



Fig. 1. (a) Variations of $f_2(\theta, \mu t)$ with μt for $\alpha = 60^\circ$. Curves for $2\theta = 10^\circ, 20^\circ, 40^\circ$ and 50° lie between curves for $2\theta = 30^\circ$ and 60° . (b) Variation of R with $\mu_\lambda t$ for $(\mu_m)_\lambda / (\mu_m)_\lambda = 0.14$. Curves for $2\theta_\lambda = 10^\circ, 20^\circ$ and 40° lie close to curve for $2\theta_\lambda = 30^\circ$.

recorded. This arrangement is also convenient because it nearly represents the condition for minimum exposure time to record λ reflexions over a range of Bragg angle from 0° to 45° .

Finally, although this investigation has been related to the geometry of the de Wolff camera, no doubt the general conclusions reached will apply to any Guinier-type camera incorporating a quartz-crystal monochromator.

References

- BRINDLEY, G. W. (1955). *X-ray Diffraction by Polycrystalline Materials*, p. 159. London: Institute of Physics.
 COX, E. G. & SHAW, W. F. B. (1930). *Proc. Roy. Soc. A*, **127**, 71.
 WOLFF, P. M. DE (1948). *Acta Cryst.* **1**, 207.

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Neutron magnetic scattering factors in the presence of extinction. By S. CHANDRASEKHAR and R. J. WEISS, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*

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One of us has recently proposed a scheme for determining a crystal structure factor in the presence of extinction by the use of polarized X-rays (Chandrasekhar, 1956). The ability to obtain polarized neutrons offers similar possibilities in magnetic substances. Consider a crystal in which the extinction is less than 20% being irradiated with monochromatic neutrons. The integrated reflexion can be written as

$$R^\theta = \alpha |F|^2 - \beta |F|^4,$$

where

$$\alpha = \frac{V \lambda^3 e^{-2W} e^{-N\sigma t}}{V_0^2 \sin 2\theta},$$

and β involves certain geometrical factors which determine the amount of extinction present. Here

- V = volume of the crystal,
 e^{-2W} = Debye-Waller temperature factor,
 $e^{-N\sigma t}$ = beam attenuation factor due to absorption, etc.,
 V_0 = unit cell volume,
 F = structure factor.

The structure factor F is the sum of the nuclear and magnetic structure factors F_N and F_P . If the neutrons are polarized, it can be arranged so that F_P is either positive or negative. For the two cases

Table 1. $R_{\downarrow}^0/R_{\uparrow}^0$ as a function of x and A

$x \backslash A$	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9
0.3	—	—	—	—	—	—	—	—	—	—
0.4	—	—	—	—	—	—	—	0.1587	0.1660	0.1734
0.5	—	—	—	—	—	0.0957	0.1012	0.1068	0.1123	0.1179
0.6	—	—	—	0.0527	0.0564	0.0602	0.0639	0.0677	0.0714	0.0752
0.7	—	—	0.0272	0.0294	0.0315	0.0337	0.0359	0.0381	0.0403	0.0425
0.8	—	0.0110	0.0120	0.0129	0.0139	0.0149	0.0159	0.0169	0.0179	—
0.9	0.0025	0.0028	0.0030	0.0033	0.0035	0.0038	0.0040	—	—	—
1.0	0.0	0.0	0.0	0.0	0.0	—	—	—	—	—
$x \backslash A$	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9
0.0	—	—	—	—	—	—	—	—	—	—
0.1	—	—	—	—	—	—	—	0.6290	0.6357	0.6424
0.2	—	—	—	0.4021	0.4109	0.4198	0.4287	0.4376	0.4465	0.4554
0.3	0.2531	0.2668	0.2755	0.2842	0.2929	0.3016	0.3103	0.3190	0.3277	0.3364
0.4	0.1807	0.1881	0.1954	0.2027	0.2101	0.2174	0.2248	0.2321	0.2395	0.2468
0.5	0.1234	0.1290	0.1346	0.1401	0.1457	0.1512	0.1568	—	—	—
0.6	0.0789	0.0827	0.0864	0.0902	—	—	—	—	—	—
0.7	0.0447	—	—	—	—	—	—	—	—	—
0.8	—	—	—	—	—	—	—	—	—	—
$x \backslash A$	3.0	3.1	3.2	3.3	3.4	3.5	3.6	3.7	3.8	3.9
0.0	—	—	—	1.0	1.0	1.0	1.0	1.0	1.0	1.0
0.1	0.6491	0.6558	0.6625	0.6692	0.6759	0.6826	0.6893	0.6959	0.7026	0.7093
0.2	0.4643	0.4732	0.4821	0.4910	0.4998	0.5087	0.5176	0.5265	0.5355	0.5444
0.3	0.3451	0.3538	0.3625	0.3712	0.3799	0.3886	—	—	—	—
0.4	0.2542	—	—	—	—	—	—	—	—	—
0.5	—	—	—	—	—	—	—	—	—	—
$x \backslash A$	4.0	4.1	4.2	4.3	4.4	4.5	4.6	4.7	4.8	4.9
0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
0.1	0.7160	0.7227	0.7294	0.7361	0.7428	0.7495	0.7561	0.7630	0.7696	0.7762
0.2	0.5533	0.5622	0.5710	—	—	—	—	—	—	—
0.3	—	—	—	—	—	—	—	—	—	—
$x \backslash A$	5.0	—	—	—	—	—	—	—	—	—
0.0	1.0	—	—	—	—	—	—	—	—	—
0.1	—	—	—	—	—	—	—	—	—	—

$$R_{\uparrow}^0 = \alpha(F_N + F_P)^2 - \beta(F_N + F_P)^4,$$

$$R_{\downarrow}^0 = \alpha(F_N - F_P)^2 - \beta(F_N - F_P)^4.$$

Eliminating β , we get

$$\frac{R_{\downarrow}^0}{R_{\uparrow}^0} = \frac{(1-x)^2}{(1+x)^2} \left[\left(\frac{1-x}{1+x} \right)^2 + Ax \right],$$

where

$$x = |F_P|/|F_N| \quad \text{and} \quad A = 4\alpha F_N^2/R_{\uparrow}^0.$$

If the nuclear scattering is known, x can be evaluated from a measurement of R_{\downarrow}^0 and R_{\uparrow}^0 . With no extinction, $A = 4(1+x)^{-2}$ and with 20% extinction on R_{\downarrow} , $A = 5(1+x)^{-2}$. Therefore, x can take all positive values between $(4/A)^{1/2} - 1$ and $(5/A)^{1/2} - 1$. Using these limits, a table (Table 1) has been prepared which gives values of $R_{\downarrow}^0/R_{\uparrow}^0$ for different values of x ranging from 0.0 to 1.0 and different values of A . These tables may be used to determine x either by extrapolation or more accurately by plotting curves connecting $R_{\downarrow}^0/R_{\uparrow}^0$ and x , after having fixed A for the particular experiment.

The above equations apply only when the neutrons are perfectly polarized and hence, in an actual experiment, the intensities have to be corrected for any depolarization.

The advantage of this technique is evidenced in a case such as nickel metal where, for the 111 reflexion, the magnetic contribution to the scattering by unpolarized neutrons is $\sim 1\%$, whereas the difference in the integrated reflexion between the two states of polarization is $\sim 40\%$. In addition, certain aspects of the band and Heisenberg theories of ferromagnetism can be studied in NiCu alloys.

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Reference

CHANDRASEKHAR, S. (1956). *Acta Cryst.* **9**, 954.