

The Lattice Spacing Variability of Intrinsic Float-Zone Silicon

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The Lattice Comparator at the National Institute of Standards and Technology (NIST) can provide individual lattice spacing comparisons with typical uncertainties of 1×10^{-8} . One of the principal uses for the machine was the generation of reference crystals that were suitable for wavelength dispersive spectrometers capable of measurements traceable to the international system of units (SI). Such crystals were invariably made from hyperpure, float zone silicon. This report provides a systematic study of lattice spacing variability from such bulk silicon materials. Recent measurements combined with those acquired over the past two decades indicate that for nearly-perfect intrinsic float-zone silicon, the variability of the lattice spacing is sufficiently small that for most diffraction applications a recommended value may be used.

The NIST Lattice Comparator is a two-crystal Laue geometry diffractometer with two silver x-ray sources, two detectors and a long (7.5 cm) first crystal to provide two nearly nondispersive x-ray paths which cross in the second crystal. Shutters allow nearly simultaneous recording of x-ray profiles by switching between the sources while the first crystal is being scanned. The first and second crystal thicknesses are chosen and matched so that the profiles exhibit pronounced Pendellösung oscillations that aid in the determination of the angular separation between the two profiles. The standard and unknown crystals reside on a transport device that allows automatic interchange of the samples. The lattice spacing difference between the standard and unknown crystals are then determined from the diffraction profile peak positions.

The comparison measurements link the unknown lattice spacing of a test crystal to a standard crystal whose lattice spacing has been accurately determined by x-ray/optical interferometry in units traceable to the definition of the meter. The crystal that serves as the standard in all the comparisons is a well characterized sample from the WASO 04 silicon boule used within the Avogadro project. The lattice spacing of the standard crystal is known with a relative uncertainty of 5×10^{-9} . With the individual lattice spacing comparison results and taking material variability into account the lattice spacing of the test materials can be determined with a relative uncertainty of a few $\times 10^{-8}$. These precision lattice spacing comparison measurements at NIST provide traceability of x-ray wavelength and powder diffraction standards to the SI.