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(kilo x unit). Uncertainty in the conversion factor between the X-ray and optical scales was the dominant contributor to the total uncertainties in the wavelength values of the sharper X-ray emission lines, such as those most frequently used in crystallography. (For a discussion of the present values in relation to previously assigned numerical values on the various scales, see Subsection 4.2.2.14.) This local unit was, for most of the time, 'officially' defined by assigning a specific numerical value to the lattice period of a particular reflection from 'the purest instance' of a particular crystal. Originally this was rocksalt; later it was calcite. In practice, most work used as *de facto* standards certain values for Cu $K\alpha_1$ and Mo $K\alpha_1$ whose inconsistency, though noted by some crystallographers earlier, was seriously addressed by Bearden and co-workers only in the 1960's (Bearden, Henins *et al.*, 1964). This early history was summarized in 1968 (Thomsen & Burr, 1968). Connection of the X-ray wavelength scale to the primary realizations of the length (wavelength) unit in the 'metric system' was primarily (at least after about 1930) through ruled grating measurements of longer-wavelength X-ray lines such as Al $K\alpha_{1,2}$.

The remainder of the X-ray wavelength database was derived from relative measurements using crystal diffraction spectroscopy. Unfortunately, even the most refined among the ruled grating measurements did not give accuracies comparable to the precision accessible by relative wavelength measurements (Henins, 1971). As noted above, in connection with establishing the previous wavelength table, Bearden introduced a new local unit, the Å*, based on an explicit value for the wavelength of W $K\alpha_1$, chosen to give a conversion factor near unity. This transitional period will not be treated further in the present documentation since, to a substantial extent, developments described in the following paragraphs have effectively eliminated the need for a local scale for X-ray wavelength metrology.

Following the demonstration of crystal lattice interferometry in the X-ray region (Bonse & Hart, 1965), efforts to combine such an X-ray interferometer with various optical interferometers were undertaken in several (mostly national standards) laboratories. Although the earliest of these, carried out at the National Bureau of Standards (NBS) (now the National Institute of Standards and Technology, NIST) (Deslattes & Henins, 1973) was, in the end, found to be burdened by a serious systematic error (1.8×10^{-6}) in later work at the Physikalisch Technishe Bundesanstalt (PTB) (Becker *et al.*, 1981; Becker, Seyfried & Siegert, 1982), it was clear that accuracy limitations associated with ruled grating measurements no longer dominated the metrology of X-ray wavelengths. The origin of the systematic error in the early NBS measurement was subsequently understood (Deslattes, Tanaka, Greene, Henins & Kessler, 1987), and, more recently, excellent results were obtained in Italy (Basile, Bergamin, Cavagnero, Mana, Vittone & Zosi, 1994, 1995) and Japan (Fujimoto, Fujii, Tanaka & Nakayama, 1997). In all cases, the goal was to obtain an optical measurement of a crystal lattice period (thus far, only Si 220) and to use the calibrated crystals in diffraction spectrometry to establish optically based X-ray wavelengths. Such exercises have been undertaken for several X-ray lines, but the most detailed and well documented results to date were obtained in Jena (Härtwig, Hölzer, Wolf & Förster, 1993; Hölzer, Fritsch, Deutsch, Härtwig & Förster, 1997), where the $K\alpha$ and $K\beta$ spectra of the elements Cr to Cu were evaluated using silicon crystals well connected with the crystal spacings measured at the PTB.

4.2.2.5. *K-series reference wavelengths*

In addition to the Jena measurements noted above, a number of characteristic X-ray lines were measured on the optically based scale at NBS/NIST. The set of directly measured reference wavelengths is given in Table 4.2.2.1 in bold type. Most of the originally published (NBS/NIST) values were burdened by the 1.8×10^{-6} error in the silicon lattice period, as noted above. These have been corrected in the numerical results summarized in the table. The directly measured elements and lines appearing in this table were often chosen to meet the need for specific reference values in locations near those of certain optical transitions in highly charged ion spectra or spectra from pionic atoms. In addition, early NBS measurements specifically addressed the lines most often used in crystallography and the W $K\alpha$ transition. In response to the needs of electron spectroscopy, Al and Mg K spectra were also determined (Schweppe, Deslattes, Mooney & Powell, 1994). In this case, the original lattice error had been previously recognized, so that no rescaling was required. The remaining directly measured entries were obtained as opportunities to do so emerged.

The optically based data set was expanded by noting that several groups of accurate (relative) measurements in the literature either contained one of the directly measured lines (bold type) in Table 4.2.2.1 or were explicitly connected to one of them. Most often this situation was realized in reports that indicated a specific reference value, *i.e.* where it was stated numerical values are based on a scale where, for example, the wavelength of Mo $K\alpha_1$ was taken as 707.831 xu. In such cases, and where other indicators of good measurement quality are presented, it is easy to re-scale the data reported so that it is consistent with the optically based data. This procedure was followed for important groups of measurements from earlier work by Bearden and co-workers, and from the X-ray laboratory at Uppsala. The rescaled numerical results are included in Table 4.2.2.1 in normal type along with the specific literature citations. The indicated uncertainties are standard uncertainties as defined by ISO (Taylor & Kuyatt, 1994; Schwarzenbach, Abrahams, Flack, Prince & Wilson, 1995).

4.2.2.6. *L-series reference wavelengths*

To date, only a very limited number of L-series emission lines have been directly measured on an optically based scale. Wavelengths for directly measured L-series lines are reported in Table 4.2.2.2 along with the literature citations. In the future, we hope to expand this limited data set by including other lines and elements that are well connected to these reference lines in the literature.

4.2.2.7. *Absorption-edge locations*

Only a small number of absorption-edge locations have been directly measured to high accuracy using the currently acceptable protocols. Some of the available data were obtained in order to provide wavelength determinations for spectra from highly charged and/or exotic atoms (Bearden, 1960; Lum *et al.*, 1981). This small group was, however, significantly expanded very recently by an important set of new measurements, extending to $Z = 51$, that are well coupled to the optical wavelength scale (Kraft, Stümpel, Becker & Kuetgens, 1996) The resulting experimental database is summarized in Table 4.2.2.3. The effort that would be needed to expand the experimental database in a systematic way is quite large. Thus, we make use of a procedure, not previously used for this purpose, that combines available electron binding energy data with emission-line locations from our expanded reference set of emission-line data and emission lines that have been rescaled to be consistent with the optically based scale. At the same time, calculation of the location of absorption thresholds within the

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