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Automated Tip Conditioning for Scanning Tunneling Spectroscopy

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" (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_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

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 $28 \times 28\,\mathrm{px}$; augment by four 90° rotations and mirror ($\times 8$ 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 ($-1.8\,\mathrm{V}$, $50\,\mathrm{pA}$), 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.