

Validation of the NRL/NIST High-energy X-ray Spectrometer (HXS) for LLE

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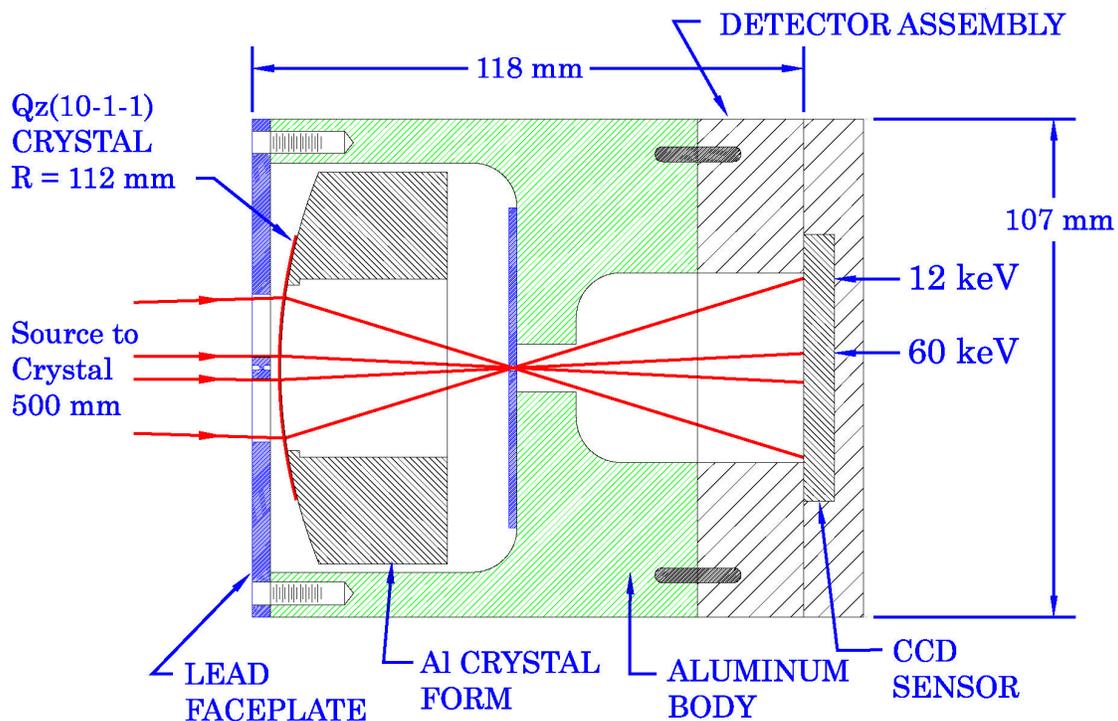
Outline:

- A. Spectrometer and Validation Overview
- B. Sensitivity to Source Size
- C. Required Pointing Precision
- D. Analysis of Spectra
- E. Determination of Plate Function
- F. Image Acquired with DEF Film

A. Spectrometer and Validation Overview

The spectrometer's layout is shown schematically below and is a modification of a design originally developed for the energy calibration of medical radiography x-ray sources (NIST US Patent #5381458, A curved crystal spectrometer for energy calibration and spectral characterization of mamographic x-ray sources, L. T. Hudson, et al. Med. Phys. **23** (1996) 1659). The instrument produces two spectral representations that are registered on a CCD detector containing 1360 rows and 1840 columns of pixels. These are mirror images of one another; each

Figure 1: **LLE CRYSTAL SPECTROMETER DESIGN**

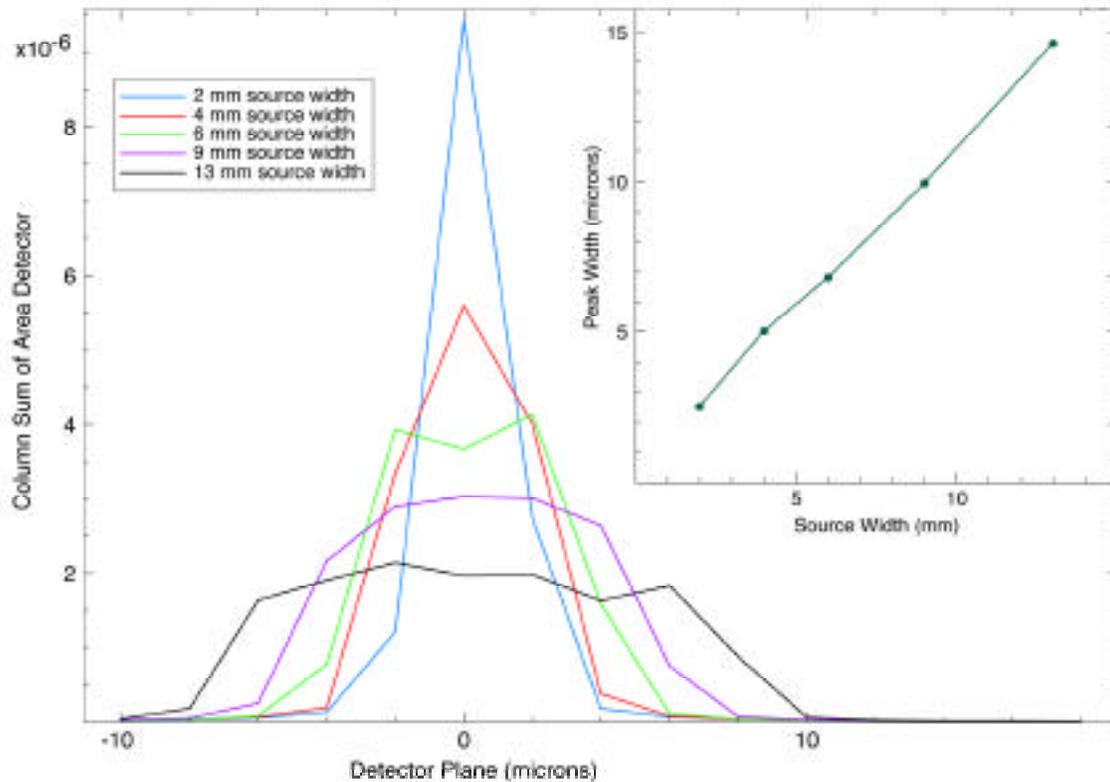


is imaged on a circle whose diameter equals the radius of curvature of the crystal after passing through a polychromatic focal spot. (Ideally, the detector would be cylindrical.) The quartz(10-1-1) crystal, which has a lattice spacing of 3.34 Å, has been aligned and cut such that spectral lines will appear vertically on the spectrometer backplane. After polishing the quartz crystal to a thickness of about 220 μm, it is etched in ammonium bifluoride to remove surface damage and finally cylindrically bent to a radius of 112 mm. Having obtained an x-ray image, a column sum of the pixel values gives a one-dimensional “line out” spectrum. The instrumental zero wavelength position lies at the bisector of any pair of corresponding spectral features. This permits the energy axis to be self-calibrated using a few x-ray lines or absorption edges. Although the wavelength dispersion is approximately constant, a very good approximation of the "plate function" which relates lateral position on the detector to energy is given by:

$$E^2 = a/x^{-2} + b$$

where a and b are constants, x is the distance from the center of the two mirror spectra to any feature of interest, and E is the energy of the spectral bin at x. During instrument validation at NIST, the crystal is rotated until the midpoint between mirror spectra coincides very nearly with the image of a pinhole situated on the center axis of the instrument. While the CCD resolution element is only 19.5 μm, the instrument resolution is somewhat greater than twice that due primarily to the scattering produced by the x-ray phosphor converter of finite thickness. Also during the NIST validation process, the sensor is rotated to coincide with the diffracting planes by making the spectral lines appear vertical on the CCD image.

Figure 2: Simulation of Source Size Sensitivity of LLE Spectrometer at E=39.2 keV (Ba Ka)



B. Sensitivity to Source Size

Monte Carlo ray-tracing software has been applied to the geometry of the HXS to predict its sensitivity to source size. A virtual monochromatic x-ray source was used with energy 39.2 keV (Ba K-alpha). Only lateral source width would affect the geometric resolution of spectral lines. Calculations were performed for source widths of 2 to 13 mm and the results are shown above in Figure 2. To a first approximation, to gauge loss of instrumental resolution, the monochromatic peak widths shown should be added in quadrature with actual lifetime widths. The results predict a geometrical broadening of less than 15 μm in all cases which is less than the instrumental resolution. It is therefore expected that modest source sizes will not cause significant degradation of resolution.



Figure 3:
NIST
Validation
Facility

C. Required Pointing Precision

Field-of-view tests were performed at NIST using a continuous microfocus (250 μm , molybdenum anode) x-ray source. Shown above is a picture of the controller, 50 kV high-voltage supply, cooling module, and calibrated step-down resistor chain that permits accurate measure of

the accelerating potential. On top of the rack can be seen a gray cube housing the x-ray tube and the HXS mounted 50 cm from the source (also shown in close up). Consider the effects of misalignment in the sense of roll, pitch, and yaw about the spectrometer center axis. Roll errors should not affect the measurements unless the source is highly asymmetric and much larger than 15 mm. Errors in pitch cause the entire spectrum to shift up or down on the sensor and should not affect energy determination but could result in some loss of signal. Yaw errors, however, are quite critical and if gross enough, can violate the diffraction condition or cause other obstructions resulting in the loss of one or both of the mirror spectra. Experimental tests using the setup of Figure 3 showed that the instrument has a lateral field of view of about ± 0.35 degrees which represents about ± 3 mm at the target. It should be noted that both pitch and yaw pointing errors can be readily quantified by noting the position of the x-ray image of the center-axis pinhole camera compared to the fiducial pinhole image position. As delivered, this position is at pixel column 907 and pixel row 669. In principle, 9 mil shims inside the sensor holder could bring the CCD into coincidence with the pinhole.

D. Analysis of Spectra

A CCD image of the molybdenum x-ray source described above is shown (in false color) in Figure 4. Visible are the K lines of molybdenum ranging from 17.4 to 20.0 keV, the continuum x-ray spectrum ranging from 12 keV at the far left to the high-energy cutoff which was 42 keV in this instance. Also seen are the images of the center-axis pinhole and, in the upper right hand of the image, a commercial logo that is not present when using the HXS drive electronics. As mentioned above, if the spectral lines are aligned with grid of the CCD, the values of the pixels can be summed by column to form a one-dimensional spectrum which is also shown on the figure with annotations. Otherwise, software image rotation is required before spectral analysis.

E. Determination of Plate Function

Spectra obtained by the aforementioned alignment and data reduction procedures have been used to energy calibrate the HXS spectrometer. We have used the K-absorption edges as well known energy markers [X-Ray wavelengths, R. D. Deslattes, E. G. Kessler, Jr., P. Indelicato, and E. Lindroth in International Tables for Crystallography, Vol. C, 1999, p. 200]. Foils of appropriate thickness were inserted into the spectrometer just before the polychromatic focal point via a filter assembly which is inserted through the lid of the spectrometer body. As shown in Figure 5, this introduces well defined absorption features into the spectra. The top spectrum of the figure shows the effect before and after insertion of a 25 μ m Mo foil. In the lower spectrum the results of a 50 μ m thick Cd foil is shown. The edge position is taken to be the inflection point in the absorption curve μx which is proportional to the logarithm of the acquired filtered spectrum [High resolution x-ray absorption spectroscopy with absolute energy calibration for the

Figure 4

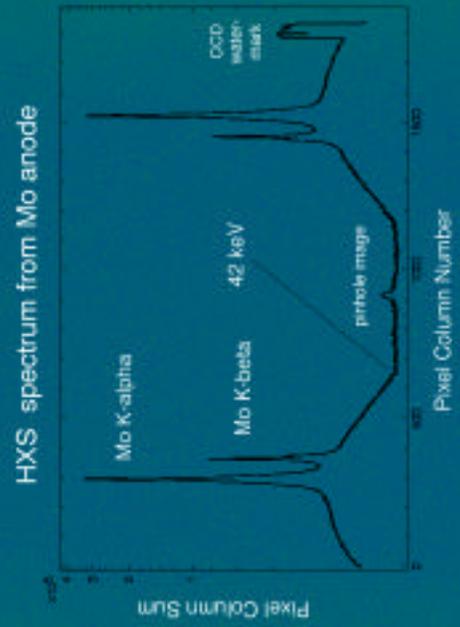


Figure 5

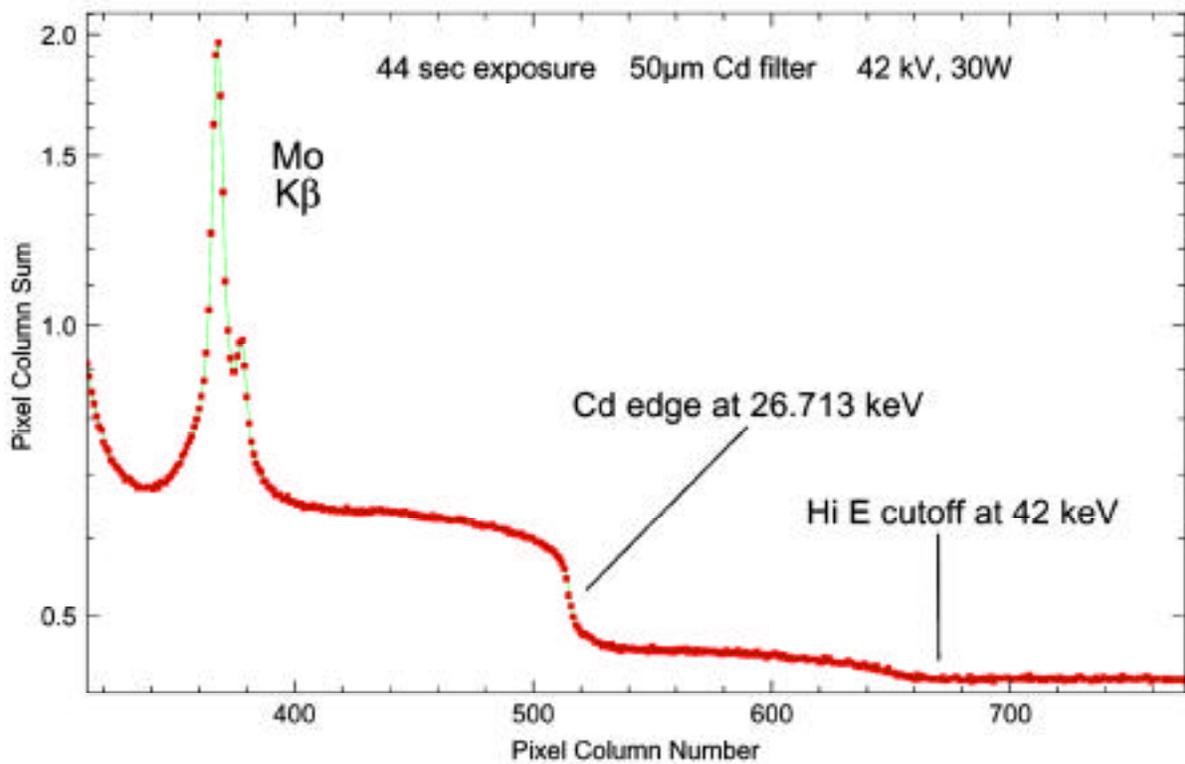
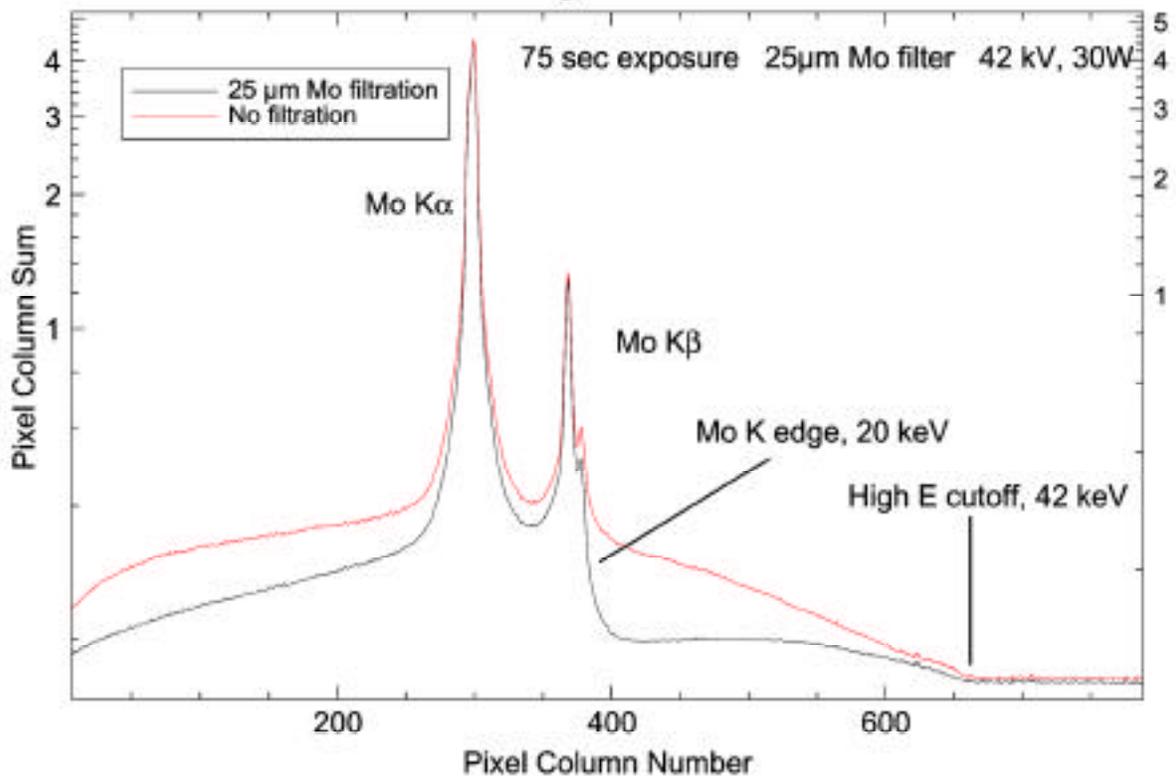
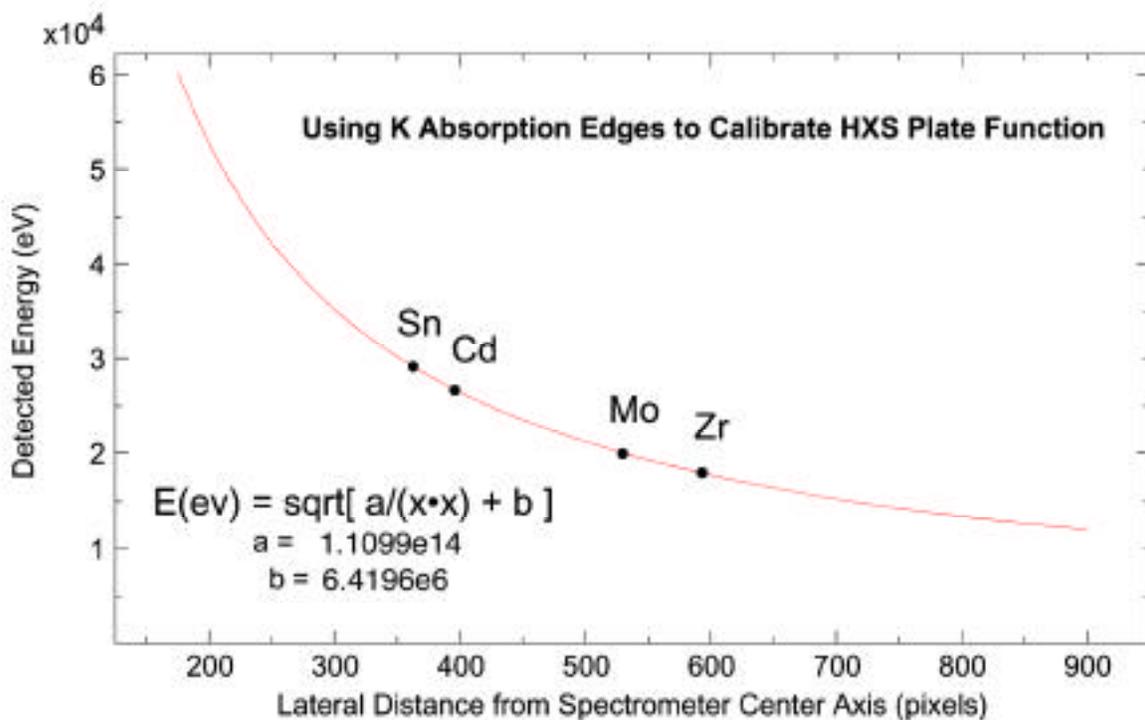
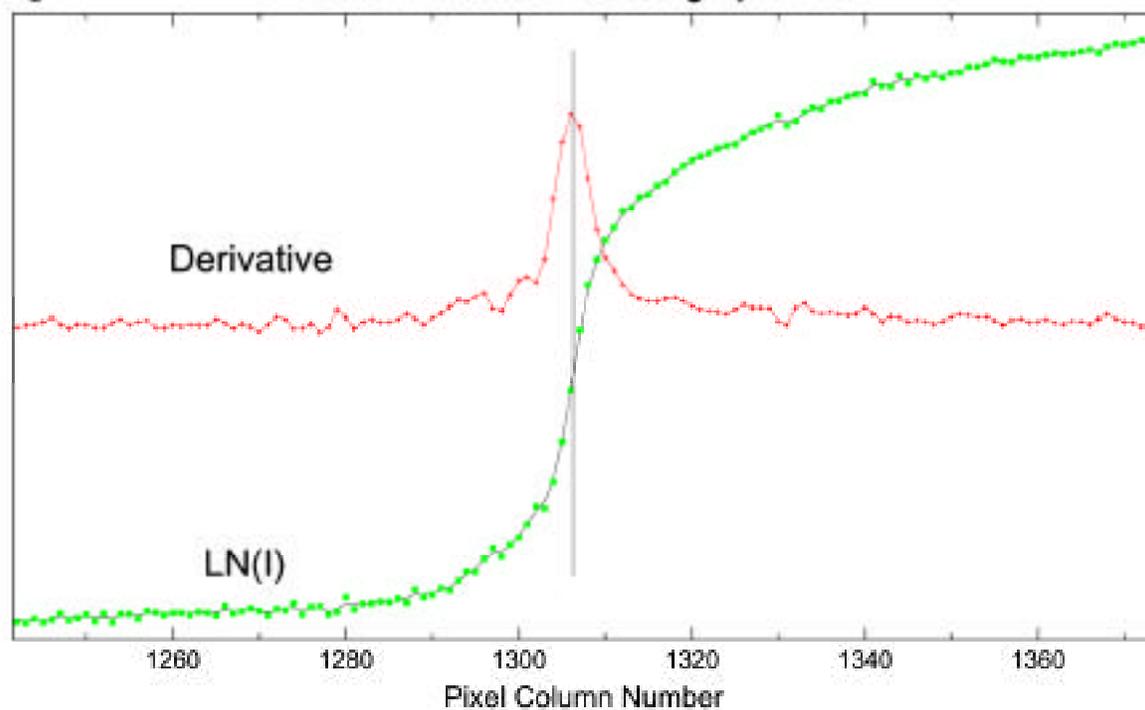


Figure 6: Determination of Cd-edge position



determination of absorption edge energies, S. Kraft, J. Stumpel, P. Becker, and U. Kuertgens, Rev. Sci. Instrum. **67** (1996) p. 681]. The top of Figure 6 illustrates the method used to determine the edge position. First, fixed pattern noise was subtracted from the spectrum using an “x-rays off” image. Then the log of the spectrum was high-frequency filtered (if needed) and the derivative of the result was fit to a Gaussian function to locate the centroid. The results for the HXS as delivered are compiled in the following table.

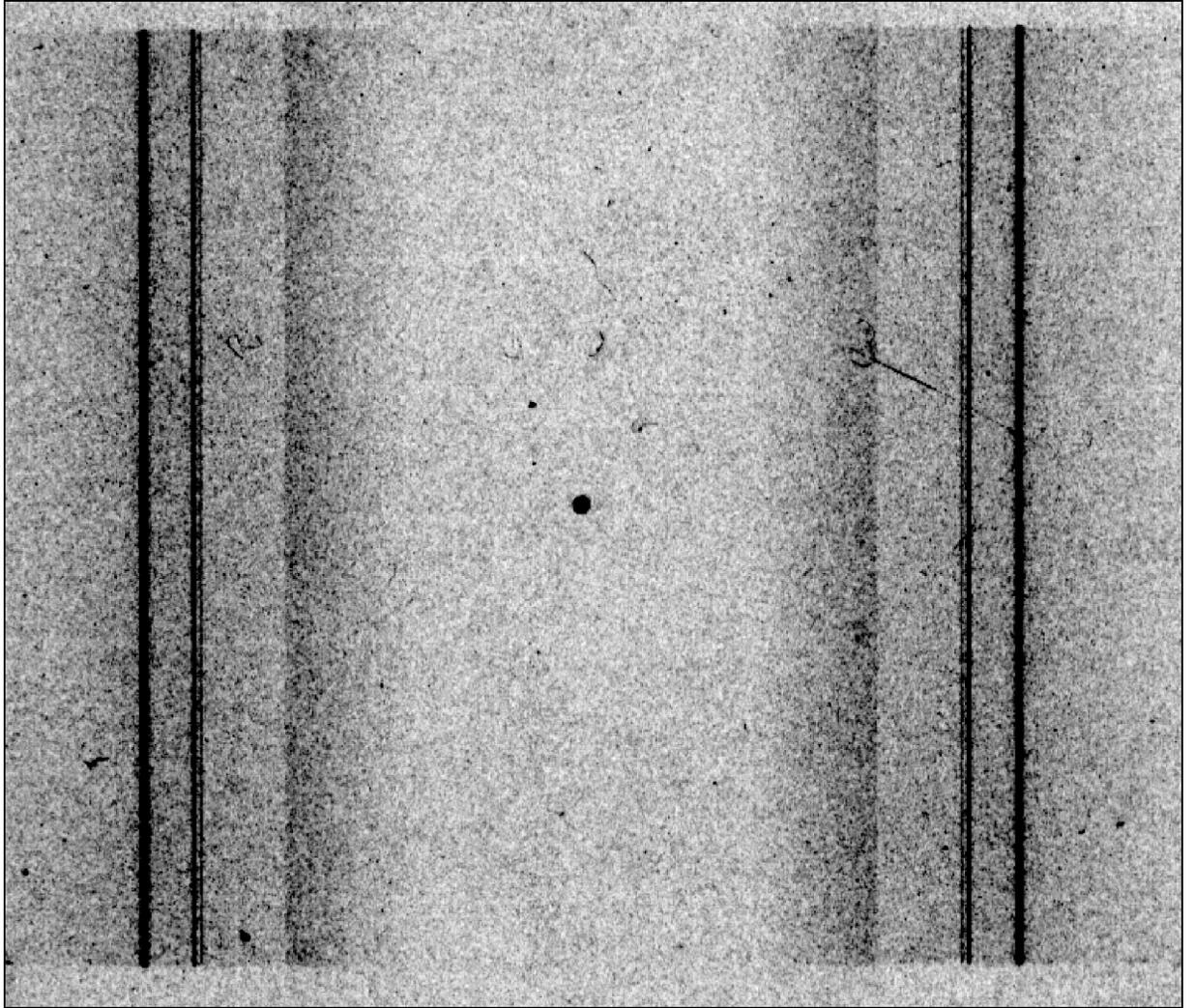
Elemental Foil	X(pixels)	E (eV)	Residuals from fitted plate function (eV)
Sn	362.70	29200	43
Cd	395.61	26713	-38
Mo	529.59	20000	-53
Zr	592.94	17996	47

The constants found for the plate function $E(\text{eV})^2 = a/x^{-2} + b$ are $a = 1.1099\text{e}14$ and $b = 6.4196\text{e}6$ giving the residuals shown in the table above. It should be noted that the plate function is modified if there are changes in the crystal-to-source distance (50 cm), spectrometer pointing errors, or rotation of the crystal with respect to spectrometer body. This crystal rotation has been carefully set at NIST and adjustment is not recommended.

F. Image Acquired with DEF Film

Finally, we include an image acquired with DEF x-ray sensitive film. Figure 7 is shown on the following pages with annotation. On the right, the digitization of the film was of sufficient resolution to reveal both resolved Mo K-alpha and K-beta lines.

If there are any questions regarding the calibration or validation of the HXS, contact Larry Hudson at NIST (301-975-2537 or larry.hudson@nist.gov).



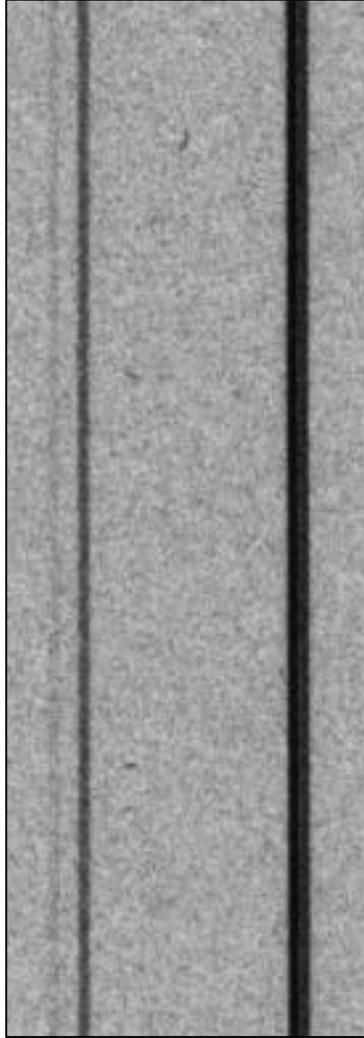


Figure 7: Top: A 40 second exposure on DEF film using a Mo anode and 45 kVp. The K α (17.374 keV and 17.479 keV) and K β (19.608 keV and 19.965 keV) characteristic x-ray lines are resolved. The enhanced absorption in the AgBr emulsion on the high-energy side of the Ag K absorption edge at 25.517 keV is also visible. Lower: A portion of the image showing the resolution of the K α and K β lines.