

## Wavelength of the W $K\alpha_1$ x-ray line

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The wavelength of the  $K\alpha_1$  line from an electron-bombarded natural W anode has been measured in terms of that of an  $I_2$ -stabilized HeNe laser. This visible laser is a reference point for current Rydberg determinations and for the present-day definition of length. The resulting wavelength value, namely 0.20901349 Å (0.90 ppm) (energy = 59.319233 keV) appears to resolve historical inconsistencies in the x-ray route to  $\gamma$  wavelengths.

The tungsten  $K\alpha_1$  x-ray line has served as a reference wavelength for both x-ray and  $\gamma$ -ray measurements. Historically, it has entered all but the most recent chains by which visible to  $\gamma$ -ray reference wavelength ratios were established. From the group of five  $K$  x-ray wavelengths whose ratios were extensively measured by Bearden and collaborators,<sup>1</sup> Bearden proposed as the scale defining entity  $\lambda(W K\alpha_1) = 0.2090100 \text{ \AA}^*$ .<sup>2</sup> This choice was based on its symmetry, relative freedom from chemical effects and its convenience for  $\gamma$ -ray standardization. On the other hand, the width of  $W K\alpha_1$  is quite large (approximately 1000 ppm) and there have been indirect suggestions of possible problems from time to time.

A particularly clear-cut instance of difficulty is found in comparing precise wavelength values for  $W K\alpha_1$  derived from distinctly different routes. In the first route a previous measurement of  $\lambda(Mo K\alpha_1)$  in terms of a visible standard<sup>3</sup> [ $\lambda(Mo K\alpha_1) = 0.7093184 \text{ \AA}$  (0.6 ppm)] is combined with the ratio  $\lambda(Mo K\alpha_1)/\lambda(W K\alpha_1)$  from Bearden *et al.*<sup>1</sup> [ $\lambda(Mo K\alpha_1)/\lambda(W K\alpha_1) = 3.393620$  (1.9 ppm)] to obtain a value for  $\lambda(W K\alpha_1) = 0.20901527 \text{ \AA}$  (2.0 ppm). Alternatively, another x-ray value can be established using the wavelength of  $Cu K\alpha_1$  from Ref. 3 and the ratio of the wavelengths of  $Cu K\alpha_1$  to  $W K\alpha_1$  from Ref. 1 with the result  $\lambda(W K\alpha_1) = 0.20901481 \text{ \AA}$  (2.1 ppm).

A third and rather different route combines a recent direct measurement of the  $^{198}\text{Au}$  411-keV  $\gamma$ -ray line<sup>4</sup> [ $\lambda(^{198}\text{Au} 411) = 3.0107788 \text{ pm}$  (0.37 ppm)] with the  $\lambda(W K\alpha_1)/\lambda(^{198}\text{Au} 411)$  ratio from Borcherth<sup>5</sup> [ $\lambda(W K\alpha_1)/\lambda(^{198}\text{Au} 411) = 6.9421377$  (3.4 ppm)] to obtain a value for  $\lambda(W K\alpha_1) = 0.20901241 \text{ \AA}$  (3.4 ppm). The three values for  $\lambda(W K\alpha_1)$  can be expressed as energies using a conventional  $V$ - $\lambda$  conversion factor to give  $E(W K\alpha_1) = 59.318728 \text{ keV}$  (2.0 ppm) from  $Mo K\alpha_1$ ,  $E(W K\alpha_1) = 59.318858 \text{ keV}$  (2.1 ppm) from  $Cu K\alpha_1$ , and  $E(W K\alpha_1) = 59.319540$  (3.4 ppm) from  $^{198}\text{Au} 411$ . The difference between the energy values from Au and Mo

is  $0.81 \pm 0.23 \text{ eV}$  and that between the energy values from Au and Cu is  $0.68 \pm 0.24 \text{ eV}$ , seriously troubling results. The wavelength of  $W K\alpha_1$  can also be derived from the two earlier less precise x-ray measurements. In the first the ratio  $\lambda(W K\alpha_1)/\lambda(Mo K\alpha_1)$  as measured by Watson *et al.*<sup>6</sup> [ $\lambda(W K\alpha_1)/\lambda(Mo K\alpha_1) = 0.294668$  (38 ppm)] was combined with the value of  $\lambda(Mo K\alpha_1)$  above to obtain  $\lambda(W K\alpha_1) = 0.2090133 \text{ \AA}$  (38 ppm). In the second a ruled grating measurement of  $\lambda(Al K\alpha)$  [ $\lambda(Al K\alpha) = 8.34034$  (9 ppm)] and the ratio  $\lambda(Al K\alpha)/\lambda(Cu K\alpha_1)$  [ $\lambda(Al K\alpha)/\lambda(Cu K\alpha_1) = 5.413782$  (4.1 ppm)] from Henins<sup>7</sup> were combined with the Bearden *et al.* ratio  $\lambda(Cu K\alpha_1)/\lambda(W K\alpha_1)$  mentioned above to obtain  $\lambda(W K\alpha_1) = 0.2090118 \text{ \AA}$  (10.0 ppm). Although both these values agree (within the uncertainty) with the result obtained via Au, the rather large uncertainties make the comparisons not particularly informative.

Because of the inconsistency in the more precise data an independent measurement of  $\lambda(W K\alpha_1)$  was undertaken which could provide not only a precise value for  $\lambda(W K\alpha_1)$  but also improve estimates of several of the wavelength ratios used above. As was the case in our previous redetermination of x-ray wavelengths<sup>3</sup> ( $Mo K\alpha_1$  and  $Cu K\alpha_1$ ) and our recent work on  $\gamma$ -ray wavelengths,<sup>4</sup> the objective for  $W K\alpha_1$  was to measure its wavelength in terms of the wavelength of a stabilized laser.

The connection of the tungsten  $K\alpha$  x-ray wavelength to this visible laser was made in three steps utilizing the lattice spacing of nearly perfect silicon crystals. In the first step a combined x-ray and optical interferometer was used to measure the lattice spacing of a particular silicon crystal in terms of the wavelength of a HeNe laser stabilized to the  $B$  peak of  $^{129}\text{I}_2$ .<sup>8</sup> The measured unit cell dimension of this crystal is  $a_0 = 5.4310280 \text{ \AA}$  (0.10 ppm) at  $22.5^\circ\text{C}$ .<sup>3,9,10</sup> A similar laser stabilized to the  $n$  peak of  $^{129}\text{I}_2$  had been interferometrically compared to Balmer  $\alpha$  in the most

recent determination of the Rydberg constant.<sup>11</sup> The frequency difference of these lasers has been measured and they have been compared to the krypton length standard.<sup>8,12</sup> Thus the unit cell measurement and the x-ray wavelength measurements reported here are on a scale directly related to the Rydberg constant and the definition of length.

In the second step, the lattice spacing of this interferometrically measured crystal was then compared to that of other silicon crystals whose size and orientation were more suitable for diffraction of the  $W K\alpha_1$  x ray. This measurement was made using a variation of a procedure suggested by Ando, Bailey, and Hart for comparison of similar crystals using surface reflections.<sup>13</sup> The surface reflection geometry was replaced with symmetric transmission geometry as shown in Fig. 1. The advantage of this method is the reduction of thermal effects by simultaneous recording of the triply diffracted reference beam (det B) and the doubly diffracted measurement beam (det A). The ratio of the lattice spacings of the interferometrically measured crystal to the crystals used in the W measurement is 1.000 000 044 (0.07 ppm) and thus the unit cell edge for the crystal used to diffract W x rays is 5.431 027 8 Å (0.12 ppm) at 22.5 °C. The lattice spacing measurements were recorded within  $\pm 1$  °C of 22.5 °C and reduced to 22.5 °C by use of  $\alpha_{Si} = 2.56 \times 10^{-6} \text{ K}^{-1}$ .<sup>14</sup>

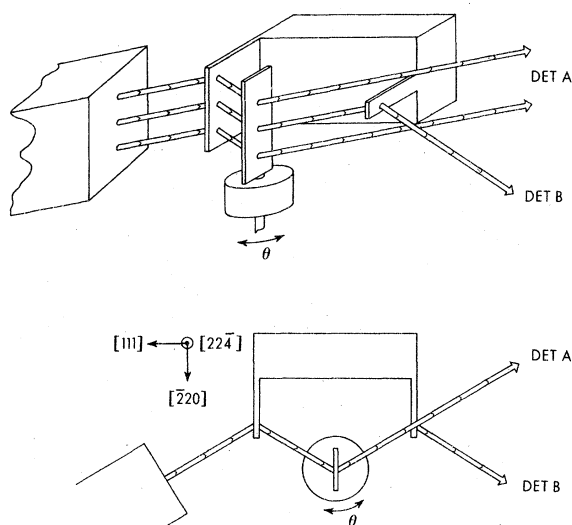


FIG. 1. Schematic diagram of the comparison of the lattice spacing of the Si crystals. The U-shaped crystal is the reference crystal, and the standard crystal and the unknown crystal are alternately placed on the rotating table. The small angular separations between the doubly (DET A) and triply (DET B) diffracted beams are measured.

In the third step, these crystals were placed on a double flat crystal spectrometer and used in the [111] orientation to diffract  $W K\alpha_1$  radiation (symmetric Laue diffraction). As noted previously,<sup>4,15</sup> this instrument is fitted with angle interferometers using polarization encoding. The resulting precision is near 0.05 marc sec while calibration accuracy near 0.1 ppm is maintained for angles in excess of 0.4 °.

The tungsten K spectrum was produced by electron bombardment of a natural W anode. Power was full wave rectified 2 kHz at 140 kV with an electron current of approximately 2 mA delivered to a focal spot area of 1.2 mm<sup>2</sup>.<sup>16</sup> The Bragg angle for the  $W K\alpha_1$  [using Si(111) planes] is 1.9°. Rocking curves were recorded with the crystals in the parallel and antiparallel positions. In the non dispersive (parallel) position, line widths of 1.8 arc sec (full width at half-maximum, FWHM) were recorded. However, in the dispersive (antiparallel) position, the line widths were 11.9 arc sec (FWHM). Almost all the measurement uncertainty results from the determination of the peak position of the dispersive rocking curve.

In order to minimize instrumental drifts, dispersive and nondispersive rocking curves were alternately recorded. In the nondispersive position, all x rays produced by the x-ray tube within the energy window of the detector were normally available. Count rates of 500 per sec at the profile maximum were recorded. Typical scanning time for recording the nondispersive profile was 10 min. In the dispersive position the count rate at the line maximum was 30 per sec. Approximately  $3 \times 10^4$  counts were accumulated in each dispersive recording which typically took about 60 min. About  $6 \times 10^5$  counts were accumulated in all the dispersive recordings. Data were recorded on seven different days with three to nine profiles being recorded on a given day.

The dispersive and nondispersive rocking curves were computer fit with a Lorentzian profile. The position, intensity, and width of the Lorentzian profile and a constant background were varied by the computer to obtain the "best" fit in a least-squares sense. Typical rocking curves and the computer fit are shown in Fig. 2.

Bragg angles were obtained from the measured angles by correcting for vertical divergence using the two-slit approximation.<sup>1</sup> The focal spot of the x-ray tube was one slit (1.2 mm) and the inter-crystal collimator was the other slit (2.7 mm). The correction was approximately 0.1 ppm.

To obtain a final wavelength value and its uncertainty, the wavelength measurements obtained on each of the seven days were weighted according

TABLE I. Comparison of wavelength ratios.

Wavelength ratio	NBS	Bearden <i>et al.</i>	Difference (NBS-Bearden <i>et al.</i> , ppm)
$\lambda(\text{Cu } K\alpha_1)/\lambda(\text{Mo } K\alpha_1)$	2.171 940 6 (1.2 ppm)	2.171 945 (1.5 ppm)	-2.0
$\lambda(\text{Cu } K\alpha_1)/\lambda(\text{W } K\alpha_1)$	7.370 803 7 (1.3 ppm)	7.370 757 (1.8 ppm)	6.3
$\lambda(\text{Mo } K\alpha_1)/\lambda(\text{W } K\alpha_1)$	3.393 648 9 (1.1 ppm)	3.393 620 (1.9 ppm)	8.5

to the number of profiles recorded and averaged. The results are  $\lambda = 0.209\,013\,49 \text{ \AA}$  (0.90 ppm) and  $E = 59.319\,233 \text{ keV}$  (0.90 ppm) where the voltage-wavelength conversion factor,  $1.239\,852\,0 \times 10^{-6} \text{ eV m}$ , from Ref. 17 was used. The components of the uncertainty are as follows: statistical uncertainty, 0.88 ppm; uncontrolled measurement systematics, 0.13 ppm (see Ref. 4); calibration uncertainty, 0.1 ppm; and lattice spacing uncertainty, 0.12 ppm. Since, in  $\text{\AA}^*$  units, the peak of the  $W K\alpha_1$  radiation has a defined value,  $\lambda(W K\alpha_1) = 0.209\,010\,0 \text{ \AA}^*$ , a conversion factor from  $\text{\AA}^*$  units to  $\text{\AA}$  units emerges as  $\Lambda^* = 1.000\,016\,7 \text{ \AA}/\text{\AA}^* (0.90 \text{ ppm})$ . By way of comparison, the most recently published adjustment of the fundamental constants recommended a value for  $\Lambda^*$  of  $\Lambda^* = 1.000\,020\,5 (5.6 \text{ ppm})$ .<sup>17</sup>

An assessment of this result may be obtained by noting that with its inclusion, there are now three x-ray wavelengths measured in terms of optical standards,  $\lambda(\text{Cu } K\alpha_1) = 1.540\,597\,4 \text{ \AA}$  (1 ppm),  $\lambda(\text{Mo } K\alpha_1) = 0.709\,318\,4 \text{ \AA}$  (0.6 ppm),<sup>3</sup> and  $\lambda(\text{W } K\alpha_1) = 0.209\,013\,49 \text{ \AA}$  (0.90 ppm). While comparisons of these values individually with previous ones depend on the particular values of  $\Lambda$  or  $\Lambda^*$  which are used, comparisons of the ratios of these three quantities with those of other experiments are independent thereof. Table I therefore shows ratios of these wavelengths and compares these with those of Bearden *et al.*<sup>1</sup> The ratios involving  $W K\alpha_1$  are clearly in disagreement with the Bearden *et al.* values which we conclude to be in error to the extent of the indicated differences.

Finally, the ratio of the wavelengths or energies of the  $W K\alpha_1$  x ray and the  $^{198}\text{Au}$  411-keV  $\gamma$  ray has been measured by other experimenters using curved crystal spectrometers.<sup>5,18</sup> Measurements of this ratio are summarized in Table

TABLE II. Comparison of W to Au wavelength ratios.

	$\lambda(W K\alpha_1)/\lambda(^{198}\text{Au } 411 \text{ keV})$
Borchert, Ref. 5	6.942 138 (3.4 ppm)
Beer and Kern, Ref. 18	6.942 216 (9.1 ppm)
NBS	6.942 1735 (1.0 ppm)
Fundamental constants	6.942 024 (17.9 ppm)

II. There it is noted that the difference of  $5.1 \pm 3.5 \text{ ppm}$  in the case of Ref. 5 is slightly troubling but not highly unlikely. The larger uncertainty from Ref. 18 makes the difference  $6.1 \pm 9.2 \text{ ppm}$  less significant but consistent with the currently reported result.

The value of this ratio can also be inferred by combining the  $W K\alpha_1$  and the annihilation radiation wavelengths from the 1973 adjustment of the fundamental constants<sup>17</sup> with a measurement of the difference between the annihilation radiation and the  $^{198}\text{Au}$  wavelengths.<sup>19,20</sup> This value is included in the table<sup>21</sup> and exhibits a discrepancy of  $\sim 20 \text{ ppm}$  from the values obtained in the direct measurements. This rather large discrepancy is primarily due to the annihilation radiation to  $^{198}\text{Au}$  411-keV comparison.

In the past compilers of  $\gamma$ -ray energies have not been able to resolve the discrepancy between the  $\gamma$ -ray scale based on tungsten and that based on Au.<sup>22</sup> The absolute measurements of the  $^{198}\text{Au}$  411-keV line<sup>4</sup> and the  $W K\alpha_1$  line reported here and the relative measurements of Ref. 5 and 18 bring the two scales into coincidence to better than the 5-ppm level.

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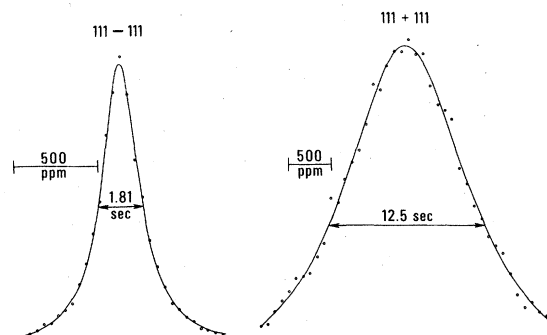


FIG. 2. Nondispersive and dispersive profiles for Si crystals at  $W K\alpha_1$  (59 keV). The dots are the data points and the curve is the computer fit.

- <sup>1</sup>J. A. Bearden, A. Henins, J. G. Marzolf, W. C. Sauder, and J. S. Thomsen, *Phys. Rev.* **135**, A899 (1964). Because the uncertainties given in this reference are probable errors (50% confidence limit), they have been expanded to one standard deviation (67% confidence limit).
- <sup>2</sup>J. A. Bearden, *Phys. Rev.* **137**, B455 (1965).
- <sup>3</sup>R. D. Deslattes and A. Henins, *Phys. Rev. Lett.* **31**, 972 (1973). The wavelengths for Cu  $K\alpha_1$  and Mo  $K\alpha_1$  given in this reference have been corrected by 0.44 ppm because of the corrections to  $a_0$  as discussed in Ref. 10.
- <sup>4</sup>E. G. Kessler, Jr., R. D. Deslattes, A. Henins, and W. C. Sauder, *Phys. Rev. Lett.* **40**, 171 (1978).
- <sup>5</sup>G. L. Borchert, *Z. Naturforsch. A* **31**, 102 (1976). In the discussion of the  $\lambda(WK\alpha_1)/\lambda(^{198}\text{Au } 411)$  ratio in Refs. 4 and 15, values from G. L. Borchert, W. Scheck, and O. W. B. Schult, *Nucl. Instrum. Methods* **124**, 107 (1975) were used. For the comparisons presented here we have chosen the more recent data associated with fluorescence sources. For a more complete discussion of the results from the Jülich group, see G. L. Borchert, 4th International Conference on Atomic Physics, Heidelberg (1974), p. 656.
- <sup>6</sup>B. B. Watson, W. J. West, D. A. Lind, and J. W. M. DuMond, *Phys. Rev.* **75**, 505 (1949).
- <sup>7</sup>A. Henins, in *Precision Measurements and Fundamental Constants*, edited by D. N. Langenberg and B. N. Taylor, National Bureau of Standards Special Publication No. 343 (U.S. GPO, Washington, D.C., 1971), p. 255.
- <sup>8</sup>W. G. Schweitzer, Jr., E. G. Kessler, Jr., R. D. Deslattes, H. P. Layer, and J. R. Whetstone, *Appl. Opt.* **12**, 2927 (1973).
- <sup>9</sup>R. D. Deslattes, A. Henins, H. A. Bowman, R. M. Schoonover, C. L. Carroll, I. L. Barnes, L. A. Machlan, L. J. Moore, and W. R. Shields, *Phys. Rev. Lett.* **33**, 463 (1974).
- <sup>10</sup>R. D. Deslattes, A. Henins, R. M. Schoonover, C. L. Carroll, and H. A. Bowman, *Phys. Rev. Lett.* **36**, 898 (1976).
- <sup>11</sup>T. W. Hänsch, M. H. Nayfeh, S. A. Lee, and I. S. Shahin, *Phys. Rev. Lett.* **32**, 1336 (1974).
- <sup>12</sup>J. Terrien, *Rev. Prog. Phys.* **39**, 1067 (1976), and references cited therein.
- <sup>13</sup>M. Ando, D. Bailey, and M. Hart, *Acta Crystallogr. Sec. A* **34**, 484 (1978).
- <sup>14</sup>R. K. Kirby (private communication).
- <sup>15</sup>R. D. Deslattes, Course No. LXVIII, "Metrology and Fundamental Constants," Enrico Fermi School of Physics, July 12–24, 1976.
- <sup>16</sup>The x-ray equipment available for this experiment was a SPX 160-kV portable x-ray unit manufactured by Sperry Division, Automation Industries, Inc.
- <sup>17</sup>B. N. Taylor and E. R. Cohen, *J. Phys. Chem. Ref. Data* **2**, 663 (1973).
- <sup>18</sup>W. Beer and J. Kern, *Nucl. Instrum. Methods* **117**, 183 (1974).
- <sup>19</sup>G. Murray, R. L. Graham, and J. S. Geiger, *Nucl. Phys.* **45**, 177 (1963).
- <sup>20</sup>G. Murray, R. L. Graham, and J. S. Geiger, *Nucl. Phys.* **63**, 353 (1965).
- <sup>21</sup>R. G. Helmer, R. C. Greenwood, and R. J. Gehrke, *Atomic Masses and Fundamental Constants 5*, edited by J. H. Sanders and A. H. Wapstra (Plenum, New York, 1976), p. 30.
- <sup>22</sup>R. C. Greenwood, R. G. Helmer, and R. J. Gehrke, *Nucl. Instrum. Methods* **77**, 141 (1970).