Acta Cryst. (1959). **12**, 701

A graphical aid for calculating structure factors.

By Luigi Cavalca and Mario Nardelli, *Structural Chemistry Laboratory, Chemical Institute, University of Parma, Italy.*

(*Received* 23 *April* 1959)

The following is a very simple method used in our laboratory for the graphical evaluation of products of the form

$$\begin{matrix}\cos\\ \sin\end{matrix}(2\pi hx)\ \begin{matrix}\cos\\ \sin\end{matrix}(2\pi ky)\ .$$

A chart is drawn with 101 equidistant parallel lines, intersected by a single perpendicular line graduated from 0 to 1·0 (Fig. 1). For each pair of x, y coordinates the values of

$$\begin{matrix}\cos\\ \sin\end{matrix}(2\pi hx) \quad \text{and} \quad \begin{matrix}\cos\\ \sin\end{matrix}(2\pi ky)$$

are read from tables. The values for

$$\begin{matrix}\cos\\ \sin\end{matrix}(2\pi hx)$$

are marked on a paper strip placed against the scale; they are labelled with the corresponding value of h and the sign, and the extreme positions of the scale are also marked on the strip.

To obtain the products

$$\begin{matrix}\cos\\ \sin\end{matrix}(2\pi hx)\ \begin{matrix}\cos\\ \sin\end{matrix}(2\pi ky)$$

for a fixed value of k the 1·0 position on the strip is placed against the

$$\begin{matrix}\cos\\ \sin\end{matrix}(2\pi ky)$$

value on the scale and the 0 position is placed on the zero line of the chart. The required product is read with the aid of the parallel lines for each h position on the strip. The signs of the products are determined immediately from the labelled signs and from the sign of

$$\begin{matrix}\cos\\ \sin\end{matrix}(2\pi ky).$$

The chart can be conveniently made from the pattern on a recorder chart. With a scale of 25 cm. for 100 divisions the third decimal figure can be obtained, and for greater accuracy the scale can be subdivided further.

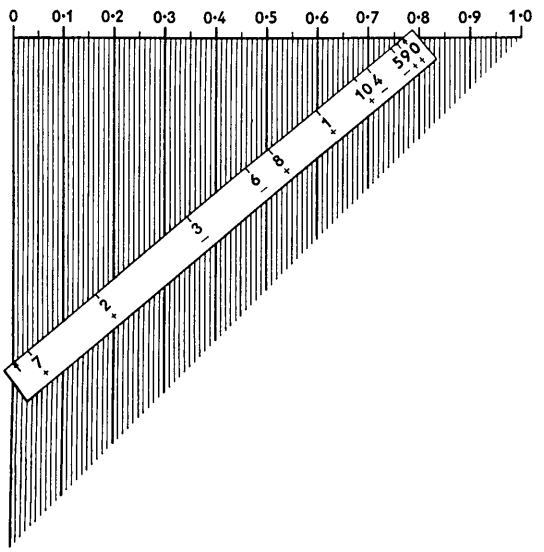

Fig. 1. Graphical evaluation of $\cos(2\pi hx)\cos(2\pi ky)$ for $x = 0{\cdot}108$, $y = 0{\cdot}537$, $h = 0, 1, \ldots, 10$, $k = 2$. As $\cos(2\pi ky) = -0{\cdot}767$ the signs of the products are opposite from those recorded on the strip.

Acta Cryst. (1959). **12**, 701

A new intermediate phase in the niobium-aluminum system.

By C. R. McKinsey and G. M. Faulring, *Metals Research Laboratories, Union Carbide Metals Company, Division of Union Carbide Corporation, Niagara Falls, New York, U.S.A.*

(*Received* 3 *March* 1959 *and in revised form* 27 *April* 1959

Two AB_3 intermediate phases in the niobium–aluminum system have been reported. $NbAl_3$ is tetragonal, with $a_0 = 5{\cdot}438$, $c_0 = 8{\cdot}601$ Å, and $c/a = 1{\cdot}582$ (Brauer, 1939), while Nb_3Al is a cubic, beta-tungsten structure with $a_0 = 5{\cdot}187 \pm 0{\cdot}002$ Å (Wood *et al.*, 1958). Corenzwit (1959) has reported the existence of an additional compound, tentatively identified as a sigma phase and believed to have a higher aluminum content than Nb_3Al. The present note confirms the existence of a sigma phase in this system and places its composition at approximately 34 atomic per cent aluminum (Nb_2Al).

Alloys containing 24·4, 28·8 and 34 atomic per cent aluminum (8·6, 10·5, and 13·0 weight per cent aluminum) were prepared from niobium roundels (0·021 weight per cent carbon, 0·04 weight per cent oxygen, and 0·017 weight per cent nitrogen) and high-purity aluminum by arc melting with a non-consumable electrode. Each 50 g. charge was remelted several times to obtain a homogeneous alloy. Since all three compositions were brittle in the as-cast condition, powder samples were easily prepared by crushing and grinding.

Powder X-ray diffraction patterns of the as-cast

Table 1. *X-ray diffraction data for* Nb_2Al

hkl	d_o (Å)	d_c (Å)	Relative intensity
101	4·599	4·599	*w*
210	4·448	4·447	*w*
111	4·171	4·174	*vw*
220	3·520	3·515	*vw*
211	3·376	3·376	*vw*
310	3·145	3·144	*w*
301	2·792	2·793	*w*
002	2·591	2·593	*w*
410	2·412	2·412	*vs*
330	2·342	2·344	*s*
202	2·305	2·299	*s*
212	2·238	2·240	*vs*
411	2·187	2·187	*vs*
331	2·137	2·136	*m*
222	2·083	2·087	*w*
312	1·998	2·001	*w*
432	1·577	1·578	*w*
522	1·503	1·504	*m*
532	1·425	1·425	*m*
710, 550, 413	1·404	1·406	*m*
333	1·389	1·391	*w*
720, 423	1·366	1·366	*m*
622	1·344	1·344	*vw*
542	1·334	1·332	*vw*
721	1·321	1·321	*vw*
513	1·292	1·294	*vw*
304	1·206	1·206	*w*
324	1·174	1·173	*w*
414	1·139	1·142	*m*
812, 742	1·114	1·114	*w*
553, 713	1·089	1·091	*vw*

alloys, obtained with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å) showed that the 24·4 atomic per cent aluminum alloy consisted of Nb_3Al with a small amount of Nb_2Al, the 28·8 atomic per cent aluminum alloy consisted of nearly equal amounts of Nb_3Al and Nb_2Al, and the 34 atomic per cent aluminum alloy consisted of Nb_2Al. The diffraction pattern of Nb_3Al was identical to that reported by Wood *et al.* (1958).

The observed X-ray diffraction data and calculated interplanar spacings for the Nb_2Al phase are shown in Table 1. The pattern could be indexed as tetragonal with $a_0 = 9{\cdot}943$ Å, $c_0 = 5{\cdot}186$ Å, $c/a = 0{\cdot}522$. The cell dimensions and relative intensities of the diffraction lines suggest a structure of the sigma type, which has 30 atoms per unit cell (Bergman & Shoemaker, 1955). The calculated density of the 34 atomic per cent aluminum alloy, assuming 30 atoms per unit cell, is 6·85 g.cm.$^{-3}$, in good agreement with the measured density of 6·87 g.cm.$^{-3}$.

This preliminary survey established the existence of the intermediate phase Nb_2Al. The structure is tetragonal and appears to be of the sigma type. If so, this niobium–aluminum phase should be of exceptional theoretical interest since all presently established binary sigma phases are composed of two transition elements from the Long Periods (Knapton, 1958).

References

Bergman, G. & Shoemaker, D. P. (1955). *Acta Cryst.* **7**, 857.

Brauer, G. (1939). *Z. anorg. Chem.* **242**, 1.

Corenzwit, E. (1959). *J. Phys. Chem. Solids*, **9**, 93.

Knapton, A. G. (1958). *J. Inst. Metals*, **87**, 28.

Wood, E. A., Compton, V. B., Matthias, B. T. & Corenzwit, E. (1958). *Acta Cryst.* **11**, 604.

Books Received

The undermentioned works have been received by the Editors. Mention here does not preclude review at a later date.

Vector Space and Its Application in Crystal Structure Investigation. By M. J. Buerger. Pp. XIV+347. With many figs. and tables. New York: John Wiley & Sons. 1959. Price $12, £4·16·0.

Dendritic Crystallization. By D. D. Saratovkin. Pp. 126 with many figs. and six tables. New York: Consultants Bureau Inc. 1959. $6·00.

Cristalofísica. By José Luis Amoros. Part 1: Propiedades continuas. Pp. XIII+233. Madrid: Aguilar. 1958.

The Determination of Molecular Structure. By P. J. Wheatley. Pp. VI+263 with many figs. and tables. Oxford: Clarendon Press, Oxford University Press. 1959. Price 35*s*.

Materialprüfung mit Röntgenstrahlen. By R. Glocker. Pp. VII+530. 4th ed. Berlin: Springer-Verlag. 1958. Price DM. 61·50.

Applications of Finite Groups. By J. S. Lomont. Pp. XI+346. New York & London: Academic Press. 1959. Price $11·00.