Title: Digitalisation route for dimensional nanometrology

Abstract

This proposal aims to establish a digitalisation route for dimensional nanometrology focusing mainly on the use of the main tool used for nanotechnology, scanning probe microscopy. The methods developed will, however, be applicable both to other areas of metrology and nanometrology. The digital chain developed will extend from the digital metre to the end user outside of the NMI. It will be realised through 'smart' samples containing a priori information (silicon steps and self-assembled structures) and the use of smart algorithms (using AI where appropriate) for the automated processing of calibration data based on direct measurement data and metadata. The whole process will conform to the FAIR principles of data management.

Keywords

Data processing, Scanning Probe Microscopy, Uncertainty, nanometrology, digitalisation, metadata,

Background to the Metrological Challenges

Many measurement methods feature a surprisingly large gap between data collection and the calculation of the measurand. One such example is Scanning Probe Microscopy (SPM) used in nanoscience and nanotechnology. It is a widely used tool for nanotechnology research or for nanometrology in many fields, including semiconductors, life sciences, quantum technology and precision engineering.

With the growth in nanotechnology-based products, the reduction in device size and tighter manufacturing tolerances, all demanded at ever increasing speeds, there is a need for improved metrology for robust SPM calibration and standardised methods for data processing. In addition, the drive towards digitalisation in industry (Industry 4.0) brings a need both for a digital calibration process for SPMs and for seamless transfer of digital SPM data in research and in manufacturing processes. Data collected in SPM are in a raw form and many pre-processing steps are needed. If such a result is used in any digital traceability chain, it can be very far from the originally measured values. It has been shown that the human influence in data processing is large and without a deeper knowledge of the data processing methods, users can handle data incorrectly leading to errors in the range of tens of percent or, even more fundamentally, data evaluation using a sub-optimal method.

SPM data processing is based on steps applied to correct for various instrument errors: tilt between probe and sample reference system, mismatch of the individual profiles, noise, tip convolution and instrument drift. This process removes valuable information about the microscope performance and subjective choices made by the operator, which can introduce bias, or lead to acquiring non-repeatable results. Recording of the application of all the data correction algorithms and adding it to the metadata, enables determination of incorrect use of correction algorithms and aid the removal of incorrect data processing. Moreover, if automated methods for scanned image quality were to exist (based either on classical or AI tools, as is increasingly the case with medical scans), images could be checked immediately after acquisition at the instrument level and re-scanned if necessary, which would open a way towards automated calibrations and improve imaging efficiency.

Even though metrology institutes have developed calibration methodologies for SPMs, there is still a large gap between their recommendations and what the real instrument users are doing, as demonstrated by an AFM comparison. Samples used to calibrate microscopes are also far from anything digital, being based on e.g., a grating with a single pitch value. When such a sample is calibrated, typically using a metrological microscope, much more information is acquired (e.g., global sample flatness, local roughness, contamination) and afterwards discarded. Moreover, novel calibration samples containing additional (a-priori) information and information with a higher metrological quality have been developed (silicon steps which are secondary realisation of metre or self-assembled patterns connected to a database of positions), but these currently cannot be treated in any special way during calibration and are not fully reflected in the traceability chain.

In data handling, existing ISO standards are infrequently used, and are unable to handle more advanced SPM big-data regimes (high-speed, force volume, etc). Data from different instruments cannot be processed using software from other instruments even though the measurand is the same and, in some cases, older data from the same instruments cannot be easily processed. The metadata does not contain the data processing steps and, in principle, the stored data methods have no means to keep raw data combined with these steps, to allow an independent review of the data processing and uncertainty propagation through it.

In the past, solutions to bridge gaps in SPM data handling were developed. Some of the authors of this PRT developed the widely used open-source software Gwyddion which brings the necessary interoperability into the SPM world, including both data handling and processing. However, the data processing methodology and its application at the instrument scale needs to be done by metrology institutes and instrument manufacturers, at the hardware level and this is the goal of this proposal. The recent development of digital calibration certificates (DCCs), and the future requirement for digital product passports, offer great opportunities for structured and standardised sharing of calibration and correction information to improve confidence in measurement data. This proposal will provide interfaces for the digital workflow of data acquisition, data analysis and uncertainty budgets to establish a seamless integration to identify areas for future focussed development of DCCs in present and future state of harmonization and standardisation to support the complete end-to-end digital traceability.

Objectives

Proposers should address the objectives stated below, which are based on the PRT submissions. Proposers may identify amendments to the objectives or choose to address a subset of them in order to maximise the overall impact, or address budgetary or scientific / technical constraints, but the reasons for this should be clearly stated in the protocol.

The proposal shall focus on developing a full traceable digital metrological infrastructure on the use of Scanning Probe Microscopy (SPM) to support European nanoscience and technology which will act as an exemplar that can be applied in other areas of metrology.

The specific objectives are:

1. To develop smart calibration samples (containing intrinsically high metrological information) for use with automated data processing of measurement data used to calibrate SPM. Samples could include silicon steps traceable to a crystal lattice, lateral standards based on self-organised and locally unique patterns (fingerprints) and programmable virtual height and lateral standards.
2. To develop a library of automated data processing routines for evaluation and quality checking, allowing propagation of calibration measurement data and associated metadata that complies with FAIR and is independent of user influence. The library will permit integration into open source and commercial microscope control software and a web-based reference platform to act as a template for digitalisation in other metrology areas. Documentary standards and good practice guides on use of developed software and algorithms will be drafted and disseminated to the SPM community and instrument manufacturers so that routines can be integrated into their software.
3. To develop tools for data management including storage of the data processing steps in the metadata in a reusable format directly associated with the data and broadening ISO compliant data formats for advanced measurement regimes (high-speed, force volume, spectroscopic, adaptive scanning) to support transfer of SPM measurement data in a manufacturing process.
4. To evaluate uncertainties associated with application of the routines leading to a digital traceability chain. To demonstrate the potential for use in length metrology with other instrumentation and at other scales (e.g., for stylus profilometers, optical profilometers, focus variation instruments). To create a database of knowledge learnt from the routines' application for transfer to other areas of metrology.
5. To facilitate the take up of the technology and measurement infrastructure developed in the proposal by the measurement supply chain (NMIs, instrument manufacturers), standards developing organisations (ISO, IEC/ISO SMART) and end users (semiconductor industry, research, precision engineering industry).

These objectives will require large-scale approaches that are beyond the capabilities of single National Metrology Institutes and Designated Institutes. To enhance the impact of the research, the involvement of the appropriate user community such as industry, standardisation and regulatory bodies, and other European Partnerships is strongly recommended, both prior to and during methodology development.

Proposers should establish the current state of the art and explain how their proposed project goes beyond this.

Proposers should note that the programme funds the activity of researchers to develop the capability, not the required infrastructure and capital equipment, which must be provided from other sources.

EURAMET expects the average EU Contribution for the selected JRPs in this TP to be 1.9 M€ and has defined an upper limit of 2.4 M€ for this proposal.

EURAMET also expects the EU Contribution to the external funded beneficiaries to not exceed 35 % of the total EU Contribution across all selected projects in this TP.

Any industrial beneficiaries that will receive significant benefit from the results of the proposed project are expected to be beneficiaries without receiving funding or associated partners.

Potential Impact

Proposals must demonstrate adequate and appropriate participation/links to the ’end user’ community, describing how the project partners will engage with relevant communities during the project to facilitate knowledge transfer and accelerate the uptake of project outputs. Evidence of support from the “end user” community (e.g. letters of support) is also encouraged.

You should detail how your proposal’s results are going to:

- Address the SRT objectives and deliver solutions to the documented needs,
- Feed into the development of urgent documentary standards through appropriate standards bodies,
- Facilitate improved industrial capability, or improved quality of life for European citizens in terms of personal health, protection of the environment and the climate, or energy security,
- Transfer knowledge to the nanometrology sector.

You should detail other impacts of your proposed JRP as specified in the document “Guide 4: Writing Joint Research Projects (JRPs)”

You should also detail how your approach to realising the objectives will further the aim of the Metrology Partnership to develop a coherent approach at the European level in the field of metrology and include the best available contributions from across the metrology community. Specifically, the opportunities for:

- improvement of the efficiency of use of available resources to better meet metrological needs and to assure the traceability of national standards
- the metrology capacity of EURAMET Member States whose metrology programmes are at an early stage of development to be increased
- organisations other than NMIs and DIs to be involved in the work.

Timescale

The project should be of up to 3 years duration.