NanoScale 2026

14th Seminar on Quantitative Microscopy (QM) and

10th Seminar on Nanoscale Calibration Standards and Methods

Dimensional and related measurements in the micro- and nanometre range

NPL, TEDDINGTON, ENGLAND
OCTOBER 20TH ~ 22ND, 2026

Organized by



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AFM 3D tip shape reconstruction using known tip characterizers with different shapes

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Keywords: AFM tip, nanometrology, known tip characterizers, computation

Atomic Force Microscope (AFM) topographies are the results of the tip-sample convolution, in which lateral measurements are mostly influenced by the tip shape. Knowing the shape and size of AFM tips is essential in several fields, such as biological applications, since it enables traceable nanomechanical measurements of biological and soft materials, and in nanoelectronics and semiconductor industries, in which there are increasing challenges in measuring nanostructures.

Between the several methodologies for AFM tip reconstruction available in the literature, the present research focus on the “known tip characterizer” methods. An open-source Python module was developed to obtain a 3D reconstruction of the tip shape by eroding the real topography with the ideal generated tip characterizer. By using a ray tracing approach, it is possible to generate multiple models of the expected size and orientation, and analyze them using an image recognition algorithm to fit the ideal structures under the measured data.
The "Known tip characterizer" method, that usually reconstruct the tip by using known simple geometries (such as spheres), suffer from slow computation time required for the processing of a single topography and lack of a robust method to estimate the position, rotation and scale of the tip characterizer.

In this work, a new methodology that overcomes these limitations is implemented. The flexibility of the method is increased by using tip characterizers of arbitrary shape, once an adequate model for the shape and size simulation is provided. Moreover, improvements in computation methodology allows to reach near real time speeds, enabling to gather information about the deconvolved sample much faster than traditional methods, providing a robust method to estimate the position, rotation and scale of the tip characterizer. The computation time was reduced by exploiting GPU-based implementation, that averages a speedup of 1000x compared to the CPU implementation for topographies of size 1024x1024 pixels, reaching speeds of 250 ms for a single reconstruction. The new algorithm proposed is based on a geometric search of the best fit of the model, which requires performing a sequence of deconvolution operations and model optimizations.

The first results show that the new method can reconstruct the tip shape with a high degree of accuracy, with values close to the tip manufacturer’s specifications.