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Contemporary x-ray wavelength metrology and traceability

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Abstract

We report recent advances in absolute x-ray wavelength metrology in the context of producing modern standard reference data. Primary x-ray wavelength standards are produced today using diffraction spectrometers using crystal optics arranged to be operated in dispersive and non-dispersive geometries, giving natural-line-width limited profiles with high resolution and accuracy. With current developments, measurement results can be made traceable to the *Système internationale* definition of the meter by using diffraction crystals that have absolute lattice-spacing provenance through x-ray-optical interferometry. Recent advances in goniometry, innovation of electronic x-ray area detectors, and new *in situ* alignment and measurement methods now permit robust measurement and quantification of previously-elusive systematic uncertainties. This capability supports infrastructures like the NIST Standard Reference Data programs and the International Initiative on X-ray Fundamental Parameters and their contributions to science and industry. Such data projects are further served by employing complementary wavelength-and energy-dispersive spectroscopic techniques. This combination can provide, among other things, new tabulations of less-intense x-ray lines that need to be identified in x-ray fluorescence investigation of uncharacterized analytes. After delineating the traceability chain for primary x-ray wavelength standards, and NIST efforts to produce standard reference data and materials in particular, this paper posits the new opportunities for x-ray reference data tabulation that modern methods now afford.

Keywords

X-ray spectroscopy; Wavelength metrology; Standards; Traceability; Reference data

Historically, the meter was defined in terms of the international prototype meter (1889). This physical artifact was replaced in 1960 by a definition based upon the wavelength of a particular transition in krypton-86, but it could be realized with a relative uncertainty $u_r \approx 4 \times 10^{-9}$ at best (Giacomo, 1984). (Herein, u_r is used to denote the fractional uncertainty reflecting the current order-of-magnitude state of the art, *i.e.*, $u_r(y) \equiv u(y)/y$ where $u(y)$ is the standard uncertainty of the measurement result y .) Since 1983, the speed of light in vacuum has been assigned an exact value ($c_0 \equiv 299\,792\,458$ m/s; $u_r = 0$), and the meter is now defined as the distance light travels in a vacuum in $(1/299\,792\,458)$ s. The second, in turn, is

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defined as the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium-133 atom. These definitions enable a calibration chain for the meter to be propagated at high accuracy through phase-locked frequency comparisons from its definition to one of the approved CIPM (*Comité International des Poids et Mesures*) radiations for the practical realization¹ of the meter (and second). These frequency/wavelength standards include stabilized lasers, spectral lamps, and other sources; when properly realized, they can have a relative standard uncertainty $u_r \approx 10^{-16}$ (Quinn, 2003). The strategy behind the 1983 *mise en pratique*² is that it can evolve with improving stability of radiation sources and better knowledge of their frequencies, while the definition of the length scale can remain unchanged.

Such an optical standard is linked to the x-ray regime using combined x-ray/optical interferometry (XROI), first demonstrated by Deslattes and Henins (1973) in 1973 at the National Institute of Standards and Technology (then National Bureau of Standards, NBS). Employing x-ray interferometry as first demonstrated by Bonse and Hart, (Bonse and Hart (1965), the motion of the analyzing x-ray crystal is simultaneously registered with optical interferometry. The ratio of the optical and x-ray fringe periods thereby scales the optical wavelength standard into the x-ray regime in terms of the lattice spacing of the analyzing crystal. Subsequent XROI measurements have been reported by three other national metrology institutes (Physikalisch-Technische Bundesanstalt (PTB), Germany (Becker et al., 1981); Istituto Nazionale di Ricerca Metrologica (INRiM), Italy (Basile et al., 1994); National Metrology Institute of Japan (NMIJ) (Nakayama and Fujimoto, 1997)) with relative uncertainties decreasing over time. (For a summary of the improvements of XROI measurements, see Section 3.1 of reference 11.) Most recently, the lattice parameter of ²⁸Si(220) was reported (Massa et al., 2015) with $u_r \approx 2 \times 10^{-9}$. It is noted that XROI, and the crystal lattice comparisons discussed below, have contributed to the international project to better determine the Avogadro constant by the counting-atoms technique, which was recently used to help redefine the artifact kilogram (Fujii et al., 2016). and the mole. Indeed, in May 2019, the redefinitions of the SI base units kilogram, ampere, kelvin, and mole were formalized by the adoption of exact numerical values for the Planck constant (h), elementary electric charge (e), Boltzmann constant (k), and Avogadro constant (N_A), respectively. The use of a constant of nature to define a unit disconnects its definition from its realization, permitting the latter to improve with superior technology or methods without adopting a new definition. One consequence of the artifact-free SI is that *a standard for a quantum of electromagnetic radiation can now be realized and transferred as a frequency (ν), a length (λ), or an energy (E) with formal equivalency*, the conversions between which are now obtained with no uncertainty: $E=hc/\lambda=h\nu$. In the context of traceability, XROI produces particular crystals with traceable absolute lattice spacing values which in principle can be used in the crystal diffraction technique to measure x-ray and gamma-ray wavelengths.

¹The list of approved radiations for the practical realization of the meter were first put forth in: BIPM Proc.-Verb. Com. Int. Poids et Mesures, 51, (1983) 25–28.

²A *mise en pratique* for the definition of a unit is a set of instructions that allows the definition to be realized in practice at the highest experimental level. Such “primary” methods also only involve measurements of quantities that do not involve the unit.

In practice, such well-characterized crystals are used to calibrate other crystal lattices that are in turn used in metrology labs to measure x-ray wavelengths, line shapes and relative yields using the crystal diffraction technique. This link of the traceability chain has been performed most often using a self-referencing lattice comparator. These instruments typically employ the symmetric Laue diffraction geometry first demonstrated by Hart (1969). By registering the angular offset between non-dispersive, double-crystal rocking curves where the second crystal is either a standard crystal (determined via XROI) or the unknown crystal, the lattice spacing difference, and therefore the lattice spacing of the unknown crystal sample can be determined. Lattice comparator instruments, with various enhancements (Kessler et al., 1994), determine lattice spacings with $u_t \approx 10^{-8}$ or better. A recent study by the NIST “delta-d” instrument (Kessler et al., 2017) has considered the last twenty years of lattice measurements of nearly-perfect float-zone (FZ) natural-isotopically single-crystal silicon. It was concluded that modern silicon crystal growth and characterization conditions permit using the CODATA (Committee on Data for Science and Technology) (Mohr et al., 2016) recommended value for the lattice spacing of modern FZ silicon, corrected for typical impurity levels, without contributing significantly to the uncertainty budget of most applications. Hence the growing relevance of the traceability pathway through the silicon lattice spacing, as a secondary realization of the definition of the meter, for nano-scale manufacturing and dimensional nanometrology applications including measurement of displacement using interferometry, calibration of transmission electron microscope magnification, and measurement of atomic step heights in the technologically prevalent single-crystal silicon (BIPM, 2019).

Primary standard x-ray wavelengths have typically been measured with double-crystal diffraction spectrometers which give line profiles with high accuracy, resolution, and precision. Such instruments (Thomsen, 1974) have been in use for over a century (Compton, 1917), but today the results can be made traceable to the definition of the meter using the traceability chain discussed above and systematic corrections discussed below. Where the lattice parameter is well known, the principal measurand in the double-crystal spectrometer is the difference angle between dispersive and non-dispersive scans of the second crystal while the first crystal orientation is fixed. This angle difference is $\pi - 2\theta_B$ where θ_B is the diffraction angle which is related to the x-ray wavelength through Bragg’s Law. In the case where multibounce crystal optics are employed, the tails of the multiplied crystal reflectivity functions are trimmed, giving natural-line-width limited profiles for most x-ray lines from neutral atoms. In contrast, when measuring x rays from highly-charged ions, instrumental broadening dominates. A recent study (Amaro et al., 2013) that employed XROI-traceable crystals demonstrated the first use of a double crystal spectrometer coupled to an electron-cyclotron resonance ion source (Amaro et al., 2014). The spectra obtained were from highly-charged ions and are part of a proposal to establish x-ray standards using few-body atoms (Anagnostopoulos et al., 2003). Such lines are advantageously narrow and possess calculable profile shapes that are typically dominated by the crystal rocking curves. These standards, however, are more challenging to experimentally realize than neutral x-ray lines.

In a double-crystal spectrometer, the angular positions and motions of the crystals are encoded; but even the best commercial encoders may not provide the desired accuracy for primary x-ray wavelength standards. Some of the best off-the-shelf angle encoders use a

periodic, optically-patterned disc that rotates with the load, in this context a mounted crystal, and acts as a diffraction grating. The disc's position is determined by illuminating the repeating pattern as it passes and registering the varying diffraction signal. The full-range error specification of such an optical encoder is generally preserved if mounted correctly, but the factory calibration curve can change due to *in situ* mounting stresses. The limitations of such encoders for precision x-ray spectroscopy and standards work are twofold. Angular accuracy is needed at an order of magnitude greater than the nominal specification, and the encoder output itself is the result of undocumented, and therefore unverifiable, internal compensation algorithms. To provide full traceability and sound error bounds, simple calibration techniques have recently been developed to generate *in situ* correction functions for both long-range errors (Kinnane et al., 2015) (errors which have periodicities of small submultiples of a full rotation) and short-period errors (Mendenhall et al., 2015) (which are nearly periodic in the spacing of the optical features on the encoder) inherent in optical disc encoders. The former uses an electronic nulling autocollimator and an optical-polygon artifact that is phased over the error function to be determined. In this method of "circle closure", *viz.*, a full rotation must equal two pi and all errors must sum to zero, both the encoder error function and polygon artifact are calibrated simultaneously with the least-squares solution of an over-determined set of linear equations. The short-period compensation method interpolates angle values between the fine optical features on the disc. Finally, for the case where a crystal rotation axis is encoded with two stacked, concentric goniometer stages, a self-calibrating angle measurement method can be adopted that uses no fixed angular artifact (Mendenhall et al., 2016). Taken together, measurements of angles can be performed from single-encoder readings (no averaging) with a standard uncertainty of a few hundredths of an arc second in the measurement of the diffraction angle.

Given advances in technology and metrology, it is clear that there is a need for both rechecking tabulated x-ray standards and re-measuring x-ray wavelengths for which there are no modern measurements or well-documented provenance. Recently such a study (Mendenhall et al., 2017) was undertaken on a newly commissioned instrument at the National Institute of Standards and Technology (NIST) that is used to certify lattice parameters of standard reference materials that are used to calibrate powder diffractometers. This work re-measured the copper K α profile, frequently used in laboratory diffraction work, using silicon crystals that had been directly compared to the silicon material which was used for the CODATA determination of (220) spacing of natural silicon. Diffraction angles were calibrated and a correction for the index of refraction of silicon was estimated, limited by form factor uncertainty. Noteworthy is the extension of the double-crystal spectrometer technique by the use of an imaging rather than photon-counting detector. This permitted new methods for determining the axial divergence correction as well as a new family of *in situ* alignment methods that assured robust quantifications of the contributions to the uncertainty budget of, e.g., crystal tilts and source-detector misalignment with respect to the plane of dispersion that aliases the apparent diffraction angle. The results of profile fitting are given to $u_t < 10^{-6}$, but it was noted that the location of the fitted top of K α_1 is very sensitive to the fit parameters, so even for this most-analyzed and most-measured characteristic line spectrum, the centroid of K α_1^0 is not a robust standard metric without further qualification. *A fortiori*, because the peak location of a spectral line is a function of

the resolving power of the measuring instrument, and spectral lines can be asymmetric in the general case, supplementary data are provided including the entire shape of the spectrum in this region, allowing it to be used in cases where simplified, multi-Lorentzian profile fits are not sufficiently accurate.

While wavelength-dispersive spectroscopy, and the double-crystal spectrometer technique in particular, is the workhorse in producing primary x-ray wavelength standards, it is not well suited for less-intense transitions such as the KM and KN lines and many of the L transitions. Energy-dispersive x-ray spectrometers are complementary to wavelength-dispersive techniques in that the former possesses broadband single-photon sensitivity while the latter provides traceability. Recent advances have also improved the resolution (e.g. 2.6 eV at 6 keV) (Doriese et al., 2016) of energy-dispersive instruments as well as their counting rates through faster electronics, novel sensor designs, and the use of sensor arrays. The next link in the calibration chain, then, can be the extension to energy-dispersive spectrometers that simultaneously observe both x-ray standards interleaved among faint x-ray emission lines under study. This was recently demonstrated (Doriese et al., 2016; Fowler et al., 2017) using arrays of superconducting transition-edge sensors (TES), microcalorimeters with high energy-resolving power. Here, the K lines of metallic titanium, chromium, manganese, iron, and cobalt ($Z = 22, 24, 25, 26, 27$) were used as primary standards to calibrate the line positions of the L lines of the lanthanides neodymium, samarium, terbium, and holmium ($Z = 60, 62, 65, 67$). Calibration functions relating pulse heights to photon energies were derived for each sensor in the array; accounting for sources of systematic variance, this resulted in typical uncertainties of 0.4 eV in the energy range of 4.5 keV–7.5 keV, or $u_r < 10^{-4}$.

Primary x-ray standards of transitions in neutral atoms are also used to calibrate Single Curved Crystal Spectrometers (SCCS), especially instruments used as diagnostics of extreme states of matter. Employing a variety of curved-crystal optics, detector technologies, and data acquisition strategies, SCCS have registered spectra from a variety of exotic x-ray sources such as electron beam ion trap (EBIT) and laser-produced plasmas. At the NIST EBIT, for example, wavelength-calibrated cylindrically-bent SCCS in reflection geometry have been coupled with thorough understanding of diffraction conditions, dispersion relations and source characterization to allow the determination of transition energies in highly charged ions (HCI) to a precision limited by statistics. Such studies permit tests of Quantum Electrodynamics (QED) atomic-structure calculations and assessment of key systematic uncertainties (Chantler et al., 2000, 2012) as well as HCI physics such as mechanisms of collisional excitation (Takacs et al., 1996). Another SCCS that was originally developed to calibrate mammographic x-ray sources (Hudson et al., 1996) has found to be particularly well suited to the high-noise environments of the latest generation of laser-plasma facilities (Hudson et al., 2006, 2007). Characterizing the spectra, time structure, and intensity of x rays emitted by ultra-intense and high-power lasers interacting with matter is critical to assessing system performance and progress as well as pursuing the new and unpredictable physical interactions of interest to basic and applied high-energy-density science. As these technologies mature, advanced diagnostic instrumentation and metrology, standard reference data, absolute calibrations and traceability of results are required.

The calibration chain for x-ray wavelength metrology is shown schematically in Fig. 1. From the definition of the meter, and its transfer from microwave to the visible in the frequency domain, to crystal lattice spacings in the spatial domain via x-ray optical interferometry. This leads to the realization of x-ray measurement standards with both wavelength-and energy-dispersive techniques and their ultimate transfer to applications by way of standard reference data. After a century of development of x-ray sources and detectors that have enabled these innovations in quantum metrology, one can posit the desiderata of next-generation x-ray reference data. A database of x-ray transition energies that will meet community needs going forward is envisioned to be actively maintained with critically-evaluated data that meet the following: the data are acquired using modern methods that possess clear SI traceability and peer-reviewed provenance; Type B uncertainties are quantified; and the excitation conditions are specified as to particle identity and energies. As mentioned above, the tabulation of line peak positions (*e.g.* NIST SRD-128 (Deslattes et al., 2005; Deslattes et al., 2003), (Arndt et al., 2006)) is not sufficient for applications requiring high precision. Accordingly, a modern x-ray database would include the entire spectral profiles on an absolute energy scale, this possibly conveying much more information (elemental, chemical bonding, many-body effects, *etc.*). For convenience, well-defined parameterizations of spectral profiles can be given, if the goodness of the models is made clear. As discussed above, it is also now possible to begin to incorporate the relatively faint L and M lines that are acquired with high-collection-efficiency energy-dispersive techniques (*e.g.* TES arrays) that have been calibrated with relatively intense x-ray standards from wavelength-dispersive techniques (*e.g.* a DCS).

A sampling of applications is given at the far right of Fig. 1. These include medical technology, nuclear weapons effects and testing, renewable energy, semiconductor fabrication, homeland security, astrophysics, and nuclear materials accounting and process monitoring. In particular, the calibration of diagnostic instruments used at novel, exotic x-ray sources is currently in demand to assess the overall system performance and progress, as well as identification of the underlying interaction mechanisms of interest to basic and applied strong-field and high-energy-density science (Hudson and Seely, 2010). And as usual, advances in measurement science and theoretical models move in referential concert.

Finally, it is noteworthy to recognize the worldwide effort known as the International Initiative on X-Ray Fundamental Parameters (Beckhoff et al., 2017). This effort brings together companies, university laboratories, and national metrology institutions involved in x-ray experiments, theory, and computation. Its goal is to take advantage of modern technologies and techniques to establish accurate critical data and standards for common use in calibrating x-ray instruments and experiments with reduced relative uncertainties. As but one example, this will include collection of much of the data needed for *ab initio* calculation of XRF profiles. For example, atomic line and edge positions are needed for numerous transition metals and rare earths where an absorption edge of a given element lies very close to an emission line of an element a few positions up on the periodic table. Very precise knowledge of these positions is critical to make it possible to calculate the absorption, and thus to quantify elements in mixtures. Without the ability to carry out this calculation from accurate published data, it becomes necessary to have a combinatorially large number of standards including mixes of elements. XRF can also benefit from tabulations of relative

fluorescence yields of peaks and peak components, as well as data for $Z < 10$ that are relevant to organic materials characterization.

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Fig. 1.

Calibration chain employed to ensure x-ray wavelength (λ) standards are traceable to the definition of the SI meter. At each step, a relative standard uncertainty, u_r , is assigned to the link in the chain that reflects the current order-of-magnitude state of the art, *i.e.*, $u_r(y) \equiv u(y)/y$ where $u(y)$ is the standard uncertainty of the measurement result y . *SI = Le Système International (d'Unités)*; N_A is the Avogadro constant; SRM = Standard Reference Material; SRD = Standard Reference Data; XRF = X-Ray Fluorescence; XRD = X-Ray Diffraction; QED = Quantum Electrodynamics. c_0 = the speed of light in vacuum; I₂-HeNe is a helium neon laser frequency-stabilized on the saturated absorption spectrum of molecular iodine (I₂); XROI = X-Ray Optical Interferometer; delta-d is the NIST lattice comparator machine; GAMS4 = the high-resolution flat-crystal gamma-ray facility at the Institut Laue-Langevin (Kessler et al., 2001); VDCS = Vacuum Double Crystal Spectrometer; PBD = Parallel Beam Diffractometer and DBD = Divergent-beam Diffractometer used to certify the lattice parameters of powder SRMs; TES = Transition Edge Sensor. The items in parentheses are particular instruments and methods that have been employed, developed or constructed by NIST.