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On the Magnetic Structure of a Manganese-Substituted Zinc Ferrite - $Zn_{0.87}Mn_{0.13}Fe_2O_4$

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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 $Zn_{0.87}Mn_{0.13}Fe_2O_4$ 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 [111] direction of the doubled cell. It is also possible to choose a simpler magnetic unit cell by the following transformation:

$$\mathfrak{a}' = \mathfrak{a} ,$$
$$\mathfrak{b}' = \mathfrak{b} ,$$
$$\mathfrak{c}' = \frac{\mathfrak{a} + \mathfrak{b} + \mathfrak{c}}{2} ,$$

where $|\mathfrak{a}| = |\mathfrak{b}| = a_o$ and $|\mathfrak{c}| = 2a_o$. a_o 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 $Zn_{0.87}Mn_{0.13}Fe_2O_4$ at 4.2 °K

(indexing on the doubled unit cell)

h_M	k_M	l_M	I_{obs}	I_{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		
3	0	7	20	16
1	0	9		
3	0	9		
2	5	1	10	13
4	1	7		

The average magnetic moment of a ferric ion in the B site was found to be ≈(3.0 ± 0.1) Bohr magnetons. Basing on the nuclear intensities at 4.2 °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

$[Zn_{0.77}Fe_{0.10}Mn_{0.13}]\,[Fe_{1.90}Zn_{0.10}]O_4$.

In connection with this study we performed neutron diffraction measurements at 4.2 °K on $ZnFe_2O_4$. Its neutron pattern showed a striking similarity in the magnetic peak distribution to that of $Zn_{0.87}Mn_{0.13}Fe_2O_4$. This suggests that the unit cell of $ZnFe_2O_4$ 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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