Table 2 (*cont.*)

hkl	d_c	I_o	I_c	
622	0·8366	26	10	29
$33\bar{2}$	0·8365		19	
$30\bar{3}$	0·8320	12	10	14
654	0·8308		4	
642	0·8257	17	11	
$41\bar{2}$	0·8175		1	
653	0·8174	17	17	22
$31\bar{3}$	0·8155		4	
655	0·8113	34	7	36
$40\bar{2}$	0·8108		29	
621, 540	0·7937		1	
631	0·7933	26	10	24
$42\bar{2}$	0·7931		13	

In this structure, each Cr(III) with point symmetry C_{3i}–$\bar{3}$ is surrounded by 6 F^- at 1·90 Å with a Cr–F–Cr angle between octahedra of 146°. The octahedra of F^- around Cr(III) are perfectly regular within experimental error since the calculated F–Cr–F angles are 89·7° and 90·3°.

At 300 °C. it is seen that the situation for CrF_3 is similar to that found in the rare earth aluminates by Geller & Bala (1956); i.e., a elongates with rising temperature faster than α increases, so that the transition to cubic for CrF_3, if it ever occurs below the melting point, should take place at a very high temperature.

It is of interest to compare this structure with the neutron-diffraction results on magnetic spin alignment. The results of Wollan *et al.* (1958) show that the magnetic space group is No. 89–$C2'/c'$ (the notation used is that of Belov, Neronova & Smirnova, 1957) in which the magnetic moments are allowed to move toward one another out of perfect antiparallel alignment without destroying the symmetry. Thus, 'weak' ferromagnetism of the type discussed by Dzialoshinskii (1957*a*, *b*) is allowed, and it was observed in the magnetization curve obtained by Bozorth & Kramer (1958) in collaboration with the author. It has also been seen by Henry, Griffel & Hansen (1955) and by Hansen (1959), who, however, attribute the spontaneous magnetization to ferrimagnetism.

The author is grateful to S. Geller for many helpful discussions. Thanks are also due R. G. Treuting for the use of and assistance with his IBM 704 programs, D. W. Mitchell, W. Masterson, and C. E. Miller for help with the experimental work.

References

Belov, N. V., Neronova, N. N. & Smirnova, T. S. (1957). *Kristallografia*, **2**, 315.

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H. & Veenendaal, A. L. (1955). *Acta Cryst.* **8**, 478.

Bond, W. L. (1958). *Rev. Sci. Instrum.* **29**, 654.

Bozorth, R. M. & Kramer, V. (1958). *Colloque International de Magnetisme de Grenoble*, paper No. 4.

Dauben, C. H. & Templeton, D. H. (1955). *Acta Cryst.* **8**, 841.

Dzialoshinskii, I. E. (1957*a*). *J. Exptl. Theoret. Phys.* (*U.S.S.R.*) **32**, 1547; translated to English in *Soviet Phys. JETP* **6**, 1259.

Dzialoshinskii, I. E. (1957*b*). *J. Exptl. Theoret. Phys.* (*U.S.S.R.*) **33**, 1454; translated to English in *Soviet Phys. JETP* **6**, 1120.

Geller, S. & Bala, V. B. (1956). *Acta Cryst.* **9**, 1019.

Gutmann, V. & Jack, K. H. (1951). *Acta Cryst.* **4**, 244.

Hansen, W. N. (1959). *J. Appl. Phys.* **30**, 304 S.

Henry, W. E., Griffel, M. & Hansen, W. N. (1955). Conference on Magnetism and Magnetic Materials (*American Institute of Electrical Engineers*, New York, 1955), p. 60.

Hepworth, M. A. & Jack, K. H. (1957). *Acta Cryst.* **10**, 345.

Hepworth, M. A., Jack, K. H., Peacock, R. D. & Westland, G. J. (1957). *Acta Cryst.* **10**, 63.

Jack, K. H. & Gutmann, V. (1951). *Acta Cryst.* **4**, 246.

Jack, K. H. & Maitland, R. (1957). *Proc. chem. Soc., Lond.* **1957**, 232.

Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.

Wollan, E. O., Child, H. R., Koehler, W. C. & Wilkinson, M. K. (1958). *Phys. Rev.* **112**, 1132.

Acta Cryst. (1960). **13**, 508

Structure factor slide rule.

By H. Fischmeister, *Swedish Institute of Metal Research* (*Metallografiska Institutet*), *Stockholm* 26, *Sweden*, and A. Niggli, *Institut für Kristallographie und Petrographie der Eidgenössischen Technischen Hochschule, Zürich, Switzerland*

(*Received* 22 *January* 1960)

Structure factor contributions of the product type,

$$F_n = f_n \cdot \frac{\sin}{\cos}(hx_n) \cdot \frac{\sin}{\cos}(ky_n) \cdot \frac{\sin}{\cos}(lz_n)$$

can be calculated conveniently by means of the device illustrated in Fig. 1. It is a composite slide rule consisting of three cyclometric scales, each covering one quarter of a period, of a straight logarithmic one for reading the product, and of a movable stage carrying a graph of $\log f_n$ *vs.* $\sin^2\theta$. The width of this stage is limited to the relative range of variation of the atomic scattering factors likely to be employed, usually less than one and a half decade. For atoms of strongly differing scattering power, the f-graphs can be brought to scale by shifting the overall zero point of the calculator.

The sign of the composite product is indicated by colour signals coupled with the cyclometric scales: the numbering of these scales is divided into four groups, printed on a white or red base according to the sign of the function. The number strips are mounted, as shown in Fig. 2, on a holder carrying a hinged flap. The whole array rests in a groove in the scale carrier; the transition from sine to cosine numbering is effected by simply inverting it in this groove.—As will be apparent from

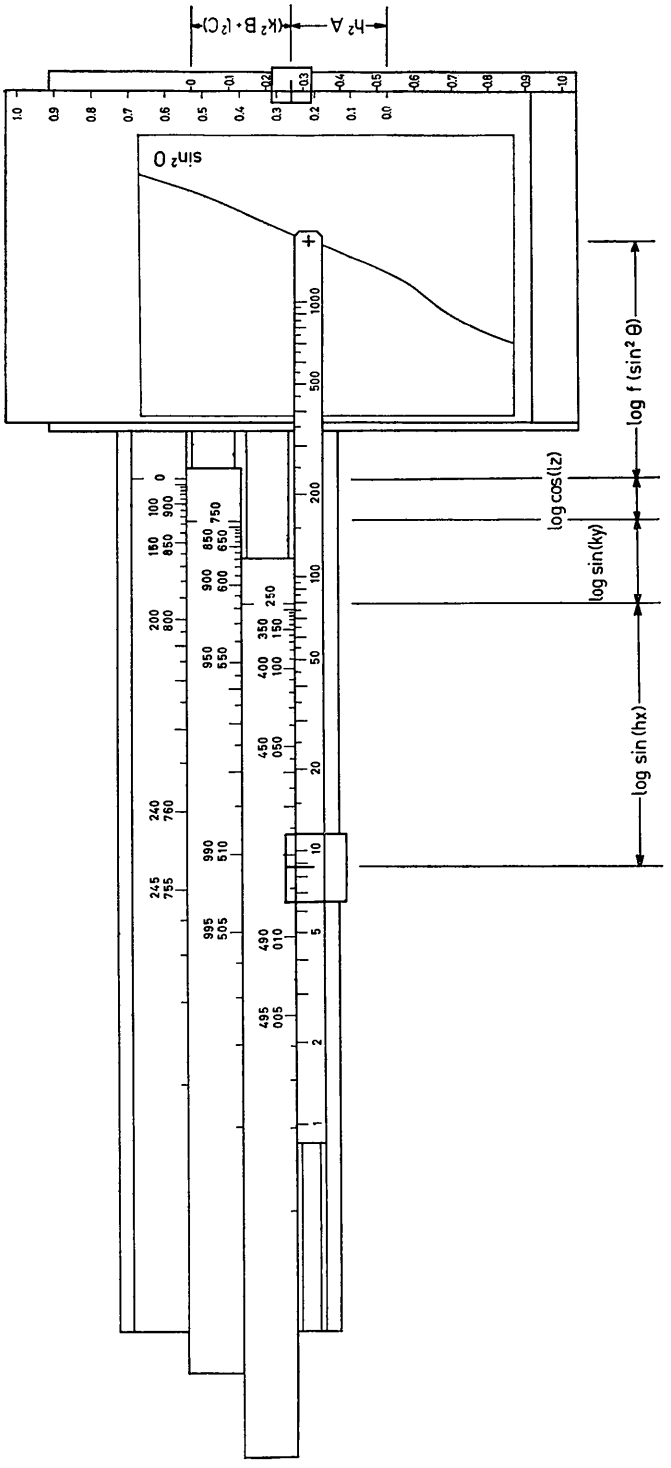

Fig. 1. Structure factor slide rule with cyclometric scales and stage for scattering factor graph.

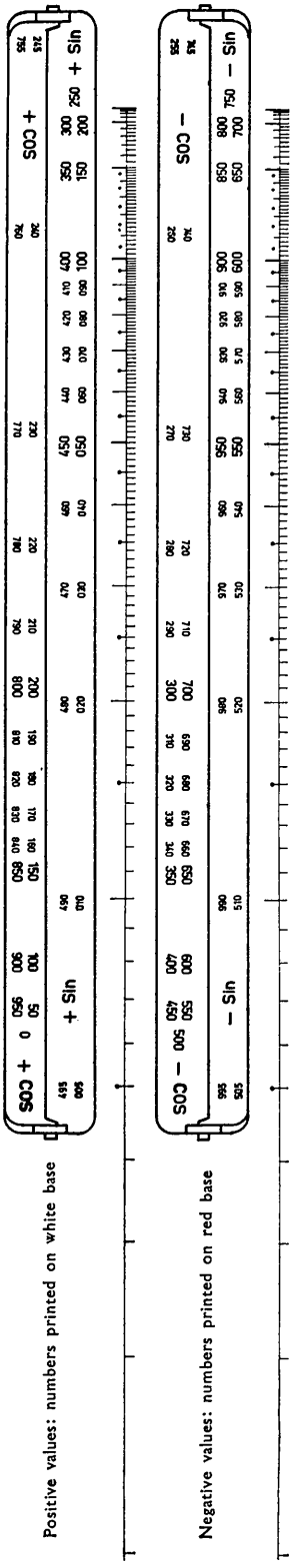

Fig. 2. Arrangement of numbering for cyclometric scales to provide colour indication of sign.

Fig. 2, values of the argument for which the function becomes negative, can be found only after throwing over the hinged flap, which will change the colour presented by the whole scale.

Calculation proceeds along a line in the reciprocal lattice, e.g., by setting the two top scales at fixed values of $k.y_n$ and $l.z_n$, and reading the triple product from the bottom scale by running the cursor through all values of $h.x_n$. (A table of the multiples of the atomic coordinates has to be prepared prior to calculation.) Before the result is read, however, the scattering factor graph is adjusted to the appropriate value of $\sin^2\theta$ and the end mark of the bottom scale made to coincide with the curve, to include the scattering factor into the product. In the high symmetry systems in which triple product formulae occur, $\sin^2\theta$ is often of the form, $h^2A+k^2B+l^2C$, so that only values of, say, k^2B+l^2C need be tabulated in advance, the third term being added graphically as indicated in Fig. 1. (The use of a different function of θ in the f-graph, such as the cylindrical coordinates of the reciprocal lattice, may be preferable where values of it had to be calculated earlier—e.g., for Lorentz-polarization correction.)

With proper care, the device can be made accurate enough even for the more advanced stages of structure determinations. In a precision model, the body was made of plexiglass and reinforced by a hard aluminium alloy base plate. The scale carriers were made of the same alloy. The scales were hand drawn and reduced photographically onto aluminium offset foil, to eliminate the uneven shrinkage of the more conventional photographic media. Care was taken to check the trueness of the photographic apparatus, a printer's reducing machine. The scales were coated with protective varnish and fastened to their carriers with araldite cement. The stage for the f-graph must have a smooth movement, which can be achieved by letting it run on small tapered wheels in a V-groove machined into its base plate. The whole f-stage is detachable from the rest of the apparatus. For this model, the standard deviation of the triple product was found to be, in 100 trial multiplications, two units in the 1000 constituting the range of the product scale. In most cases, the uncertainty due to the temperature and atomic scattering factors will be greater than this.

An alternative possibility is to use blank cyclometric scales on which, by matching them against a master scale, only those values of $\cos hx_n$ or $\sin hx_n$ are marked that are actually needed; the index h, k or l is written down, and different colours are used for positive and negative values. In this way, the interpolations are made once for all, and large series of structure factors can be calculated in a shorter time. On the other hand, the accuracy may be somewhat lower, depending upon the care taken in drawing the ad-hoc scales.

The first model of this device was built in 1955, when both authors were guests at the Institute of Chemistry at Uppsala University. We wish to record our gratitude to Prof. G. Hägg for his permission to have a prototype built in the workshop of the Institute. We also gratefully acknowledge the grants that formed the basis of our sojourns at Uppsala: from Statens Naturvetenskapliga Forskningsråd—the Swedish Natural Science Research Council—(H. F.), and from Schweizerische Stiftung für Stipendien auf dem Gebiete der Mineralogie (A. N.).

Acta Cryst. (1960). **13**, 510

The effect of lattice imperfections on the interference function centroid.

By Robert Asimow,
Engineering Division, California Institute of Technology, Pasadena 4, California, U.S.A.

(*Received* 7 *October* 1959)

For a large perfect crystal, the interference function distribution in reciprocal lattice space is well known. The function has appreciable values only for positions very near reciprocal lattice points, and further the distribution is symmetric about each lattice point. As a result, the precise measurement of lattice parameters for crystals of high perfection is a relatively straight-forward procedure. For crystals containing a large number of imperfections, as in a cold worked metal, the interference function has appreciable values over a large region of reciprocal lattice space. Further there is no obvious relationship between the interference function distribution and the corresponding distribution of lattice strains in the crystal. Thus, if diffraction techniques are to be used to obtain precision parameter measurements for imperfect crystals, it is necessary to show that some property of the interference function can be used to define a mean lattice parameter. In this paper it is shown that the centroid of the interference function for the region surrounding the (h, k, l) reciprocal lattice point corresponds very nearly to the mean reciprocal (h, k, l) interplanar spacing.

We start by using a method similar to that developed by Warren & Averbach (1950) and Warren (1955). An imperfect crystal is considered in which the unit cells are displaced from their correct positions. The crystal axes (a, b, c) are chosen in a manner convenient for this problem. The c axis is taken to have a component normal to the (h, k, l) plane which is equal in length to the mean interplanar spacing and the other two axes are fixed in the (h, k, l) plane. In terms of these three axes, the position of any unit cell is given by

$$r_{uvw}=ua+vb+wc+ax_{uvw}+by_{uvw}+cz_{uvw}\,, \qquad (1)$$

where u, v, w are integers and x, y, z represent the displacement of the u, v, w unit cell from its regular position. It is assumed that the lattice strains in the deformed crystal are small; therefore, x, y, z are small compared to u, v, w respectively. The magnitudes and direction of a, b, c are fixed by the condition that

$$\bar{x}=\bar{y}=\bar{z}=0\,, \qquad (2)$$

where $\bar{x}$ is the mean value of x averaged over all u, v, w, and similar definitions apply to $\bar{y}$ and $\bar{z}$.