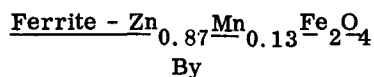


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On the Magnetic Structure of a Manganese-Substituted Zinc



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In the course of neutron diffraction studies on spinel-type ferrites in which the B-B magnetic interactions are comparable with the A-B ones, a Mn-substituted zinc ferrite with the composition  $\text{Zn}_{0.87}\text{Mn}_{0.13}\text{Fe}_2\text{O}_4$  was investigated.

Neutron diffraction patterns of a polycrystalline sample taken at 4.2 °K showed the presence of strong and well-shaped magnetic peaks which could be readily indexed on the basis of a magnetic unit cell obtained by doubling the chemical unit cell in one direction. The observed magnetic indices obeyed the rule

$$h_M + k_M + l_M = 2n$$

with  $l_M$  odd only.

Using a computer programme a large number of simple and complex magnetic structures was surveyed including those with the magnetic order in the B sites as well as in the A sites. However, the best agreement between the observed and calculated magnetic intensities was obtained for a collinear model with antiferromagnetic ordering in the B sites only. Considering the doubled spinel-type unit cell, the spin direction denoted by + is associated with magnetic ions in the following positions:

1/8, 1/8, 5/16; 1/8, 7/8, 11/16; 7/8, 7/8, 13/16; 7/8, 1/8, 3/16; 7/8, 3/8, 1/16;  
5/8, 7/8, 15/16; 3/8, 1/8, 7/16; 1/8, 5/8, 9/16.

The same spin direction appears at further 8 ions connected with those above by the (1/2, 1/2, 1/2) translation. The magnetic ions with opposite spin direction are situated in the positions obtained by adding (0, 0, 1/2) to the above 16 sets of coordinates.

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The minimum value of the R-factor for the magnetic intensities ( $R = 0.04$ ) was obtained for the spins aligned in the  $[11\bar{1}]$  direction of the doubled cell. It is also possible to choose a simpler magnetic unit cell by the following transformation:

$$\begin{aligned}a' &= a, \\b' &= b, \\c' &= \frac{a+b+c}{2},\end{aligned}$$

where  $|a| = |b| = a_0$  and  $|c| = 2a_0$ .  $a_0$  is the lattice constant of the chemical unit cell. In the new magnetic unit cell the spins are parallel to the  $c'$ -direction.

The observed and calculated intensities for 8 observable magnetic reflections are collected in Table 1.

Table 1

Magnetic intensities in  $\text{Zn}_{0.87}\text{Mn}_{0.13}\text{Fe}_2\text{O}_4$  at  $4.2^\circ\text{K}$

(indexing on the doubled unit cell)

$h_M$	$k_M$	$l_M$	$I_{\text{obs}}$	$I_{\text{calc}}$
1	0	1	480	475
1	0	3	20	17
2	1	1	33	33
1	2	3	108	112
1	0	5		
3	0	1	36	45
3	2	5	26	22
4	1	3	20	16
3	0	7		
1	0	9		
3	0	9	10	13
2	5	1		
4	1	7		

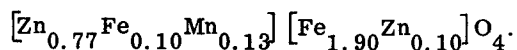
The average magnetic moment of a ferric ion in the B site was found to be  $\approx (3.0 \pm 0.1)$  Bohr magnetons. Basing on the nuclear intensities at  $4.2^\circ\text{K}$  the

oxygen parameter and the inversion coefficient at this temperature were determined to

$$x = 0.3857 \pm 0.0005,$$

$$i = 0.10 \pm 0.05$$

leading to  $R = 5\%$ . The cation distribution is thus



In connection with this study we performed neutron diffraction measurements at 4.2 °K on  $\text{ZnFe}_2\text{O}_4$ . Its neutron pattern showed a striking similarity in the magnetic peak distribution to that of  $\text{Zn}_{0.87}\text{Mn}_{0.13}\text{Fe}_2\text{O}_4$ . This suggests that the unit cell of  $\text{ZnFe}_2\text{O}_4$  should be described as doubled in one direction only, contrary to the previously reported data (1).

#### References

- (1) J. M. HASTINGS and L. M. CORLISS, Phys. Rev. 102, 1460 (1956).

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