tip apex and target positions on both the sample and a clean reference metal.
   - Use piezoceramic scanner commands (via Nanonis V5 API) to maneuver the tip between regions.
2. **Sample Survey & Site Identification**
   - Acquire a coarse topographic map of the sample area.
   - Identify regions of interest (flat, debris-free patches) on both the sample and the clean metal for imaging and conditioning.
3. **Tip-Shaping Loop**
   1. **Imprint Generation**: Gently impinge the tip onto the clean reference metal to leave an atomic-scale imprint.
   2. **Imprint Imaging**: Scan the imprint region to produce an image that reflects the tip's geometry.
   3. **Quality Assessment**: Measure **area** and **circularity** of the imprint; compare against predefined thresholds.
   4. **Conditional Shaping**:
      - If criteria are met → tip deemed "sharp."
      - If not → perform a more aggressive poke at a new location on the metal and repeat steps 1-4.
4. **Resumption of Data Acquisition**
   - Once the imprint satisfies quality metrics for two consecutive assessments, automatically return the tip to the sample of interest and resume STM imaging or spectroscopy.

Key Findings & Recommendations

1. **Software Compatibility** Scanbot is compatible with any STM system controllable via **Nanonis V5**.
2. **Modular Design** All core functionalities are hook-based, allowing labs to plug in custom imaging or conditioning routines without modifying the Scanbot core.
3. **Imprint-Based Metrics** Quantitative analysis of imprint geometry (area & circularity) provides a robust, microscope-agnostic metric for tip quality.
4. **Performance** Demonstrated reliable convergence to high-quality tips in a handful of shaping cycles, reducing manual overhead.

Short Method Summary

Scanbot leverages **Nanonis V5** control software to orchestrate a closed-loop sequence, camera-guided tip positioning, imprint-based tip-shaping on a clean reference metal, and quantitative image analysis, automatically restoring and maintaining an atomically sharp STM probe before returning to the sample for uninterrupted, high-resolution data acquisition.

Automated Scanning Probe Tip State Classification without Machine Learning

[4] D. S. Barker, P. J. Blowey, T. Brown, and A. Sweetman, "Automated Scanning Probe Tip State Classification without Machine Learning," *ACS Nano*, vol. 18, no. 3, pp. 2384–2394, Jan. 2024, doi: 10.1021/acsnano.3c10597.

Method Overview

Barker et al. (2024) present a template-matching (TM)–based approach to classify STM tip state directly from a single topographical image without requiring large labeled data sets or machine learning. Their LabVIEW scripts interface with an RC5 **Nanonis** controller to automate image acquisition, classification, and in situ tip conditioning via bias pulses and nano-indentations.

Workflow Steps

1. **Image Acquisition & Preprocessing**
   - Acquire constant-current STM topographs (20×20 nm^2, 720×720 px) at system-specific biases and setpoints (e.g., 2 V/200 pA for Si(111) 7×7).
   - Flatten images and remove bottom scan lines to avoid creep artifacts.

2. **Template Matching Classification**

   1. **Cross-Correlation (CC)**
      - Choose a small reference template (e.g., corner-hole on Si(111) 7×7 or dangling bond on B:Si(111)).
      - Compute the cross-correlation ratio (CCR) feature map by scanning the template over the input image.
      - Aggregate top N CCR peaks to derive a single metric; classify as **Good** or **Bad** based on an empirically determined threshold.

   2. **Circularity Measurement (for adatoms)**
      - Locate adatom via CC; normalize and binarize the region at multiple thresholds (0.4-0.7).
      - Compute circularity $C(r) = \frac{\sigma(r)}{\bar{r}}$ across thresholds; classify based on threshold (e.g., C $<$ 0.035 denotes **Good**).

3. **Automated Tip Preparation Loop**
   - Repeatedly acquire images and classify tip state.
   - If **Bad**, move 200 nm away, apply bias pulses and indentations of increasing magnitude to condition the tip.
   - After a set number of shaping attempts or upon classification as **Good**, return to imaging site or shift scan area using the coarse motor.

Key Findings & Recommendations

1. **Accuracy & Precision** TM classifier achieves 90% accuracy and >95% true-positive precision (TPP) on Si-based surfaces, comparable to CNN models and human operators.

2. **Minimal Overhead** Requires only a single **Good** reference image; no training or large labeled data sets needed.

3. **Wide Applicability** Effective on systems with repeating surface features; flexible to new substrates by selecting appropriate templates.

4. **Robust Automation** Integrated within LabVIEW and RC5 **Nanonis** for a fully autonomous tip conditioning tool, achieving a **Good** tip in 12 shaping events (10 min).

Short Method Summary

A LabVIEW–driven tool using an RC5 **Nanonis** controller automates STM tip state classification via cross-correlation and circularity template matching, then performs bias-pulse and indentation conditioning until consecutive **Good** classifications restore an atomically sharp tip for uninterrupted high-resolution imaging.

Automated Structure Discovery for Scanning Tunneling Microscopy*

[5] L. Kurki, N. Oinonen, and A. S. Foster, “Automated Structure Discovery for Scanning Tunneling Microscopy,” *ACS Nano*, vol. 18, no. 17, pp. 11130–11138, Apr. 2024, doi: 10.1021/acsnano.3c12654.

Method Overview

Kurki et al. (2024) present **ASD-STM**, a machine-learning pipeline that predicts atomic structure directly from bond-resolved STM images by training an Attention U-Net on simulated STM/AFM datasets. No real-time STM control is required; the method operates on acquired images

Workflow Steps

1. **Synthetic Dataset Generation**
   - Compute electronic states for ~81,000 organic molecules using FHI-aims (PBE functional).
   - Simulate constant-height STM images via PPSTM (Bardeen tunneling theory) and AFM images via PPAFM over a range of tip–sample distances.
   - Generate atomic disk descriptors (size $\propto$ covalent radius, brightness $\propto$ height) for training
2. **Machine Learning Model Training**
   - Formulate as an image-to-image task: STM image $\rightarrow$ atomic disk descriptor.
   - Develop an Attention U-Net with encoder-decoder blocks and attention gating.
   - Train in PyTorch for 50 epochs on 180 k training images (with noise and cut-outs), validate on 20 k, and test on 35.5 k images
3. **Inference & Validation**
   - Apply the trained model to experimental bond-resolved STM images of various organic molecules.
   - Assess performance: ~1 % mean absolute error on simulated images; ~91 % atom-level and ~74 % ring-level accuracy on hydrocarbons.
   - Demonstrate qualitative chemical identification (H vs C vs O) and discuss limitations on challenging cases

Software Requirements

1. FHI-aims for electronic structure calculations
2. PPSTM & PPAFM for STM/AFM simulations
3. PyTorch for ML model implementation and inference

Key Findings & Recommendations

1. **High Prediction Accuracy** Mean absolute error ~1 % on simulated images; ~91 % atom accuracy on experimental STM
2. **No Real-Time Control Needed** Decouples ML from instrument operation: runs post-acquisition on standard STM images.
3. **Generalizable Pipeline** Synthetic-dataset approach enables extension to diverse molecules without modifying STM control software.
4. **Future Directions** Incorporate simultaneous AFM signals, vary tip-orbital contributions, and tailor datasets for specialized molecular domains.

Short Method Summary

ASD-STM trains an Attention U-Net on a large, simulated STM/AFM image dataset (via FHI-aims, PPSTM, PPAFM), then predicts atomic structure from a single experimental STM image with high accuracy, requiring only PyTorch for inference and no specialized STM control software.

Bibliography

[1] S. Wang, J. Zhu, R. Blackwell, and F. R. Fischer, "Automated Tip Conditioning for Scanning Tunneling Spectroscopy," *The Journal of Physical Chemistry A*, vol. 125, no. 6, pp. 1384–1390, Feb. 2021, doi: 10.1021/acs.jpca.0c10731.

[2] M. Rashidi and R. A. Wolkow, "Autonomous Scanning Probe Microscopy in Situ Tip Conditioning through Machine Learning," *ACS Nano*, vol. 12, no. 6, pp. 5185–5189, Jun. 2018, doi: 10.1021/acsnano.8b02208.

[3] J. Ceddia, J. Hellerstedt, B. Lowe, and A. Schiffrin, "Scanbot: An STM Automation Bot," *Journal of Open Source Software*, vol. 9, no. 99, p. 6028, Jul. 2024, doi: 10.21105/joss.06028.

[4] D. S. Barker, P. J. Blowey, T. Brown, and A. Sweetman, "Automated Scanning Probe Tip State Classification without Machine Learning," *ACS Nano*, vol. 18, no. 3, pp. 2384–2394, Jan. 2024, doi: 10.1021/acsnano.3c10597.

[5] L. Kurki, N. Oinonen, and A. S. Foster, "Automated Structure Discovery for Scanning Tunneling Microscopy," *ACS Nano*, vol. 18, no. 17, pp. 11130–11138, Apr. 2024, doi: 10.1021/acsnano.3c12654.