Short Communications

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Redetermination of the scattering length of yttrium.

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The scattering length of yttrium was redetermined from a neutron powder pattern of Y_2O_3 which was analysed by the profile-analysis technique. The study confirmed the structural parameters of the single-crystal investigation of O'Connor and Valentine and yielded a scattering length of $b_Y = 0{\cdot}765$ ($\sigma = 0{\cdot}007$) 10^{-12} cm. This value is supported further by the results of a current study of yttrium iron garnet (YIG) by polarized neutrons.

Introduction

In the course of our present polarized-neutron study of yttrium iron garnet (YIG) (Bonnet, Delapalme, Tcheou & Fuess, 1974) discrepancies in the interpretation of data occured which could not be solved using the scattering lengths of yttrium available in the literature (Table 1). All scattering lengths in this note are given in terms of 10^{-12} cm.

Table 1. *Scattering length of yttrium for thermal neutrons*

Authors	Compound	b_Y
Prince (1957)	$Y_3Al_5O_{12}$	$0{\cdot}80 \pm 0{\cdot}01$
Villain (1957)	Y_2O_3	0·71
Fert (1962)	Y_2O_3	$0{\cdot}79 \pm 0{\cdot}02$
Kuz'minov, Yamzin, Mal'tsev & Belov (1962)	Y_2O_3	$0{\cdot}816 \pm 0{\cdot}07$
Atoji (1961)	YC_2	$0{\cdot}786 \pm 0{\cdot}017$
Rustadt (1964)	Transmission	$0{\cdot}775 \pm 0{\cdot}015$
Paton & Maslen (1965)	Y_2O_3	$0{\cdot}781 \pm 0{\cdot}008$

We therefore decided to re-examine the value of the yttrium scattering length by means of a neutron powder diffraction study using the profile analysis technique (Rietveld, 1967, 1969; Hewat, 1973*a*). For this purpose we choose the oxide Y_2O_3 which is easily available in high purity (99·95% from Pechiney-St. Gobain). A neutron single-crystal study has been reported by O'Connor & Valentine (1969). These authors refined the positional and thermal parameters and used the scattering length determined by Paton & Maslen (1965). The crystal data for Y_2O_3 are: space group $Ia3$, $Z = 16$, $a = 10{\cdot}604$ Å. The atoms occupy the following positions:

Y(1) in 8(*b*)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	*etc.*
Y(2) in 24(*d*)	u	0	$\frac{1}{4}$	*etc.*
O in 48(*e*)	x	y	z	*etc.*

Experimental

The powder pattern was registered at the D1A powder instrument at a thermal guide tube at ILL. The wavelength was 1·510 Å from the (533) plane of a Ge monochromator. Owing to the guide tube no λ/n contamination was present and the high take-off angle of the monochromator $2\theta_M = 116°$ yielded a fairly flat resolution curve.

53 reflexions were recorded between $2\theta = 14°$ and 72°. The background level was about 400 counts/point and the maximum counting rate about 10000 counts/point for a counting time about 8 min.

Refinement

The refinement was carried out by minimizing the function M with respect to the parameters;

$$M = \sum w_i \left\{ Y_i(\text{obs}) - \frac{1}{c} Y_i(\text{calc}) \right\}^2 .$$

The reliability value for the profile, R_{pr}, is given by

$$R_{pr} = 100 \left\{ w_i \left[Y_i(\text{obs}) - \frac{1}{c} Y_i(\text{calc}) \right]^2 / \sum w_i [Y_i(\text{obs})]^2 \right\}^{1/2},$$

where c is a scale factor, Y_i(obs) and Y_i(calc) the observed and calculated intensities at any point i, and $w_i \propto 1/\sigma_i^2 \simeq 1/Y_i$(obs) is the weighting factor for this point.

The background was determined by averaging any three points in the pattern which were not attributed to a reflexion.

Table 2. *Crystallographic parameters of* Y_2O_3 *and scattering length of yttrium*

Standard deviations in parentheses.

	u	x	y	z	B_{Y1}	B_{Y2}	B_O	b_{Y1}	b_{Y2}	b_Y	R_{pr}	R_B
Present work	−0·0326 (2)	0·3911 (2)	0·1519 (2)	0·3806 (3)	0·09*	0·305*	0·351*	0·764 (10)	0·765 (5)	0·765 (7)	5·65	1·80
O'Connor & Valentine	−0·0327 (3)	0·3907 (3)	0·1520 (3)	0·3804 (3)		Anisotropic		0·788*	0·788*	0·788*		
Paton & Maslen	−0·0333 (3)	0·3889 (9)	0·1551 (10)	0·3789 (9)		Anisotropic		–	–	X-rays		

* These parameters were not refined.

Owing to the limited range in 2θ the thermal parameters are not well defined. We therefore fixed them on the best refined values of a preceding cycle without further refinement which gave considerably better standard deviations for all other parameters (see Table 2). An attempt to refine anisotropic temperature factors (Hewat, 1973*b*) gave negative temperature factors for one of the atoms as a result of the limited amount of data.

The crystallographic positional parameters are in excellent agreement with the single-crystal neutron refinement of O'Connor & Valentine (1969); the agreement is not so good with the X-ray study of Paton & Maslen (see Table 2).

The parameter varied in the least-squares refinement was in fact the occupation number of the two yttrium sites, which is linearly dependent on the scattering length. We found in fact good agreement between the scattering lengths of the two crystallographic sites.

Three values of the scattering length of oxygen are given in the literature. We carried out refinements of the yttrium occupation numbers with all three values and found the following ratios b_Y/b_O.

b_O	Reference	b_Y/b_O	b_Y
0·577	Hughes & Schwartz, 1958	1·3189	0·760
0·575	Bacon, 1962	1·3172	0·758
0·580	Bacon, 1972	1·3182	0·765

The reliability values quoted are R_{pr} which is defined above and the reliability value R_B based on the Bragg reflexions:

$$R_B = 100 \sum_i \left| F_i^2(\text{obs}) - \frac{1}{c} F_i^2(\text{calc}) \right| / \sum_i F_i^2(\text{obs}) .$$

The final value of the scattering length of yttrium with the latest value of the oxygen scattering length of $b_O = 0{\cdot}580$ and with fixed values of the thermal parameters is $b_Y = 0{\cdot}765$ ($\sigma = 0{\cdot}007$).

Further support is given by our single crystal study of yttrium iron garnet (YIG) by the polarized neutron technique (Bonnet, Delapalme & Fuess, 1975).

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The calculation of peak heights on Fourier maps.

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The paper describes a method for the rapid calculation of expected peak heights on Fourier maps for each atom type over a range of temperature factors, given the crystal data and the number of independent reflexions collected. An algorism is presented for assigning unidentified peaks to specific atom types.

Scattering factors, f, for atoms at rest can be approximated by the series $f = \sum A_j \exp(-a_j s^2)$ over j terms, where $s = \sin\theta/\lambda$ (Forsyth & Wells, 1959; Moore, 1963; Cromer, Larson & Waber, 1968; Lee & Pakes, 1969). Usually, $j = 3$, and $a_3 = 0$, so that the correction for the real component of anomalous dispersion can be added algebraically to A_3. Sakurai (1967) pointed out that this representation of f enabled the height, H_i, of a peak on a Fourier map due to an atom of type i to be calculated independently of the production of the map. If reflexions are collected out to a limiting value, l, for $\sin\theta/\lambda$, and the temperature factor, U_i, is known, then, since the effective radius of the limiting sphere is $2l$,

$$H_i = 8 \int_0^l 4\pi s^2 \sum_j A_{i,j} \exp\left[-(a_{i,j} + 8\pi^2 U_i) s^2\right] \mathrm{d}s . \quad (1)$$

Sakurai published a table of values for H for all atoms over a range of values for $B(=8\pi^2 U)$ with values for l of infinity, and the values for the limiting spheres for Cu $K\alpha$, and for Mo $K\alpha$ radiations. This paper presents a routine solution for equation (1) for any limiting value for $\sin\theta/\lambda$, and any values for U.

It is convenient to drop subscripts temporarily, and to use the substitutions:

$$E = (a + 8\pi^2 U); \quad x = 2Es^2; \quad \chi^2 = 2El^2$$

so that equation (1) is converted into (2*a*):

$$H = (8\pi/\sqrt{2}) \sum AE^{-3/2} \int_{x=0}^{x=\chi^2} [x^{1/2} \exp(-x/2)] \mathrm{d}x . \quad (2a)$$

The integral is a standard one, of value $\sqrt{2\pi} P(\chi^2, 3)$, where the function P is the χ^2 integral for three degrees of freedom. Table 1, derived by linear interpolation from the values of P as a function of χ^2 (Pearson & Hartley, 1954), gives the values of χ^2 which provide an equally spaced series of values for the integral; between these values the