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Point Cloud Data Processing in Scanning Probe Microscopy

Petr Klapetek[1], *Miroslav Valtr*[1], *David Nečas*[2], *Edward Heaps*[3], *and Andrew Yacoot*[3]
[1] Czech Metrology Institute, Okružní 31, 638 00 Brno, Czech Republic
[2] CEITEC, Brno University of Technology, Purkyňova 123, 612 00 Brno, Czech Republic
[3] National Physical Laboratory, Hampton Road, Teddington, Middlesex, TW11 0LW, United Kingdom
pklapetek@cmi.cz

Summary: This work describes the methods for processing general XYZ data clouds which are the primary data coming from metrological Scanning Probe Microscopes (SPM).They can also be obtained also with other SPM instrumentation. XYZ data are more general than the normal raster scan data, typically used in SPM. The transition from raster data to point clouds allows much more complex scanning patterns to be used easily and makes the SPM sampling closer to that used in other 3D measurements systems such as coordinate measuring machines. The with all the benefits and drawback of this approach for scanning probe microscopes are discussed.

Keywords: Data Processing, Scanning Probe Microscopy, Metrology

Introduction

Scanning Probe Microscopy is a widely used measurement technique, suitable for determining dimensional and physical properties with nanometre resolution and with no need for sample preparation. It is based on use of a sharp probe that is physically scanned across the sample surface, while the force between the probe and surface is detected and used to establish a probe-sample distance feedback.

Conventional microscopes perform measurements in a raster pattern, *i.e.* the sample is scanned using an equidistant set of points lying on a rectangular grid. The benefit of this approach is that the results can be easily visualized. However, information on the sample is only rarely distributed homogeneously, so the sampling resolution is therefore in principle too low or too high on different areas of the scanned surface. Increasing the scan resolution, however, means increasing the scanning time, which leads to low throughput and increased impact of parasitic effects like thermal drift. When it comes to large area SPMs[1], designed to study industrially relevant sample areas scanning over millimetre ranges, raster patterns become highly ineffective. They are also unsuitable for high-speed SPMs[2], designed mostly for life-sciences applications as they contain too sharp turnarounds, leading to mechanical vibrations.

A solution is to use non-raster patterns, either optimized to obtain the information with density adapted to its local content or optimized to provide smooth mechanical motion. However, data processing techniques for non-raster data in SPM are highly underdeveloped. Here we describe some algorithms developed for the open source software Gwyddion[3] to treat general XYZ data, i.e. point clouds.

XYZ data acquisition

XYZ data sets are organized in a manner such that every sampled point comprises an x, y and z coordinate value. This is a natural way to store data from metrological systems where interferometric sensors are used to determine the probe or sample position in space.

To drive a microscope in a non-raster pattern we have used a Gwyscope open hardware digital signal processor[4] which is fully designed to work with general XYZ data sets. On top of it, every point is stored also with its timestamp, relative to the measurement start time. The microscope was based on use of a large area air bearings and voice coil motor based stage combined with a high-speed stage using piezoelectric transducers. Positions of both stages were measured using interferometers, as illustrated in Fig. 1.

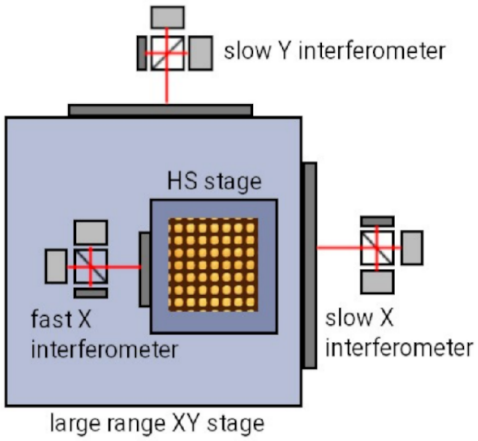

Fig. 1: Dual stage system with interferometers used to measure the XYZ data set

XYZ data processing

The XYZ point clouds in Gwyddion open source software are loaded as a special data type and dedicated data processing modules are provided for them. This includes the key operations that are needed to pre-process and evaluate the data: cropping data in time or space, organizing the point clouds data (merging, splitting, sorting), assigning the scales and units to them, etc. The data can be also filtered using Fast Fourier Transform, assuming that they were generated at constant sampling speed and they can be leveled to remove probe-sample tilt. Drift in the data can be estimated from the crossing points in the sampling pattern. Data can be at any moment rasterized to a regular grid to enable use of much wider set of data processing algorithms developed for the conventional scans, however this is not the goal. Algorithms are being developed for direct processing of XYZ data, e.g. for fitting a geometrical shape on it. All the algorithms discussed here are available in the open source software Gwyddion (http://gwyddion.net).

Results

Here we show an example of processing a XYZ data cloud from a measurement on a chessboard pattern calibration sample. The measurement was performed using a combination of a high-speed short range stage scanning in the x direction and large area stage moving in both x and y direction. This leads to a complex scan pattern on the surface. As the measurement was done using a simple setup that was not thermally optimised, there is a significant z drift in the data. In traditional raster data it would be easy to remove it by adjusting individual scan lines, however, for a general point cloud this is not possible. The drift was therefore detected from the crossing points,*i.e.* points where the scan path intersects itself. As all the data points also include a timestamp, we could evaluate the evolution of the z coordinates as a function of time and fit a polynomial drift model on these data. By removal of this polynomial the drift was significantly reduced, as seen in Fig. 2. It should be noted that there are also some other parasitic effect coming from mechanical oscillations of the test setup, nevertheless the data were significantly flattened using this approach.

Conclusions

A set of algorithms for XYZ point clouds generated in Scanning Probe Microscopy was developed and included in the Gwyddion open source software. It enables running advanced SPM experiments with more complex sampling patterns without need for developing the data processing tools from scratch. XYZ point clouds are a natural way how to extend the SPM functionality towards larger area and higher speed measurements.

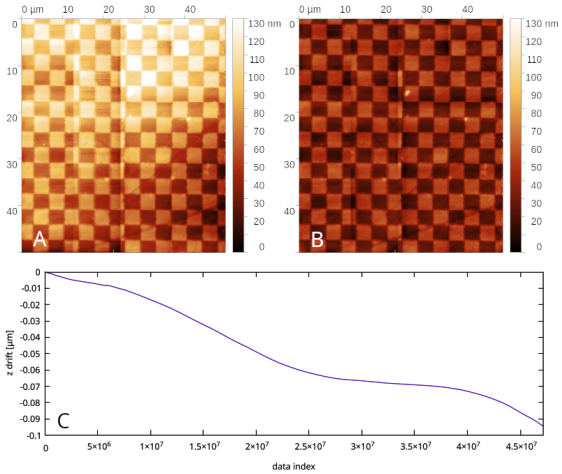

Fig. 2: Drift removal from XYZ data clouds measured on the checkerboard grating: A) raw data, B) processed data, C) estimated drift.

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