NIST SRM 2000 - A HIGH RESOLUTION X-RAY DIFFRACTION STANDARD REFERENCE MATERIAL

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In 2008, the National Institute of Standards and Technology completed a Standard Reference Material (SRM) for calibration of high resolution X-ray diffraction (HRXRD) laboratory, synchrotron, and fabrication-line instrumentation. Here we present our strategy for providing the HRXRD community with International System of Units (SI) traceable determination of the substrate Si lattice constant for SRM 2000. We will also provide an approach for using this SRM in the field for instrumentation calibration and discuss our future plans for SRM recertification to include reference values from refinement of the SRM's nominal 50 nm, SiGe epitaxial layer structure.

HRXRD measurements usually treat the substrate Si lattice constant as a known quantity, measuring peak shifts from the substrate position to infer information on strained, epitaxial surface features. This first generation of HRXRD calibration reference offers an absolute reference for the substrate lattice, $d_{substrate}$, allowing for accuracy comparisons between different samples and different instruments. One limitation is that the SRM can provide either calibration of an HRXRD instrument's monochromator wavelength or its angle measurements, but not both simultaneously. This is especially relevant to systems where angle measurement is not encoded or where instruments undergo large, thermal environmental changes between calibrations.

The determination of an accurate Si substrate lattice parameter was performed using a 4θ transmission, Bond measurement of the Si (220) substrate peak on SRM 2000 and on an internal reference standard obtained from the Avogadro Project and qualified using the NIST Lattice Comparator. We referred to this internal calibration of our instrumentation as a "sequential delta-d" method. This approach provided expanded uncertainties on the lattice spacing of less than a femtometer (10^{-15} meters). The same approach to SI-traceability will be used in future NIST HRXRD, X-ray reflectometry, and powder diffraction SRM projects.

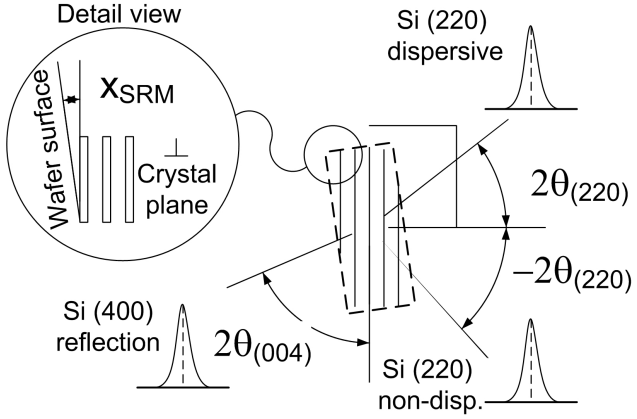

Figure 1. Diagram of HRXRD measurements on SRM 2000: Si (220) in transmission and Si (004) in reflection.