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# Considerations for tool-to-tool matching across a fleet of X-ray metrology tools

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# Outline

1. Introduction
2. Traceability
3. Goniometer calibration
4. Gauge Repeatability & Reproducibility

# Introduction

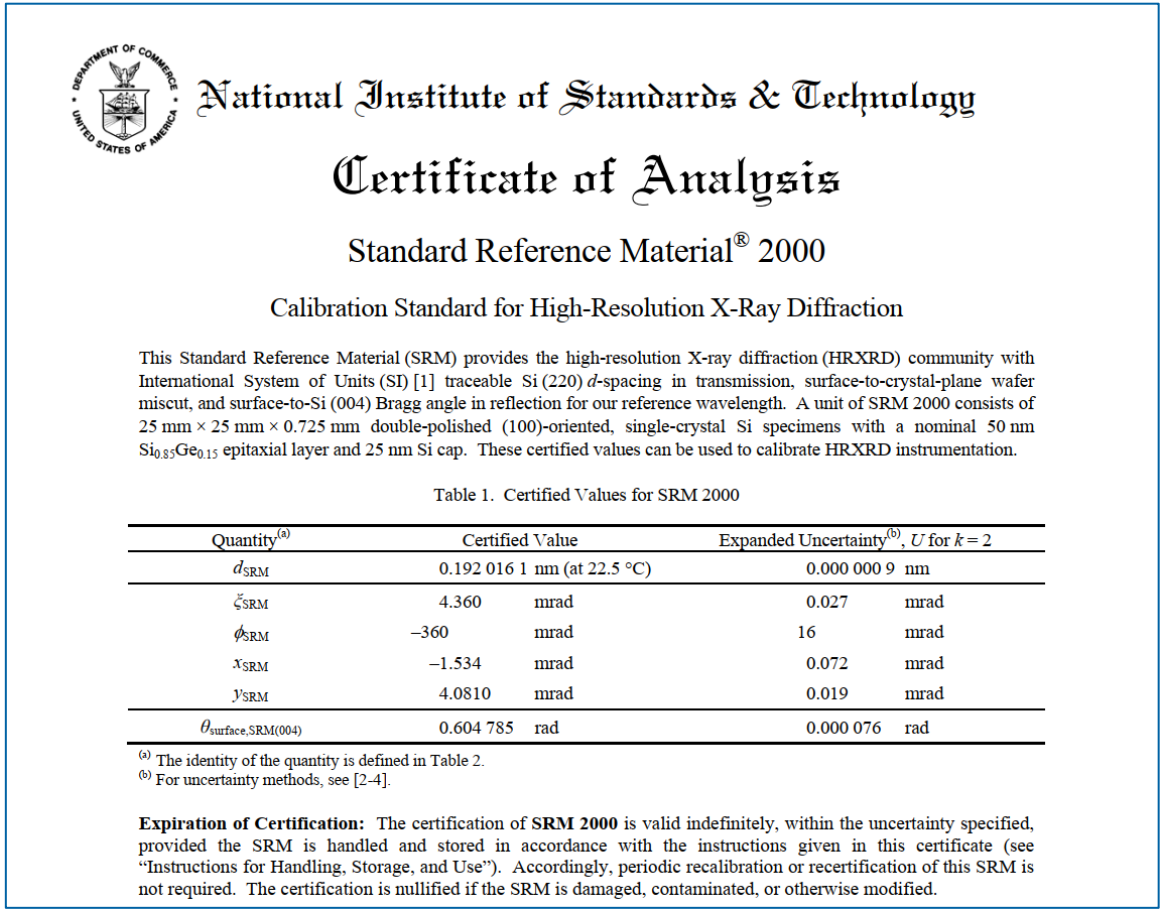
- Fleets of metrology tools, across multiple sites and countries, used by different operators, need to be capable of ensuring customer products can ship reliably
  - Same metrology performance required across the fleets
- Bruker ensures its tools are calibrated and qualified under an ISO9001-2015 quality management system
- Bruker uses NIST-certified standard samples when available, and secondary standards when not
- This allows customers to be confident that their measurement tools are well calibrated, giving stable and reliable results

# What is important to measure in X-ray metrology of semiconductor materials?

- Application dependent – but for elastic scattering techniques: intensity vs. scan angles
  - HRXRD
  - XRD
  - XRR
- So we need accurate angle calibration over the scan range of the scanning axes
- Linearised detector
- Impact of improper calibration directly impacts the accuracy of:
  - Thickness (HRXRD, XRR)
  - Lattice parameter / strain (HRXRD, XRD)
  - Composition (and relaxation) of epilayers (HRXRD)

# Traceability for goniometer angle calibration (Omega, 2Theta)

- NIST SRM 2000
  - Single crystal Si substrate with SiGe epilayer
  - Si(220) lattice plane spacing is certified
  - The method of use described in the standard is not possible on many X-ray tools as it requires measurement of diffraction peaks on either side of $2\theta = 0$
  - An alternative method was developed and has been successfully used for several years



National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 2000

Calibration Standard for High-Resolution X-Ray Diffraction

This Standard Reference Material (SRM) provides the high-resolution X-ray diffraction (HRXRD) community with International System of Units (SI) [1] traceable Si (220) *d*-spacing in transmission, surface-to-crystal-plane wafer miscut, and surface-to-Si (004) Bragg angle in reflection for our reference wavelength. A unit of SRM 2000 consists of 25 mm × 25 mm × 0.725 mm double-polished (100)-oriented, single-crystal Si specimens with a nominal 50 nm $Si_{0.85}Ge_{0.15}$ epitaxial layer and 25 nm Si cap. These certified values can be used to calibrate HRXRD instrumentation.

Table 1. Certified Values for SRM 2000

| Quantity[a] | Certified Value | | Expanded Uncertainty[b], $U$ for $k = 2$ | |
|---|---|---|---|---|
| $d_{SRM}$ | 0.192 016 1 nm (at 22.5 °C) | | 0.000 000 9 | nm |
| $\xi_{SRM}$ | 4.360 | mrad | 0.027 | mrad |
| $\phi_{SRM}$ | –360 | mrad | 16 | mrad |
| $x_{SRM}$ | –1.534 | mrad | 0.072 | mrad |
| $y_{SRM}$ | 4.0810 | mrad | 0.019 | mrad |
| $\theta_{surface,SRM(004)}$ | 0.604 785 | rad | 0.000 076 | rad |

[a] The identity of the quantity is defined in Table 2.
[b] For uncertainty methods, see [2-4].

**Expiration of Certification:** The certification of **SRM 2000** is valid indefinitely, within the uncertainty specified, provided the SRM is handled and stored in accordance with the instructions given in this certificate (see "Instructions for Handling, Storage, and Use"). Accordingly, periodic recalibration or recertification of this SRM is not required. The certification is nullified if the SRM is damaged, contaminated, or otherwise modified.

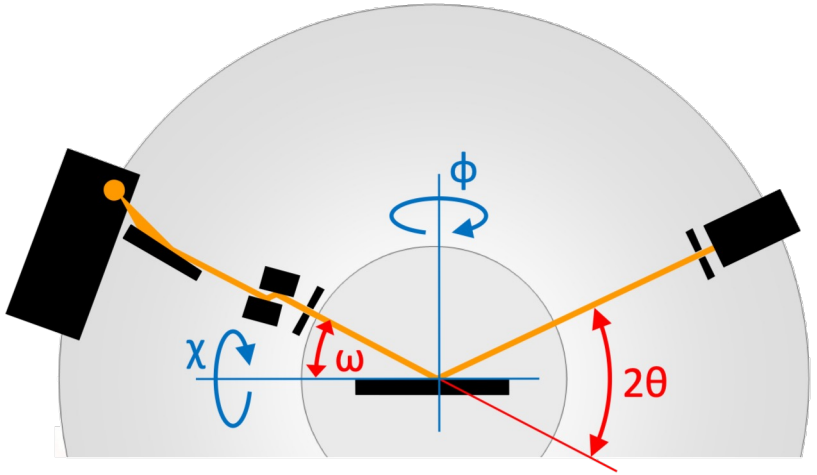
https://tsapps.nist.gov/srmext/certificates/2000.pdf
https://shop.nist.gov/ccrz__ProductDetails?sku=2000&cclcl=en_US

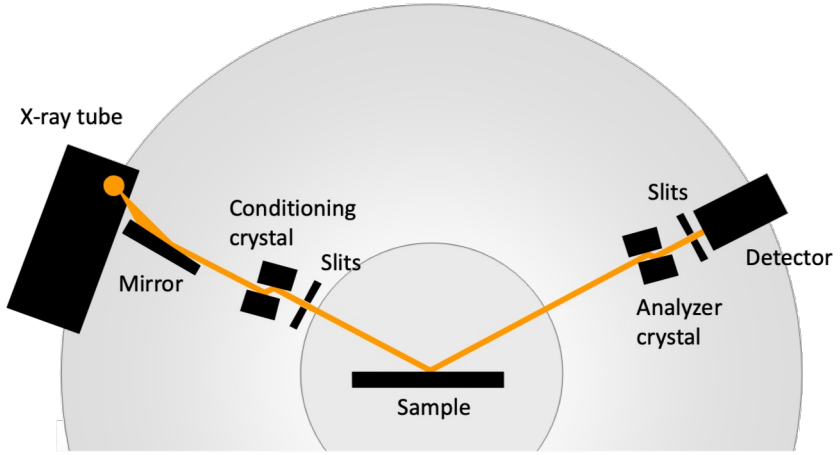
# Process

- ISO9001-2015 Quality Management System
  - QMS assessed every six months to maintain certification
- For a customer to be ISO-compliant, our tools need to be ISO-compliant

# Goniometer calibration method

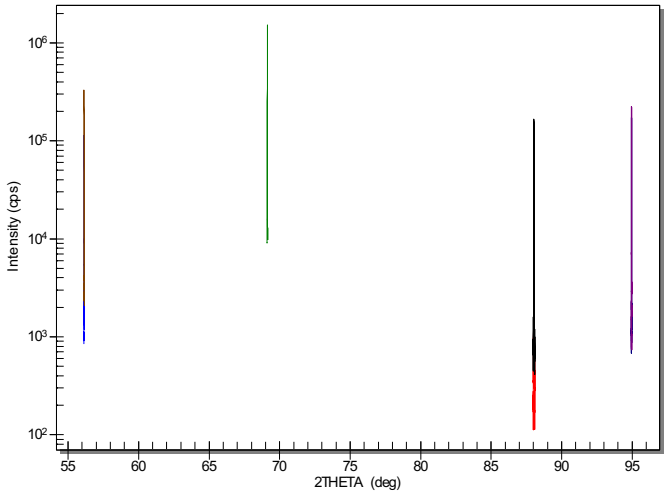
- Pre-requisite: minimisation of sphere of confusion (centre of rotation of all axes; beam incident here)
- Find diffraction from multiple diffraction planes (hkl)
  - Symmetric (004)
  - Several asymmetric planes
    - Grazing incidence geometry
    - Grazing exit geometry
  - → Multiple reference angles around the range of Omega and 2Theta
- Minimise the deviation from differences between nominal diffraction angles for traceable sample
  - Not using absolute angles
  - Only measure diffraction peak positions on one side of 2θ = 0.0, which is an output of the calibration process
- Update calibration parameters



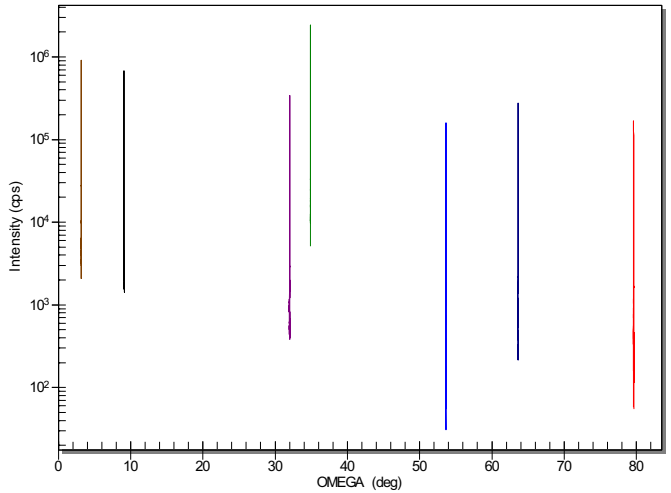



# Multiple reference angles around the range of Omega and 2Theta

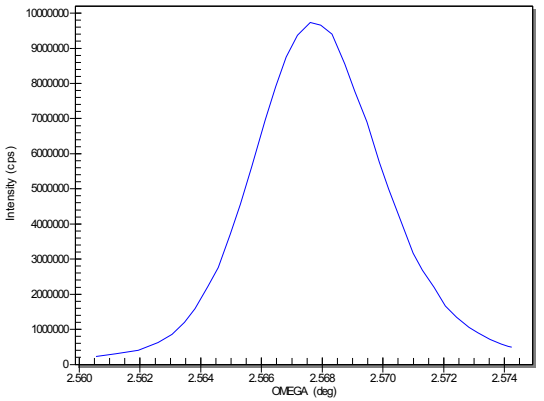
- Non-linear regression process to fit the measured diffraction peak positions from different reflections (hkl) to determine the angular scale over a wide range
- Update goniometer calibration parameters, i.e. steps / unit angle
- Repeat – check accuracy
- Fully automated process (alignment, measurement, peak fitting and position regression) with qualification report




2Theta triple axis scans across the various peaks




Omega rocking curves over the angular range




Example rocking curve: Si(113)GI

# Pre-shipment tests – repeatability

- Recipe-driven
- Robot loading (where applicable)
- Functional tests
  - Axes movement repeatability; hardware limits; homing
  - Direct beam intensity
  - Intensities and FWHM of rocking curves of Si for the beam conditioning optics configurations fitted

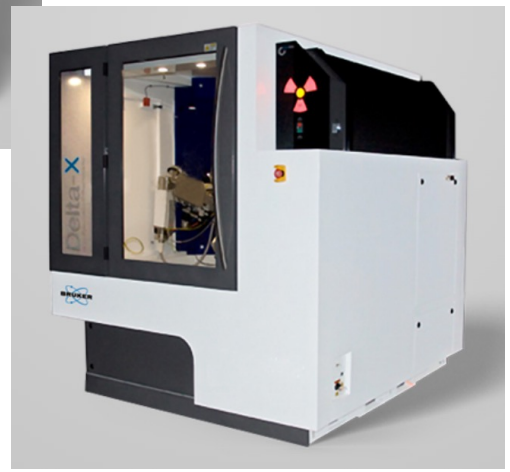
- Applications tests
- Cover a range of measurements for which the tools are used
  - XRD, GI-XRD, in-plane GI-XRD
  - HRXRD
  - XRR

# Gauge Repeatability & Reproducibility (GR&R)

- Basic calibrations may not be sufficient for the customer for tool acceptance – customer-specific tests may be required
- GR&R compliance enabled by tool calibration
- GR&R < 10% typical industry requirement
- Customer samples, customer spec agreed
- Calculation may be customer-specific
- “Range method”
  - Take ranges of results and averages
  - Some magic numbers relating to population size
  - Factor relating to how tight the customer requirement is on the GR&R result
  - LSL, USL
- Samples may be a number of wafers, with a number of sites on each – always comparing like with like
- Repeated runs
- Range of values on a single tool – “single tool gauge capability”
- Tool to tool matching (TTTM)

# Applies to…

- 7300L, 7300LSI, Delta-X (NIST SRM)


- QCVelox series, QC3 (secondary standards)


# Summary

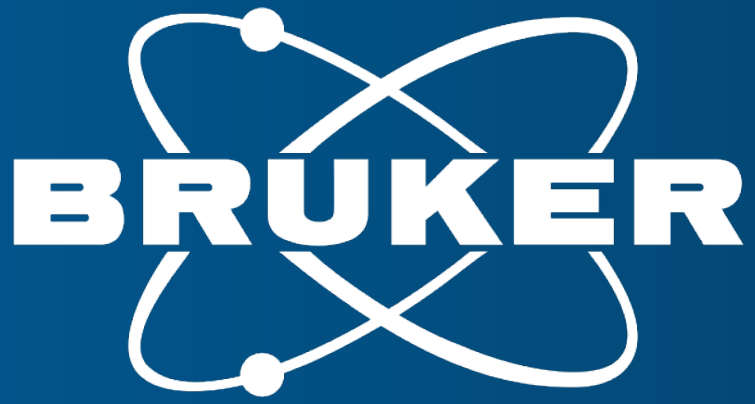
- NIST-traceable standard sample for base calibration of the goniometer given as an example
  - Additional standards from certification agencies such as NIST are highly desirable for more application-specific tests as X-ray metrology continues to move from R&D labs to HVM manufacturing
- ISO9001-2015 oversight of process
- Tool users can have confidence that the same equipment can get the same metrology results, regardless of where in the world the equipment is or who is operating it


- D. Keith Bowen, David Joyce, Paul Ryan and Matthew Wormington, “Accuracy and Repeatability of X-Ray Metrology ”, Characterisation and Metrology for ULSI Technology 2005, pp. 604-609

# Acknowledgments


- Mark Vermeulen
- Lucas Fuhl
- John Wall
- Matthew Wormington
- Richard Bytheway
- Kevin Matney

- Thank you for your attention
- Any questions?




Innovation with Integrity