$$F(\hat{\mathbf{K}})=\iint_S \Phi_s(\mathbf{r}_s)\exp\{-i(\mathbf{K}\cdot\mathbf{r}_s)\}d\mathbf{r}_s\,. \tag{A–2}$$

If the distance between the light source and the slit is large enough this tends to F_L (equation (6)) asymptotically.

Next we consider a vector field $\mathbf{H}_s$, which has the form of equation (13). The Fourier transform of the diffracted wave due to slit S is then

$$\mathbf{F}(\hat{\mathbf{K}})=\iint_S \tilde{M}\Phi_s\exp\{-i(\mathbf{K}\cdot\mathbf{r}_s)\}d\mathbf{r}_s \tag{A–3}$$

using Kirchhoff's approximation again. Carrying out the operation of $\tilde{M}$:

$$\begin{aligned}\mathbf{F}(\hat{\mathbf{K}})&=-\iint_S \operatorname{rot}(\mathbf{J}\Phi_s)\exp\{-i(\mathbf{K}\cdot\mathbf{r}_s)\}d\mathbf{r}_s\\ &=-\int_C \mathbf{J}\Phi_s\exp\{-i(\mathbf{K}\cdot\mathbf{r}_s)\}d\mathbf{r}_s\\ &\quad+\iint_S[\mathbf{J}\Phi_s\times i\mathbf{K}]\exp\{-i(\mathbf{K}\cdot\mathbf{r}_s)\}d\mathbf{r}_s\,,\end{aligned} \tag{A–4}$$

where $\int_C$ means a line integral along the periphery of the slit, at which Φ_s should be zero according to the boundary conditions. Therefore,

$$\mathbf{F}(\hat{\mathbf{K}})=i[\mathbf{J}\times\mathbf{K}]F(\hat{\mathbf{K}})\,. \tag{A–5}$$

Accordingly,

$$\mathbf{H}=[\mathbf{J}\times\nabla]\Phi=\tilde{M}\Phi\,, \tag{A–6a}$$

since Φ has the form of equation (4).

The same methods can be applied also to the electric field using the operator $\tilde{N}$; thus,

$$\mathbf{E}=\tilde{N}\Phi\,. \tag{A–6b}$$

Repeating the same argument we can conclude that the diffracted vector waves due to an arbitrary slit system can be expressed in the form of equation (A–6*a*), (A–6*b*).

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References

KATO, N. (1952*a*). *J. Phys. Soc. Jap.* **7**, 397.

KATO, N. (1952*b*). *J. Phys. Soc. Jap.* **7**, 406.

KATO, N. (1960*a*). *Acta Cryst.* **13**, 349.

KATO, N. (1960*b*). *Z. Naturforsch.* **15a**, 369.

KATO, N. & LANG, A. R. (1959). *Acta Cryst.* **12**, 787.

LANG, A. R. (1959). *Acta Cryst.* **12**, 249.

SCHIFF, L. I. (1948). *Quantum Mechanics*, chap. X. New York: McGraw-Hill.

STRATTON, J. A. (1941*a*). *Electromagnetic Theory*, p. 361. New York: McGraw-Hill.

STRATTON, J. A. (1941*b*). *Electromagnetic Theory*, p. 395. New York: McGraw-Hill.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

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The refinement of the Co_2Al_5 structure.

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The Co_2Al_5 compound has a hexagonal unit cell with dimensions:

$$a=7\cdot656_0\ \text{Å},\ c=7\cdot593_2\ \text{Å}\,.$$

The structure was originally determined from powder photographs taken with Fe $K\alpha$ radiation in a 19 cm. camera. Systematic absences were consistent with the space group D_{6h}^4–$P6_3/mmc$. There are 28 atoms per unit cell in the following positions (Bradley & Cheng, 1938):

$2\ Al_1$ in $2(a)$: $0, 0, 0$;
$6\ Al_2$ in $6(h)$: $x, 2x, \frac{1}{4}$ with $x=0\cdot467$;
$12\ Al_3$ in $12(k)$: $x, 2x, z$ with $x=0\cdot196$, $z=-0\cdot061$;
$2\ Co_1$ in $2(d)$: $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$;
$6\ Co_2$ in $6(h)$: $x, 2x, \frac{1}{4}$ with $x=0\cdot128$.

No statement was made on the accuracy of the atomic parameters, nor was the reliability index given.

Compounds with similar structures have been reported in some other systems. The structure of π(AlFeNi) with

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the ideal formula Fe_3NiAl_{10} resembles Co_2Al_5 in that it has 28 atoms per unit cell with nickel and iron atoms in place of manganese (Bradley & Taylor, 1940). The structure of β(AlMnSi), though similar to Co_2Al_5, characteristically differs from it in having two unoccupied atomic sites which would correspond to the $2(d)$ positions (Robinson, 1952).

The structural similarity of these three compounds was accounted for in terms of a prominent Brillouin Zone with an inscribed Fermi distribution corresponding to 1·68 electron states per atom. It was concluded that the unoccupied atomic sites (or 'holes') in the β(AlMnSi) structure occur so as to preserve the electron-to-atom ratio in the neighbourhood of 1·68. On the assumption that aluminium and silicon contribute 3 and 4 free electrons per atom respectively, this result was consistent with a suggestion (Raynor, 1944) that Mn absorbed 3·66 free electrons per atom. Similarly, valencies were ascribed to iron, cobalt and nickel in the related structures, which were also consistent with the negative valencies for these elements. On the basis of such arguments, these compounds were considered to be electron compounds (Robinson, 1952).

More recently it has been shown that β(AlMnSi) can take up some zinc and that zinc replaces manganese, atom for atom. This fact is not compatible with the above explanation for the occurrence of these compounds (Damjanovic & Black, 1959).

For a further discussion of these compounds, it was felt desirable to re-determine the Co_2Al_5 structure with improved accuracy.

An alloy of composition Co_2Al_5 was prepared under argon in an induction furnace. Special precautions were taken in order to obtain a homogeneous ingot. The alloy was slowly cooled to room temperature in order to produce large crystals, and a single crystal was chipped from the ingot. A complete structural analysis was carried out, using both oscillation and Weissenberg photographs, taken with Mo $K\alpha$ radiation. Intensities were measured by visual comparison and corrected for various effects in the usual way. From F_o and $F_o - F_c$ Fourier projections on (0001) and $(10\bar{1}0)$ the following atomic parameters were obtained:

For Al_2 in $6(h)$: $x = 0{\cdot}470_2$,
For Al_3 in $12(k)$: $x = 0{\cdot}194_6$, $z = -0{\cdot}058_0$,
For Co_2 in $6(h)$: $x = 0{\cdot}126_8$.

Using the equations of Booth (1946) and of Booth & Britten (1948), the following values for standard deviations in atomic positions were estimated:

$$\text{Co: } \sigma(r) = 0{\cdot}001_5 \text{ Å}, \quad \text{Al: } \sigma(r) = 0{\cdot}003 \text{ Å}\ .$$

With these values standard deviations in interatomic distances are not greater than $\sigma(d) = 0{\cdot}008$ Å, and for most distances they will be less than this. Differences greater than 0·02 Å between interatomic distances may be considered significant. Interatomic distances are listed in Table 1.

Table 1. *Interatomic distances in* Co_2Al_5

Atom	Neighbour	Number of neighbours	Interatomic distances
Al_1–	Co_2	6	$2{\cdot}53_6$ Å
	Al_3	6	$2{\cdot}61_8$
Al_2–	Co_1	1	$2{\cdot}60_6$
	Co_2	2	$2{\cdot}41_3$
	Al_2	2	$3{\cdot}14_4$
	Al_3	4	$2{\cdot}73_9$
	Al_3	4	$2{\cdot}96_8$
Al_3–	Co_1	1	$2{\cdot}34_7$
	Co_2	2	$2{\cdot}69_7$
	Co_2	1	$2{\cdot}50_6$
	Al_1	1	$2{\cdot}61_8$
	Al_2	2	$2{\cdot}73_9$
	Al_2	2	$2{\cdot}96_8$
	Al_3	1	$2{\cdot}91_6$
	Al_3	2	$2{\cdot}72_7$
	Al_3	2	$3{\cdot}18_6$
Co_1–	Al_2	3	$2{\cdot}60_6$
	Al_3	6	$2{\cdot}34_7$
Co_2–	Co_2	2	$2{\cdot}91_2$
	Al_1	2	$2{\cdot}53_6$
	Al_2	2	$2{\cdot}41_3$
	Al_3	2	$2{\cdot}50_6$
	Al_3	4	$2{\cdot}69_7$

Though Bradley & Cheng's results were obtained with the powder method and with Fe $K\alpha$ radiation, they do not differ much from those obtained in this work. However, the new atomic parameters and interatomic distances are more accurate and therefore more suitable for a discussion of the relationship of Co_2Al_5 to similar structures.

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References

Booth, A. D. (1946). *Proc. Roy. Soc.* A, **188**, 77.
Booth, A. D. & Britten, K. H. V. (1948). *Proc. Roy. Soc.* A, **193**, 305.
Bradley, A. J. & Cheng, C. S. (1938). *Z. Kristallogr.* **99**, 480.
Bradley, A. J. & Taylor, A. (1940). *J. Inst. Met.* **66**, 53.
Damjanovic, A. & Black, P. J. (1959). *Acta Cryst.* (in press).
Raynor, G. V. (1944). *J. Inst. Met.* **70**, 531.
Robinson, K. (1952). *Acta Cryst.* **5**, 397.