Advances in SI-Traceable Wavelength Metrology

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A collaboration was begun within NIST to combine wavelength- and energy-dispersive X-ray methods to provide traceability to the definition of the meter in the international system of units (SI). The Vacuum Double Crystal Spectrometer (VDCS) [1] measures wavelength-dispersive spectra in the 2 keV to 12 keV X-ray energy range. These reference spectra then can be used for the calibration of transition edge sensor (TES) arrays to obtain high resolution energy-dispersive spectra of much weaker X-ray transitions.

The X-ray Fundamental Parameters (FP) project should include the characteristic X-ray spectra of the elements. In contrast, current line lists [2] and databases [3] are limited to a list of peak positions for the X-ray transition energies with a single numerical value listed corresponding to the energy profile maxima. Even the strongest lines in the characteristic X-ray spectra of neutral atoms naturally include various satellites that alter the line shapes in the spectra yielding asymmetric peaks. Furthermore, the peak position for any asymmetric peak is a function of instrumental resolution and analysis method. A better approach is to provide reference spectra for each X-ray transition in a critically-evaluated database, with an accounting of all instrumental and systematic effects, giving parameterization of the intrinsic spectra.

The VDCS employs crystals whose lattice spacings are traceable to the definition of the meter through X-ray optical interferometry to a relative uncertainty $<10^{-8}$. In a double crystal spectrometer X-ray wavelength measurements are based on precision angle difference measurements for which the rotation stages of VDCS have been calibrated using the circle closure method for accurate, absolute angle measurement [4]. A vacuum compatible Dectris, Pilatus 100 area detector allows for the quantification of various aberration functions contributing to the observed line shape. The detector and the use of a thin lamella as the first crystal facilitate the alignment of the diffraction elements. Using these new techniques X-ray spectra are registered with the VDCS producing results at the relative uncertainty of 10^{-6}. These reference spectra, in turn, may provide the energy calibration of high resolution TES arrays with uncertainties better than 10^{-4}. In this way, the VDCS provides a few, intense standard fiducials, and the TES X-ray spectrometers can contribute many interleaved and often weak X-ray standards to the future FP databases.

[1] R. D. Deslattes, *Rev. Sci. Instrum.* **38**, 616-620 (1967).

[2] R. D. Deslattes *et al.*, *Rev. Mod. Phys.* **75**, 35-99 (2003).

[3] NIST Standard Reference Database 128: https://www.nist.gov/pml/X-ray-transition-energies-database

[4] M. N. Kinnane, L. T. Hudson, A. Henins, M. H. Mendenhall, *Metrologia* **52**, 244-250 (2015).