AFM tip reconstruction with known tip characterizers in Python environment

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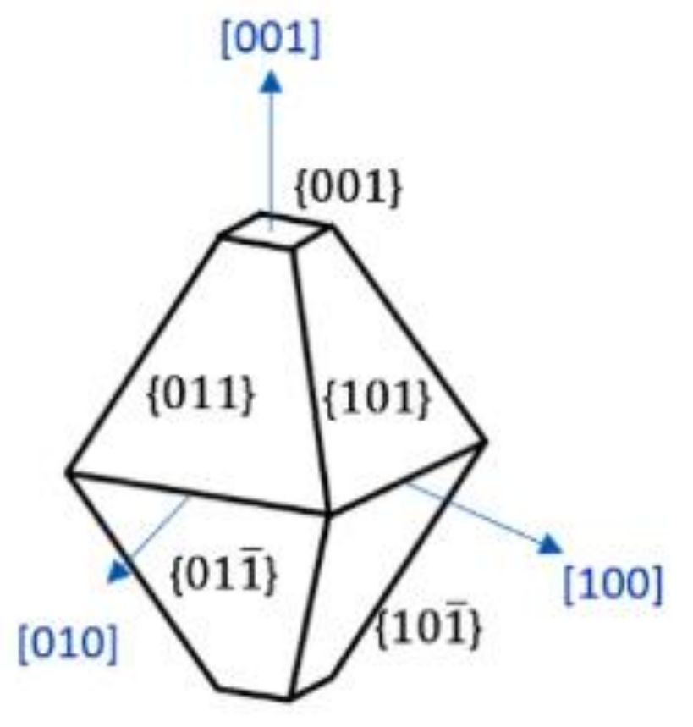
ABSTRACT

Nanometrology covers a wide range of techniques for the characterization and measurement of different kind of materials at the nanoscale. In particular, Atomic Force Microscopes (AFMs) are used to measure topographies with high resolution on the Z axis. The tip of the microscope plays a fundamental role in the reconstruction of the real image, and its shape must be reconstructed before analysing the collected data. Several methods for AFM tip reconstruction are presented in literature, which can be divided into two main approaches for in situ characterisation, which are blind reconstruction and known tip characteriser techniques. In [1, 2, 3] a geometrical method for tip reconstruction, using TiO_2 nanosheets, tobacco mosaic viruses as known characterizers was described.

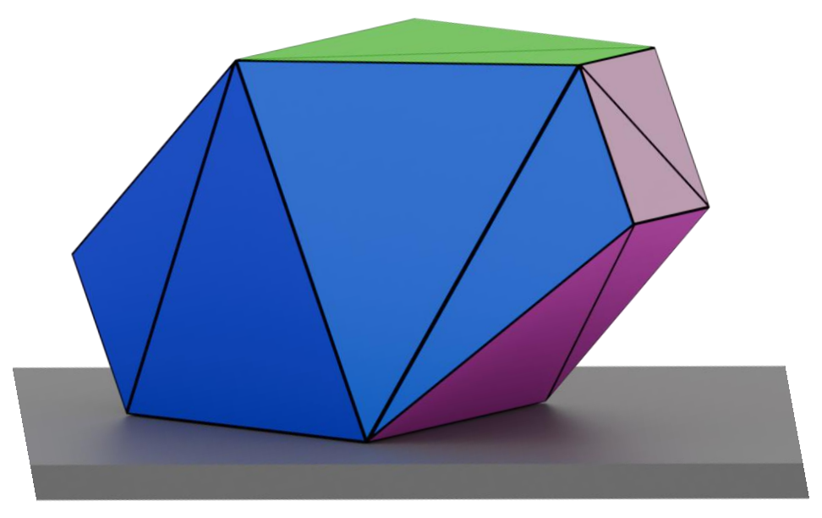
In this work, we generalize this approach to any ideal structure, and we implement routines for the procedural generation of height maps with multiple tip characterisers. Our goal is to create a Python module that helps generating the ideal topography of the tip characteriser, and then reconstructs the tip shape by eroding the real measurement with the generated structure.

RAY TRACED STRUCTURE GENERATION



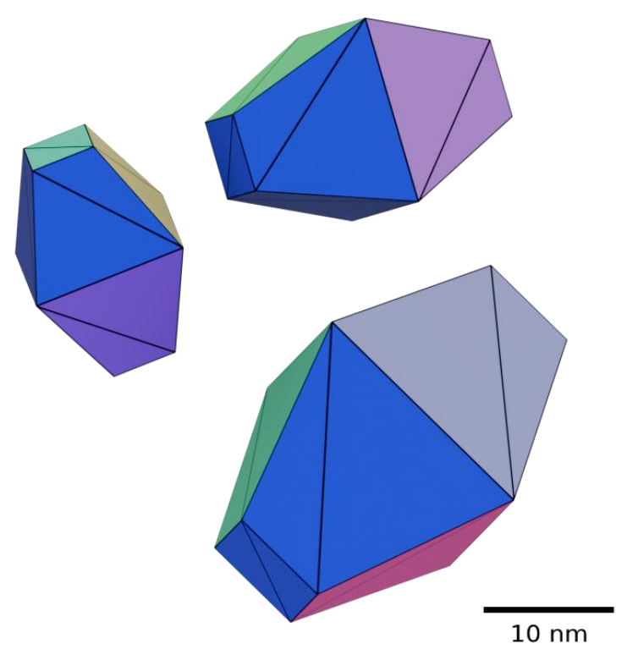
Crystalline structure of an anatase TiO₂ bipiramid

MODEL



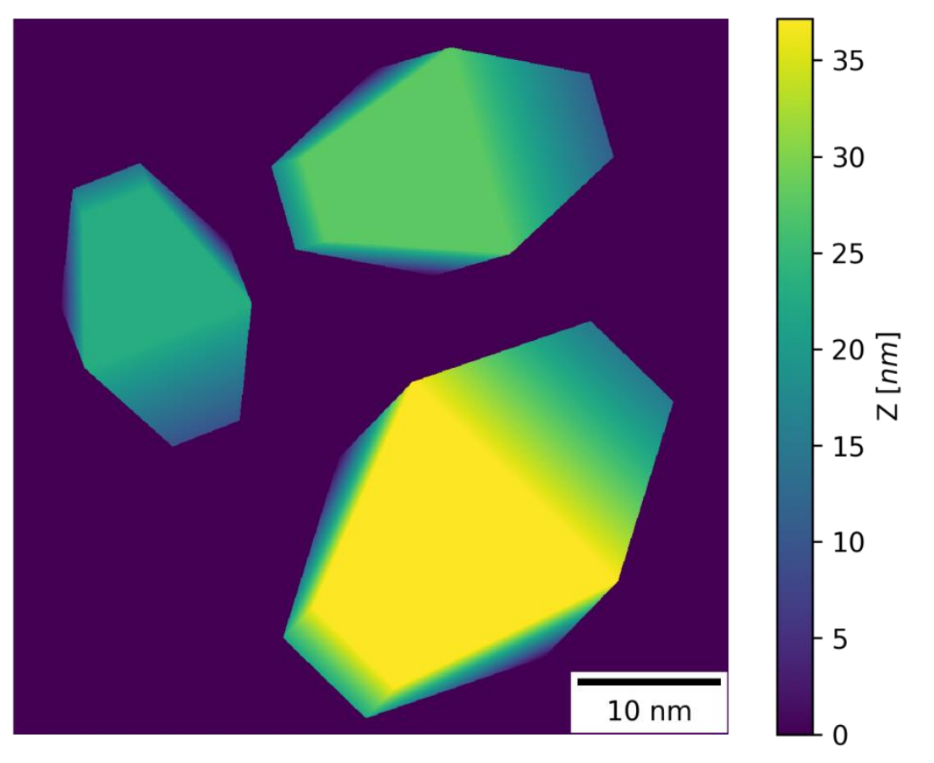
Generated model of a nanoparticle lying on a substrate

MESH



Generated mesh of multiple nanoparticles

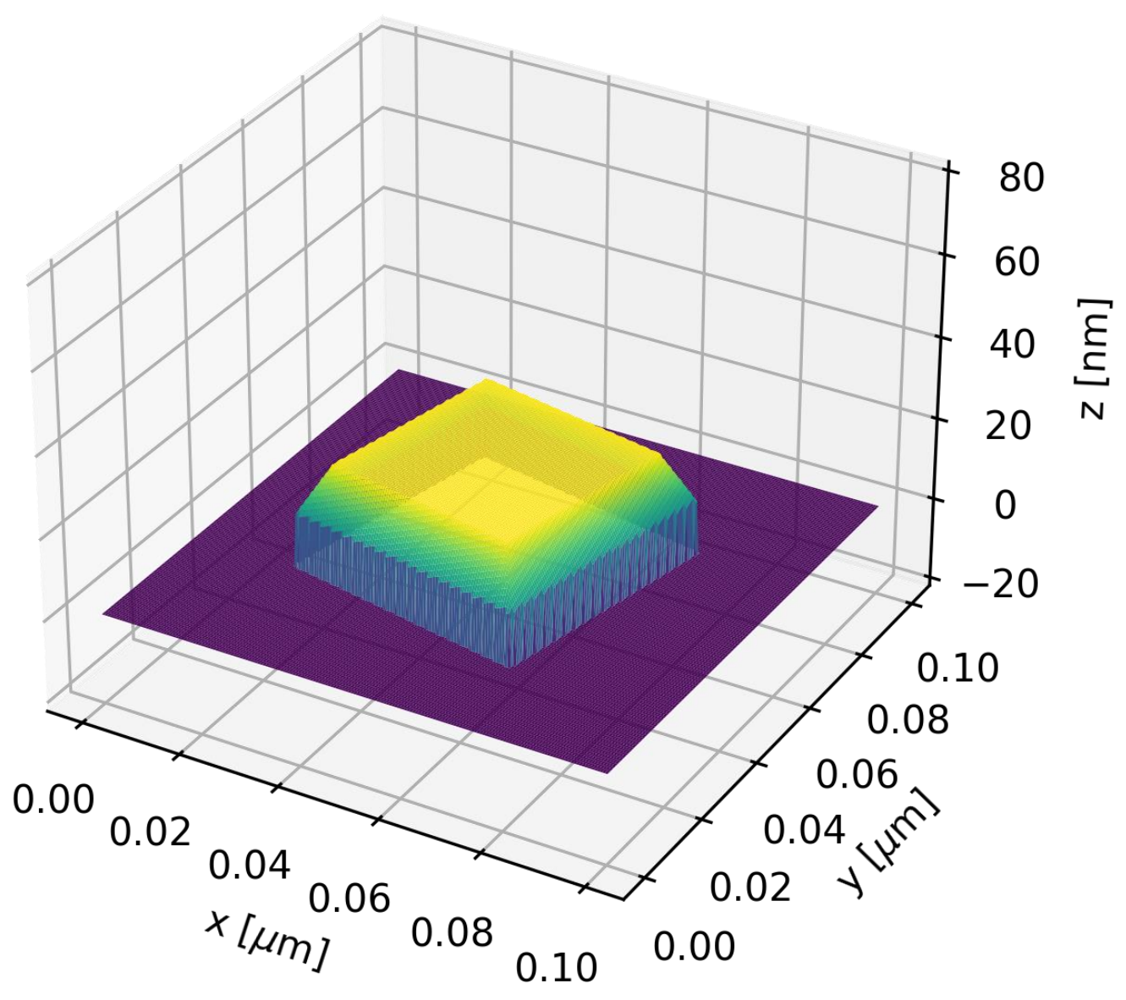
RASTERIZATION



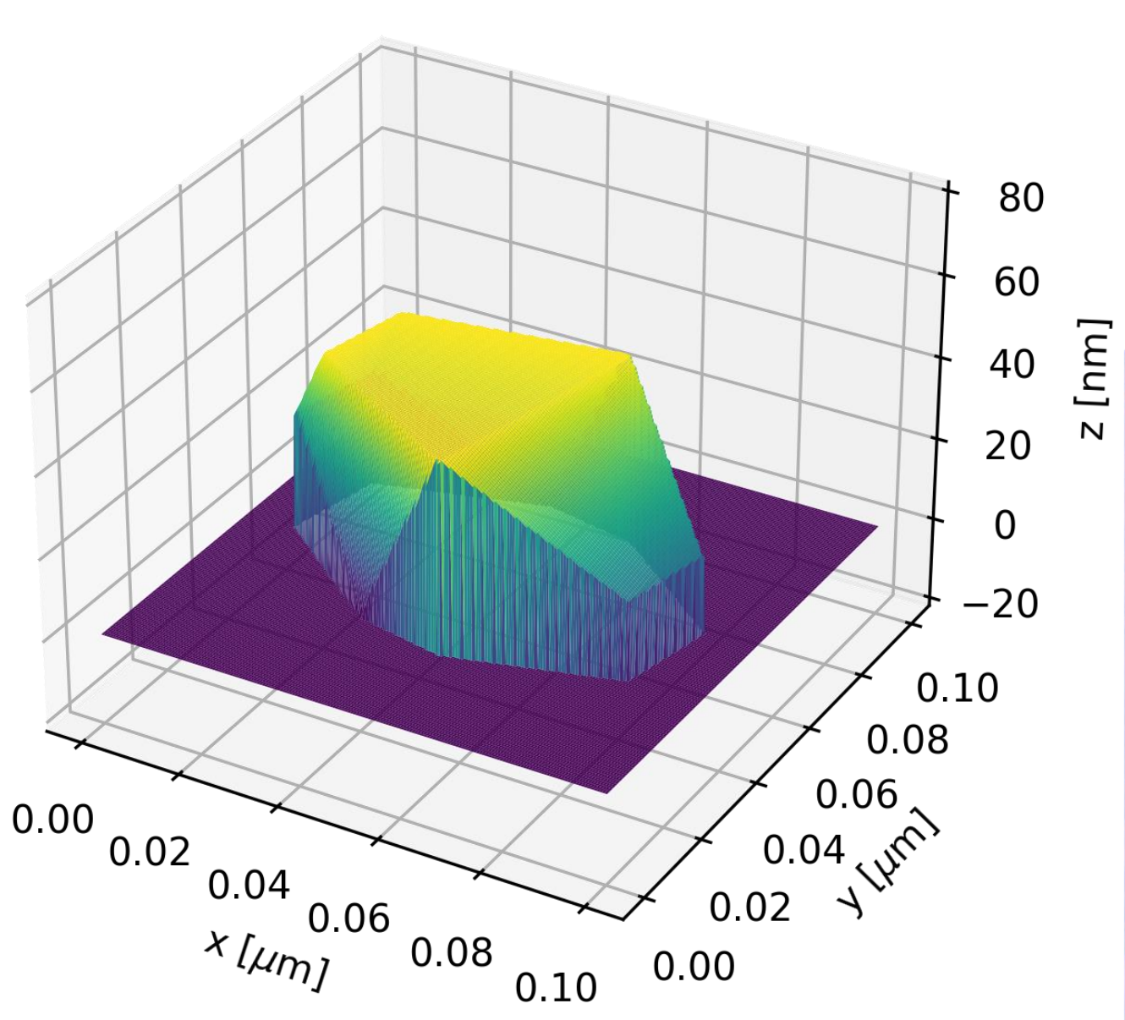
Generated ideal topography

The general method used to create different structures is based on the generation of meshes made of triangles using known dimensional parameters. These meshes can then be rendered using a technique called z-test (also known as depth-test) which relies on testing the distance at which a certain point is from the planar camera. If another point that should be drawn in the same pixel results to be closer, it will substitute the previous one thus ensuring a correct occlusion handling. We can then create a standard and normalized model of each structure we want to study (spheres, cubes, steps, etc..) and given an external input of parameters generate the model of the correct size, orientation and position using scaling, rotation and translation operators.

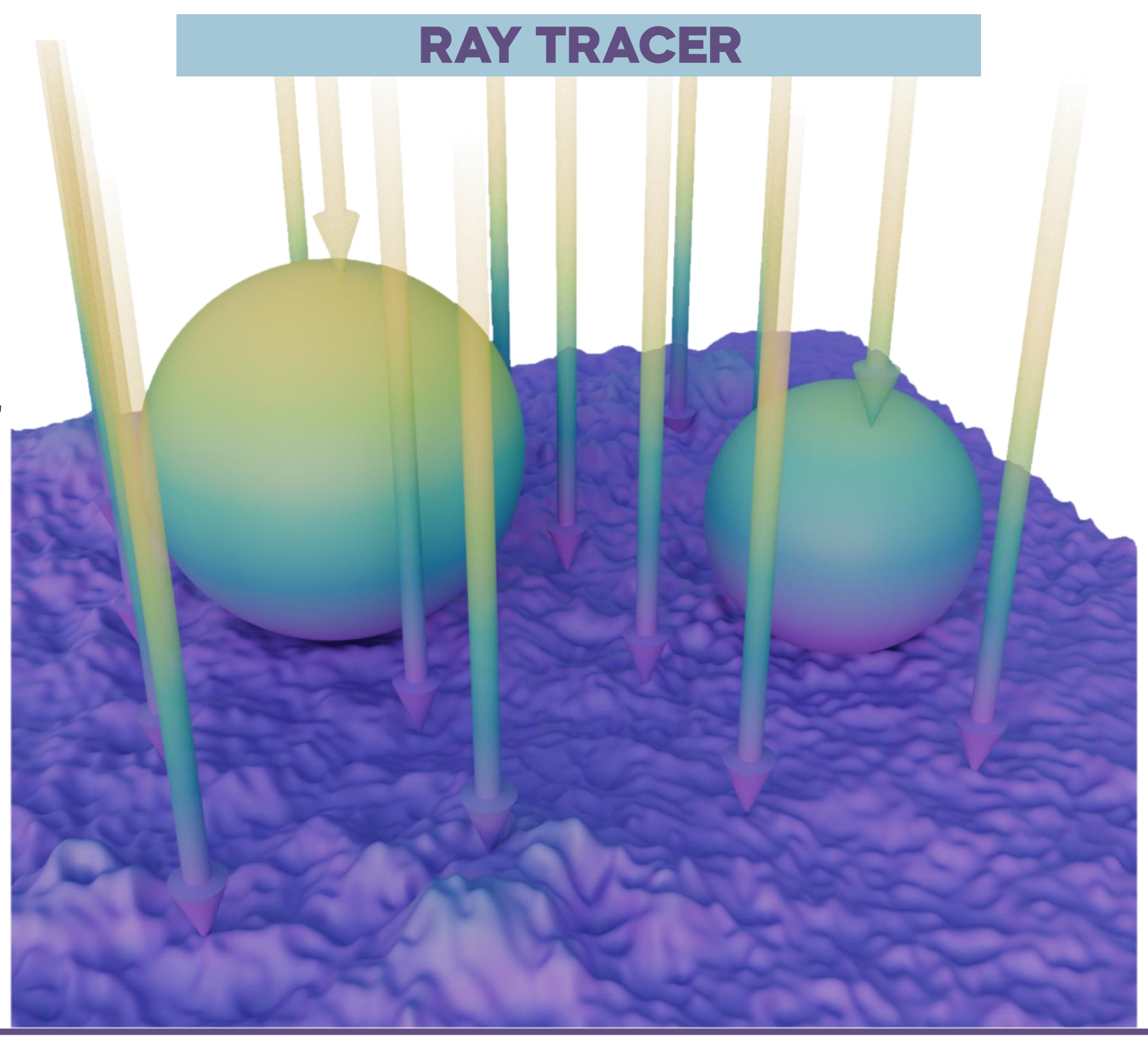
TiO_2 NANOSHEET



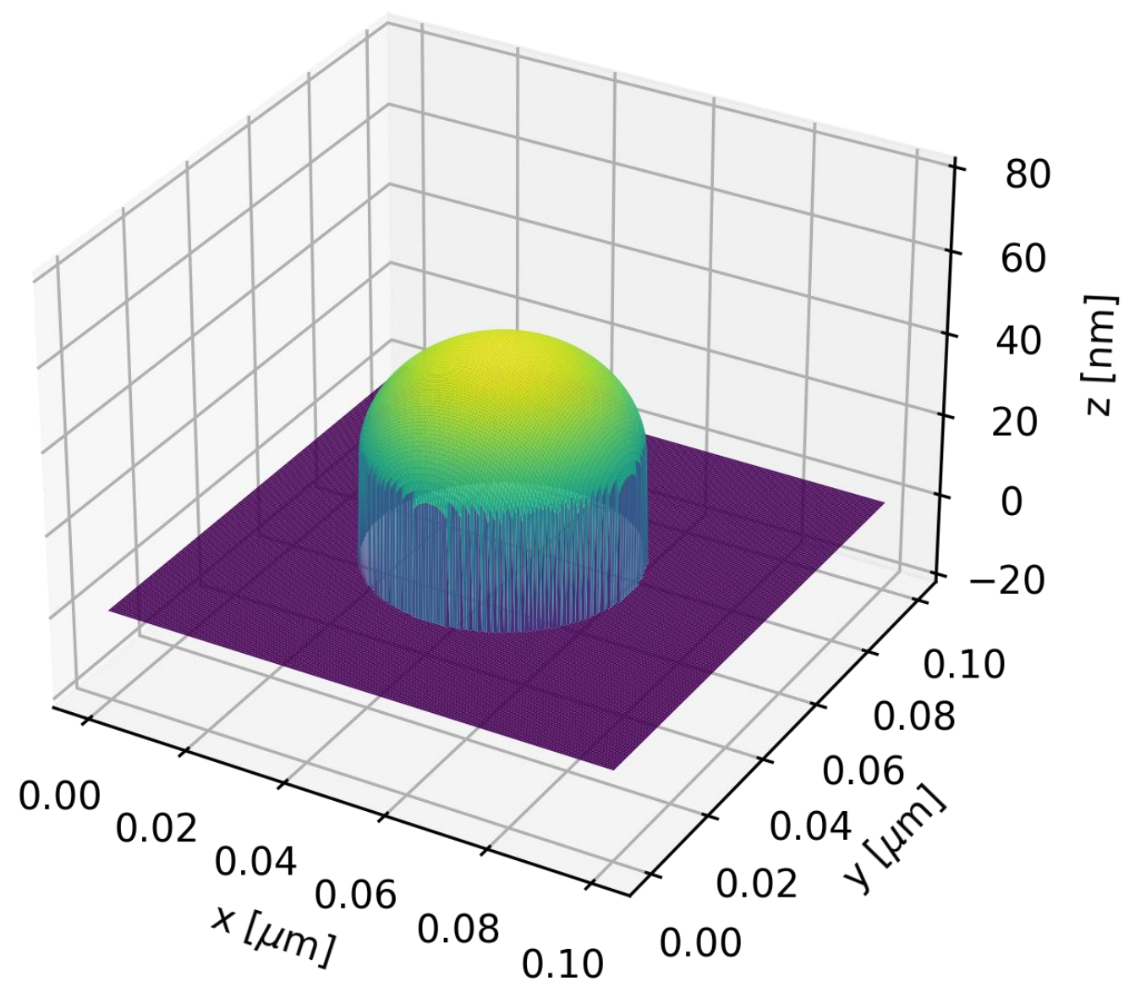
TiO_2 BIPIRAMID



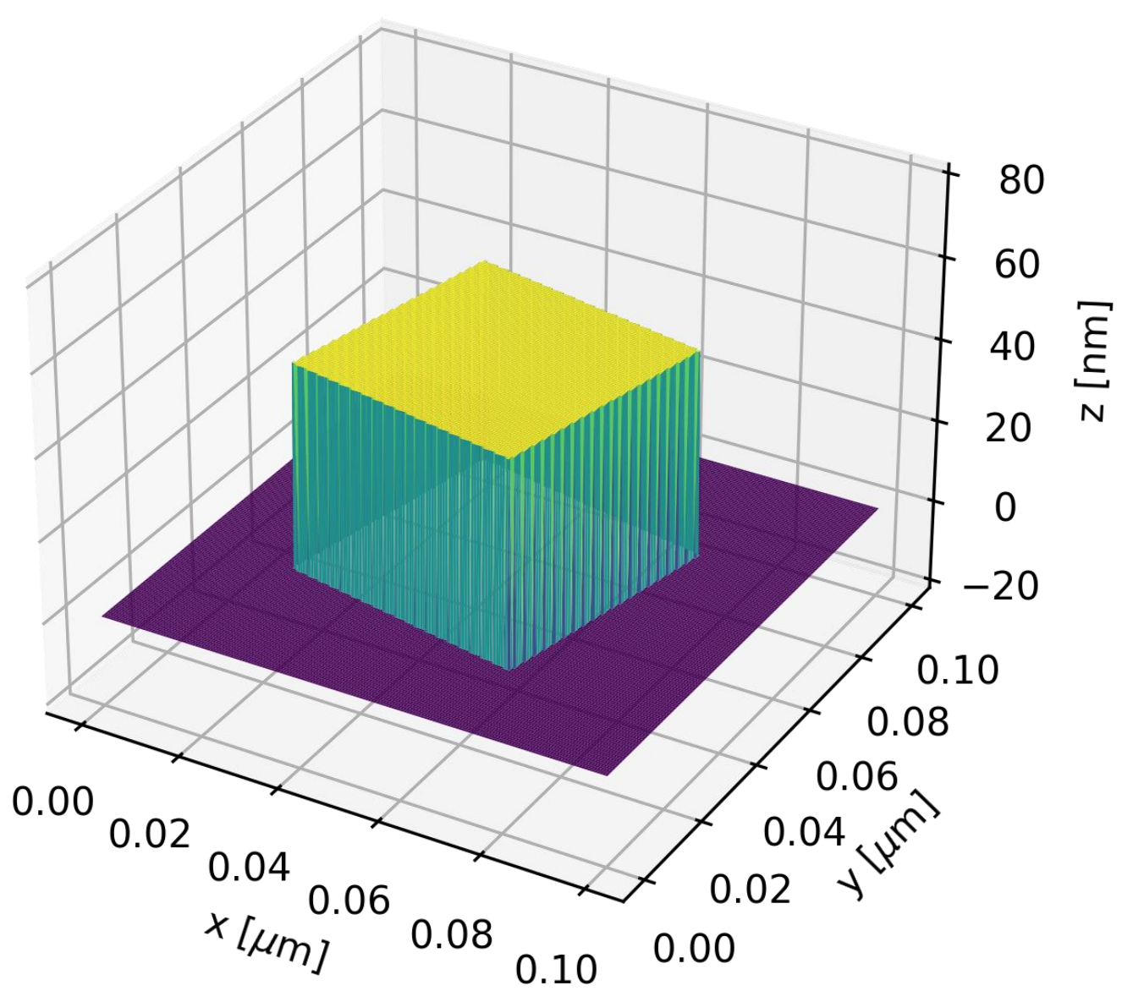
RAY TRACER



SPHERE

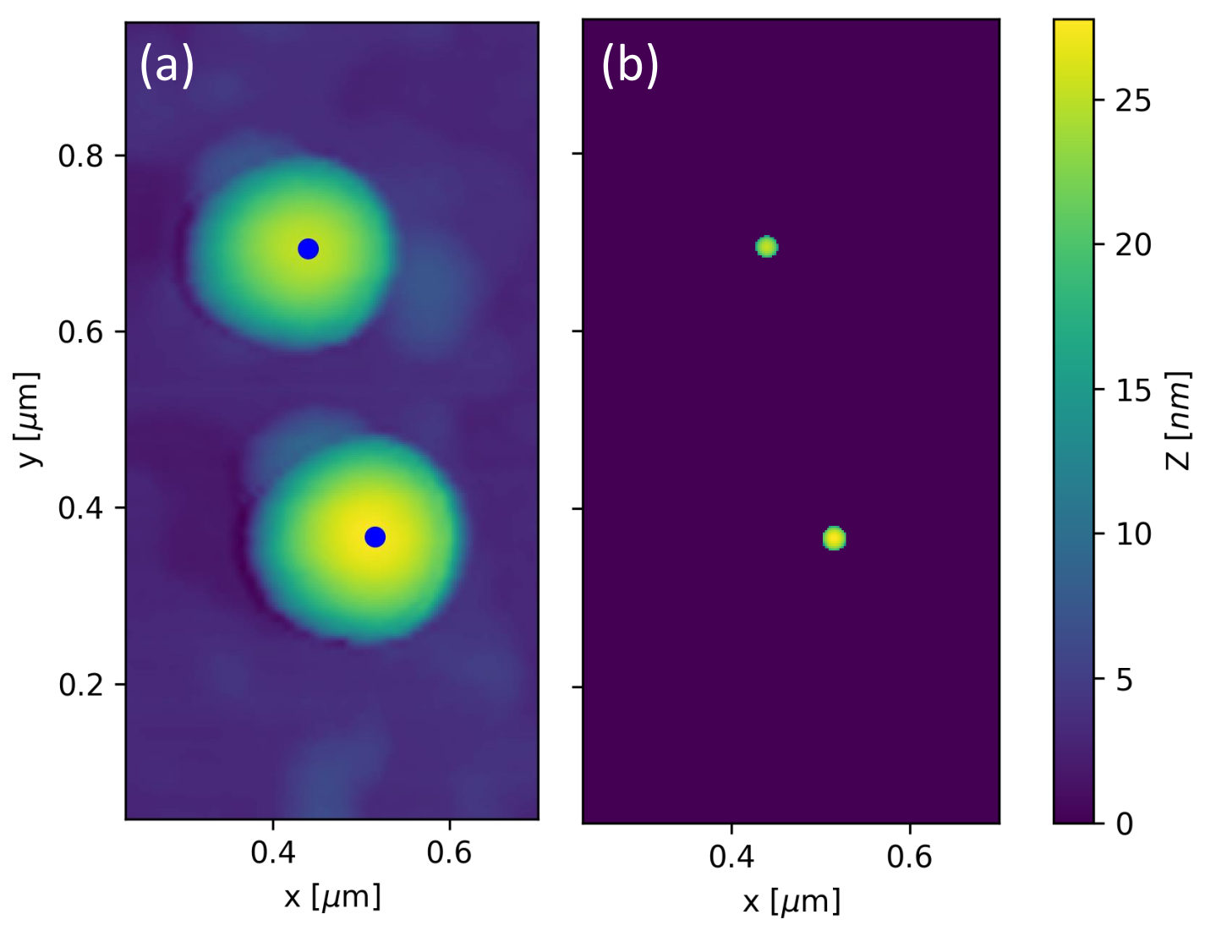


CUBE



STRUCTURE FITTING AND TIP DECONVOLUTION

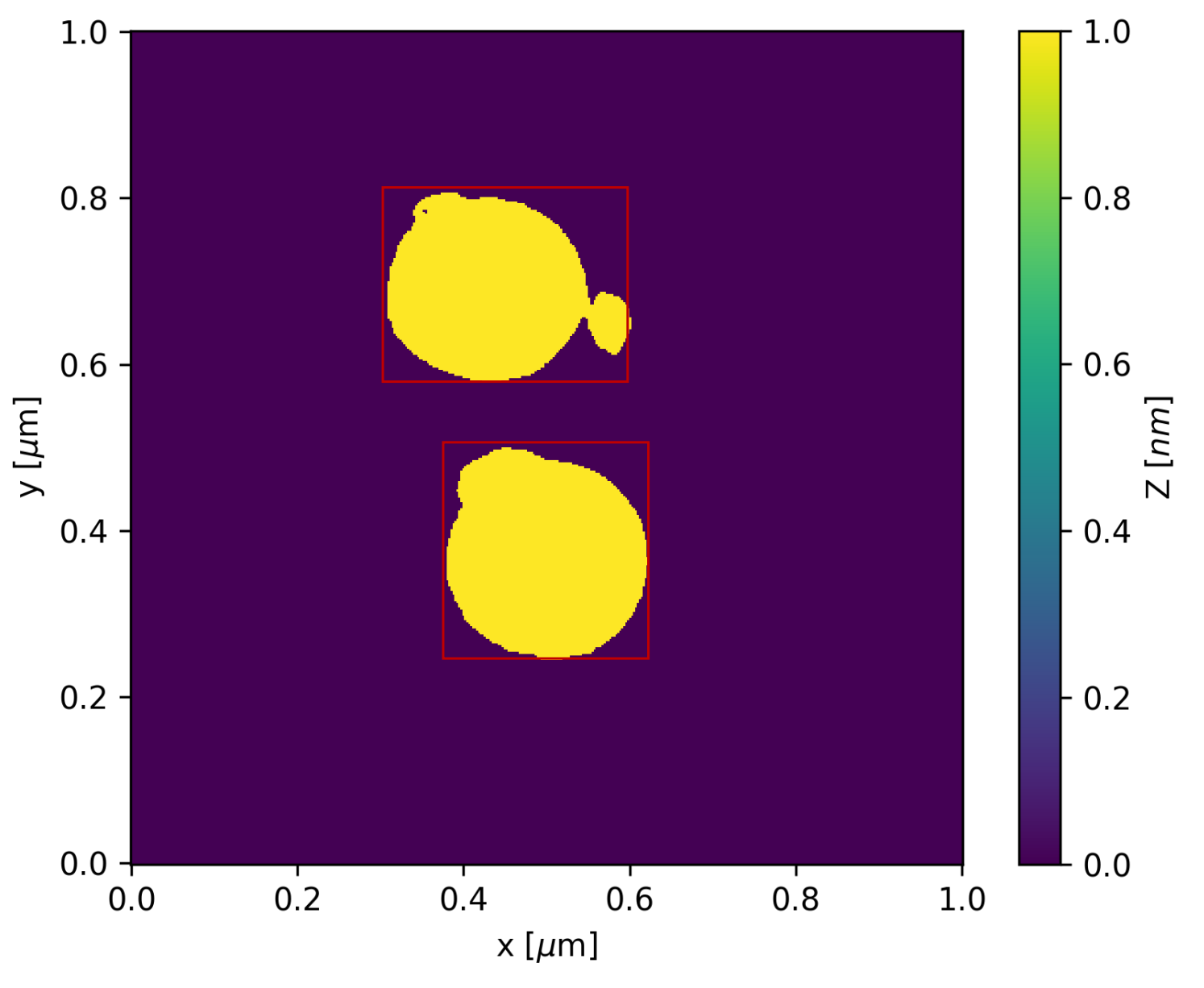
1. STRUCTURE FITTING



(a) measured topography with maximum filter, (b) reconstructed structure

This algorithm is used to find the best position and parameters of an ideal structure that needs to be fitted under the measured AFM data. The program begins by finding the maximum peaks in the image using a maximum filter. Then it calculates the best parameters of the structure under analysis and generates it in the best position and rotation using the ray tracer pipeline described before.

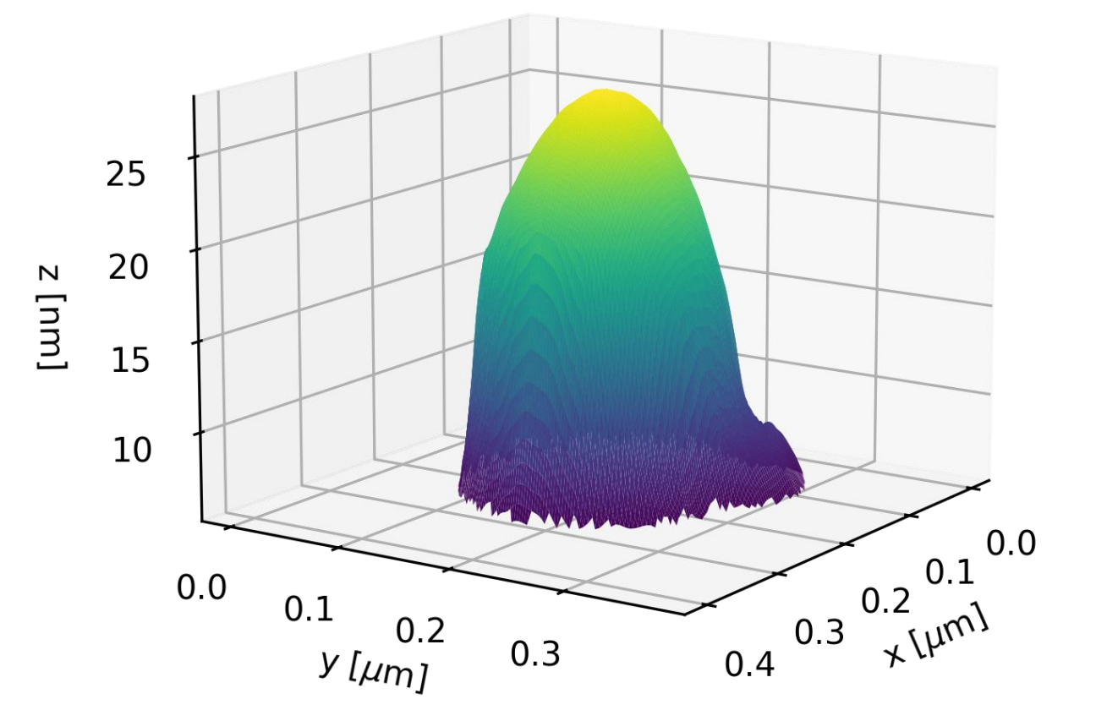
2. TIP SIZE ESTIMATION



Boolean mask and particle bounding box size

The tip matrix size must be estimated to cover the largest sample present in the image. Using a Boolean mask of the measured topography it is possible to detect the dimensions in x and y directions of the nano-particles.

3. TIP RECONSTRUCTION

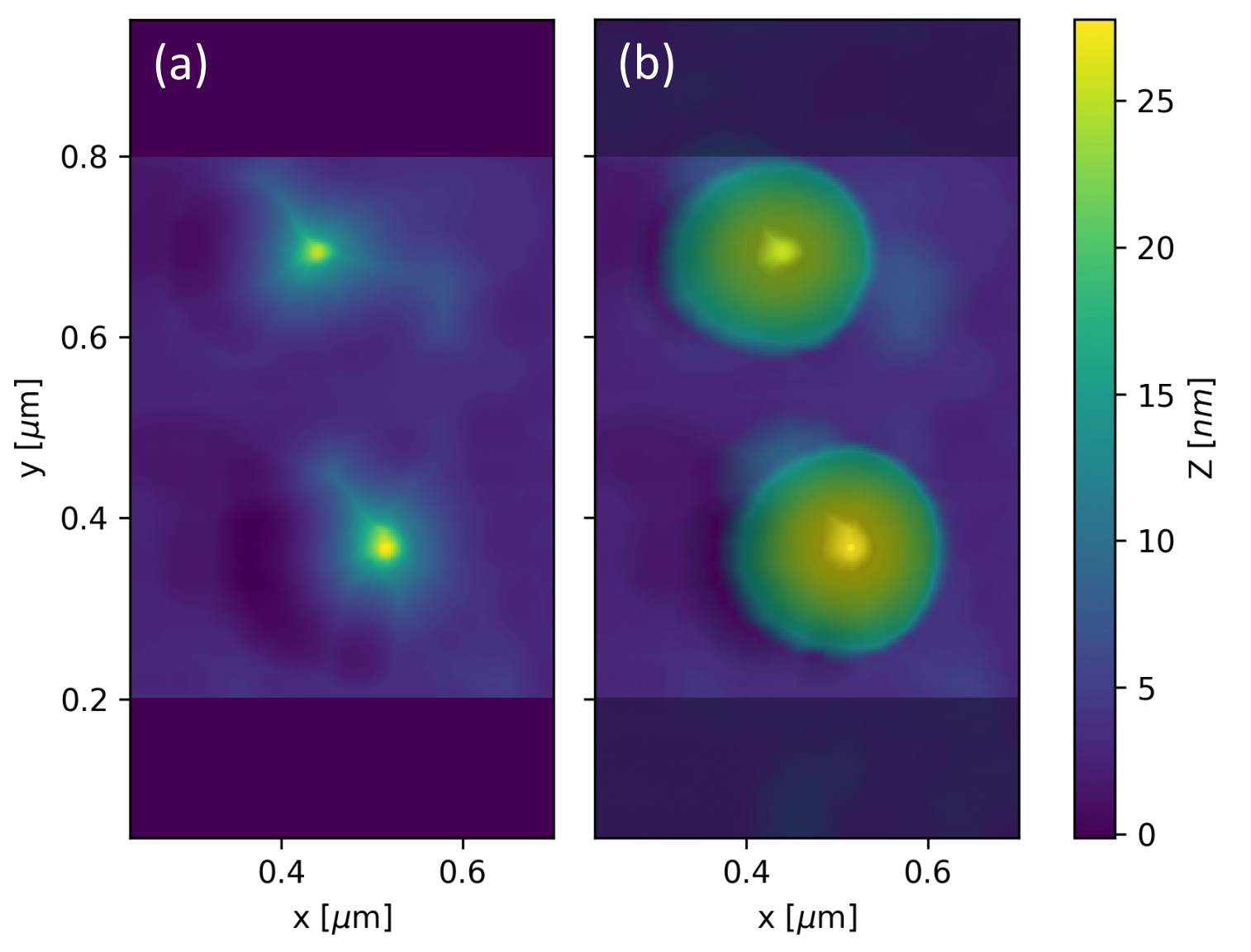


Reconstructed tip using the erosion algorithm

The tip is reconstructed using the erosion algorithm proposed by Villarrubia [4] for image deconvolution. Since we are interested in reconstructing the tip shape we erode the original image with the ideal reconstructed surface reduced on each side by half of the tip size.

$$T(x,y) = I \ominus S = \min_{u,v}[i(x+u,y+v) - s(u,v)]$$

4. IMAGE DECONVOLUTION



(a) deconvoluted topography, (b) superposition with original topography

The measured topography is eroded once more by the reconstructed tip and the resulting topography is compared to the original image and the reconstructed ideal structure.

CONCLUSIONS

We presented a technique that gives the possibility to generate structures that are far more complex to describe using mathematical equations.
The starting meshes are simple to create using open source software, such as Blender, and can be used to generate structures with multiple nano-particles of different shape and size oriented and positioned anywhere.

Future studies:
- comparison of reconstructed tip with Villarrubia
- Implementation of structure fit for each particle shape
- Study of tip wear
- Deconvolution accuracy determination

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