line of intersection of the lattice plane with the plate, and E and R are the corresponding points on the extinction and reflexion Kikuchi lines respectively. An elementary calculation gives

$$\delta_{\text{rel}}=(RP-PE)/(RP+PE)=\operatorname{tg}\theta\operatorname{tg}(\theta+\gamma)\,. \qquad (9)$$

Here θ is the Bragg angle and γ is the deviation of the diffracting beam from the direction of the incident beam.

It is useful to consider in individual cases whether it is better to use equation (5) (with the approximation given above) or equation (4) (where we need to know the wavelength). For practical details of pattern measurement see Wilman's (1948) paper.

Conclusion

Using the Kikuchi model the equation of Kikuchi lines has been derived in a quite general case, in which diffraction by the triclinic lattice in an arbitrarily chosen position takes place. Thus, we have shown the possibility of performing various crystallographic measurements with good accuracy.

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A Measurement of the Absorption Coefficients of Mn, Fe, and Ti for Ag *Kα* Radiation

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The absorption coefficients of Mn, Fe and Ti have been measured to an accuracy of better than ±0·6% with monochromatic Ag *Kα* radiation. The absorption coefficient for Fe is in excellent agreement with Cooper's measured value.

Cooper (1965) measured the mass absorption coefficients of Al, V, Cr, Fe, Co, Ni and Cu. Utilizing Walter's (1927) empirical equation:

$$(\mu/\varrho)\frac{A}{N}=2{\cdot}64\times10^{-26}Z^{3{\cdot}94}\lambda^{3} \qquad (1)$$

in which μ/ϱ = mass absorption coefficient
A = atomic weight
N = Avogadro's number
Z = atomic number
λ = wavelength

one may plot these values of $(\mu/\varrho)A$ *versus* $Z^{3{\cdot}94}$ and determine by interpolation the mass absorption coefficient of the other elements of this series. However, this method can lead to values which are only accurate to within 2% whereas precise intensity measurements require a determination of the absorption coefficient to less than 1%. This investigation is a direct determination of the mass absorption coefficients of Mn, Fe and Ti.

The experimental set-up employed a standard General Electric XRD-5 spectrogoniometer with a high intensity Ag target tube operated at 40 kV, 25 mA, a singly bent lithium fluoride monochromator and palladium filters. Scintillation counters were used to monitor the beam as well as determine I/I_0. Positional micrometers located different areas of the specimen in the beam path. The monochromator geometry was adjusted until the lattice parameter, a_0, of a silicon single crystal (using a Cohen least-squares analysis) agreed with the most precise value of a_0 available (Straumanis, Borgeaud & James, 1961).

Three Mn specimens and one each of Fe and Ti were utilized in the absorption measurements. In order to optimize the accuracy of transmission measurements the thickness of all specimens was approximately equal to $2/\mu$. The three electrolytic Mn plates,* purity 99·78%, were approximately 0·006″ thick. The first

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* The authors wish to thank Mr C. C. Whiting of Union Carbide Corporation for supplying the Mn plates.

two plates were irregular in shape, the third was cut with a micro-sandblaster to a rectangular shape $\frac{3}{4}''\times 1\frac{3}{4}''$. To determine the area of the Mn specimens the plates were photographed on calibrated graph paper, the photographs enlarged, and the area measured with a planimeter. Corrections were applied to compensate for nonuniform film shrinkage.

Since the Mn plates may have been electrodeposited in the γ phase, a check was made to determine if the plates had completely transformed to α-Mn. Plate no. 1 was baked in a vacuum oven at 150 °C for two minutes to insure transformation to the α form. The transmission measurements were unaffected. The Mn plates were checked for pits and irregularities by scanning the entire area of the plates with the X-ray beam and observing any intensity change on a ratemeter chart recorder. Intensity changes were negligible.

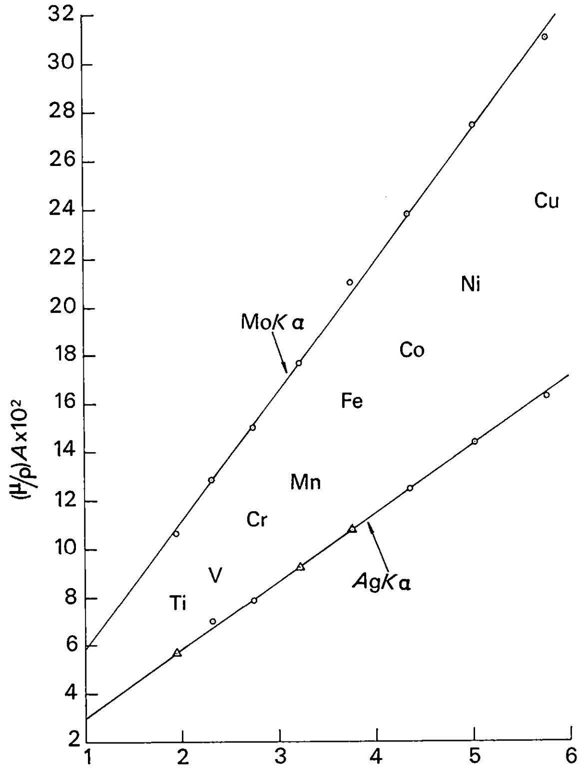

Fig. 1. Values of $(\mu/\varrho)A$ *versus* $Z^{3\cdot94}$. The circles represent Cooper's values and the triangles represent the values of the present investigation.

The Ti plate was formed from six $\frac{3}{4}''\times 2''$ rectangular foils (commercial Ti 99·5%), each 0·0015″ thick, sandwiched between aluminum frames. The area of each foil was determined with a Bausch and Lomb comparator.

The Fe plate was composed of seven $9/16''\times 2''$ rectangular foils 0·0007″ thick, chemical purity 99·9%. The areas were measured and the foils framed in the same manner as for Ti. Both sets of foils were obtained from A. D. Mackay, Inc. All the specimens were weighed on a Sartorius semi-micro balance.

The dead time of the scintillation detector was measured and found to be 3·8μ sec, employing a number of palladium filters in a fixed positional sequence following the procedure of Klug & Alexander (1954). All measurements (I and I_0) were corrected for dead time.

Transmission measurements were taken at 20 to 30 different places across the face of the absorber so that the readings would be truly representative. All intensity measurements were conducted for a sufficiently long time to insure that the probable error was less than 0·1%. Each transmission measurement was preceded and followed by a measurement of I_0, all measurements being corrected relative to the monitored count. The I_0 counting rate was adjusted by adding palladium filters to obtain a dead-time correction of less than $1\frac{1}{2}$%.

A determination of the amount of scatter was obtained by holding the absorbers normal to the beam and scanning around the absorber with the detector. The I/I_0 measurements were corrected for scatter in order to obtain the photoelectric absorption coefficient τ, and the correction amounted to $\frac{1}{2}$% for Ti and Fe, and 1% for Mn.

The results of this investigation, exhibited in Table 1, show excellent agreement between our values of μ/ϱ for Fe and Mn and Cooper's values. Fig. 1 is a plot of Cooper's values of $(\mu/\varrho)A$ *versus* $Z^{3\cdot94}$ for Mo and Ag radiation as well as the values of the present investigation. Note that on the Ag $K\alpha$ curve our values fall full on the line connecting Cr, Fe, Co and Ni, the only points deviating being the $(\mu/\varrho)A$ of V and Cu. From the straight line fit for Mo $K\alpha$ and Ag $K\alpha$, a

Table 1. *Values of maximum deviation, D, photoelectric absorption coefficient, τ, and mass absorption coefficients, μ/ϱ* (cm^2.g^{-1}) *of the specimens investigated, with a comparison of Cooper's values*

Specimen	Number of measurements	D*	μ/ϱ	τ	Cooper's values μ/ϱ
Fe	7	2·7 %	19·34 ± 0·10	19·29 ± 0·10	19·38 ± 0·10
	4	2·0	19·42 ± 0·10	19·37 ± 0·10	
Ti	18	0·7	11·83 ± 0·05	11·78 ± 0·05	11·53†
Mn	20	4·4	16·82 ± 0·10	16·74 ± 0·10	16·67†

* D = Maximum deviation in transmission due to a variation in thickness .
† Interpolated values.

determination of the constant in equation (1) resulted in a value of $2{\cdot}48 \times 10^{-26}$ instead of $2{\cdot}64 \times 10^{-26}$. We also obtained a value of $\lambda^{2 \cdot 8}$ instead of λ^3, the former being in qualitative agreement with Weiss (1966). It is interesting to note that on the Mo radiation curve the $(\mu/\varrho)A$ for Fe appears to be high even though Cooper's value is verified by Batterman, Chipman & DeMarco (1961).

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The Interpretation of X-ray Diffraction Photographs with the Use of Computers

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The large number of reflexions which are recorded on diffraction photographs make it necessary to use automatic instruments for measuring the integrated intensity of reflexion. One class of such instruments requires the photographic film to be positioned automatically in the correct position for scanning over each spot in turn. The present paper sets out the way of computing the coordinates of spots on films so that a microdensitometer, with automatic setting along two mutually perpendicular directions, can set the film in the required positions. An alternative approach to this problem involves finding, instrumentally, the coordinates on the film of each spot and computing the indices of the reflecting plane. It is shown what programs are necessary to do this for oscillation, Weissenberg and precession photographs.

Introduction

The determination of the structure of a crystal frequently requires the measurement of the integrated reflexions of some thousands of spots on oscillation or Weissenberg or precession photographs. Eye estimation has been used extensively but it is tedious and not sufficiently accurate for many purposes. Efforts have therefore been made in recent years to develop automatic instruments capable of carrying out measurements, for each spot on a photograph, of its linear coordinates and its integrated intensity. The method described by Abrahamsson (1966) is very thorough. The intensity at every point on a 1/10th mm grid covering the whole film is registered, and the information stored magnetically. This means that some millions of measurements are made on each film. Subsequently this information must be sorted and the integrated intensities determined for each spot. A computer of considerable capacity is clearly required for this purpose. It seems likely that a more economical approach to the problem would involve calculating the position of each possible reflexion and using this information to examine and integrate the intensity in the region round this calculated position. This method has the merit that spurious 'reflexions' are not recorded along with the genuine ones. It also has the advantage over a method which depends on an automatic searching for the spots of intensity above a certain value, that no reflexion is too weak to be studied. The following paragraphs attempt to set out a method of calculating the position of spots on various types of photograph. The assumption is made that the cell dimensions and orientation of the edges of the unit cell relative to the photographic instrument are known.

Calculation of coordinates on the film of spots corresponding to given indices *hkl*

The unit-cell sides referred to Cartesian coordinates

Whatever the symmetry of the crystal and whatever the orientation of the unit cell with respect to the photographic instrument, it is always possible to write down the Cartesian coordinates of the axes, $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ of the reciprocal unit cell as follows:

$$\begin{matrix} p_{a^*} & q_{a^*} & r_{a^*} \\ p_{b^*} & q_{b^*} & r_{b^*} \\ p_{c^*} & q_{c^*} & r_{c^*} \end{matrix} \qquad (1)$$