phys. stat. sol. (b) 91, K83 (1979)

Subject classification: 18.3; 22.8.2

Institute of Physics, Jagiellonian University, Cracow[1] (a)
and Institute of Physics, Silesian University, Katowice (b)

On the Exchange Integrals in Nickel Ferrite

By

Z.M. STADNIK (a) and W. ZAREK (b)

Nickel ferrite $NiFe_2O_4$ is a collinear Néel ferrimagnet with a completely inverted spinel structure /1 to 3/.

Using the Mössbauer effect method, Morel /4/ measured the reduced magnetizations of Fe^{3+} ions in the tetrahedral (A) and octahedral (B) sites in this ferrite. By a molecular field analysis he deduced from the experimental data the exchange integrals $J_{12} = -18.8$ K, $J_{13} = -24.44$ K, and $J_{23} = 20.68$ K, assuming that $J_{11} = J_{22} = J_{33} = 0$; the indexes 1, 2, and 3 refer to Fe^{3+} in the A and B sites and Ni^{2+} in the B site, respectively. Reduced sublattice magnetizations were measured only for $T < 0.57\ T_c$, as at higher temperatures it was not possible to separate hyperfine fields acting on ^{57}Fe in the A and B sites.

However, as it is well known /5/, the molecular field theory is a good approximation only for high temperatures. Therefore, exchange integrals derived from the low temperature region, where reduced magnetizations are weakly dependent on temperature, may be incorrect. What more, the values of exchange integrals were rather guessed /4/ than obtained from a fit. Therefore, we felt it useful to determine exchange integrals in $NiFe_2O_4$ from more complete experimental data and without neglecting any of them. For that purpose the specific magnetization measurements have been carried out from 77 K up to T_c. The experimental details are described elsewhere /6/.

Let us express the exchange integrals in $NiFe_2O_4$ through $J_{12} = J$; $J_{11} = xJ$, $J_{22} = yJ$, $J_{33} = zJ$, $J_{13} = rJ$, and $J_{23} = qJ$. Then, using the molecular field theory for the case of three collinear sublattices, one can obtain the following equations for reduced sublattice magnetizations:

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1) Reymonta 4, 30-059 Cracow, Poland.

$$m_1(T) = B_{5/2}\left[50\,xJ\,\frac{m_1(T)}{T} + 75\,J\,\frac{m_2(T)}{T} + 30\,rJ\,\frac{m_3(T)}{T}\right],$$

$$m_2(T) = B_{5/2}\left[75\,J\,\frac{m_1(T)}{T} + \frac{75}{2}\,yJ\,\frac{m_2(T)}{T} + 15\,qJ\,\frac{m_3(T)}{T}\right],$$

$$m_3(T) = B_1\left[30\,rJ\,\frac{m_1(T)}{T} + 15\,qJ\,\frac{m_2(T)}{T} + 6\,zJ\,\frac{m_3(T)}{T}\right]. \tag{1}$$

The resulting reduced magnetization gets the form

$$m(T) = m_3(T) + \frac{5}{2}\left[m_2(T) - m_1(T)\right]. \tag{2}$$

At the Curie temperature T_c sublattice magnetizations vanish, leading to the equation

$$T_c^3 - \frac{2}{3}J(35\,x + \frac{105}{4}y + 6z)\,T_c^2 + \frac{20}{9}J^2\left[\frac{63}{2}(yz - q^2) + 42(xz - 3r^2) + \right.$$

$$\left. + \frac{735}{4}(xy - 3)\right]T_c - \frac{4900}{3}J^3\,(xyz + 6qr - 3r^2y - 3z - q^2x) = 0 \tag{3}$$

In our calculations the value $T_c = 856.73$ K, which is the weighted average of the most reliable experimental data, has been used. The experimental data ($m_1(T)$ and m_2T from /4/, and our data for m(T)) have been fitted, using 1 ERN computer subroutines /7 to 9/, with exchange parameters satisfying (3) and the non-linear equations (1). The best fit has been obtained for the following values: $J_{11} = J_{22} = J_{33} = 0$, $J_{12} = -15.84$ K, $J_{13} = -29.20$ K, and $J_{23} = 26.26$ K. The strong ferromagnetic Fe(B)-Ni(B) interaction is in accordance with theoretical predictions by Goodenough /10/.

Fig. 1 and 2 show the theoretical curves calculated using Morel exchange integrals and those obtained in this paper. As can be seen, the agreement between molecular field theory and experiment at high temperatures is better in Fig. 2 than in Fig. 1. The discrepancy between calculated curves and experimental data remains in the low temperature region. This is a consequence of the limitations of the molecular field approach. More precise theoretical methods, using e.g. temperature-dependent Green function theory or the random phase approximation, while giving better results for simple magnetic systems (e.g.

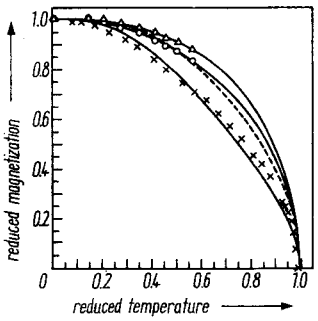

Fig.1

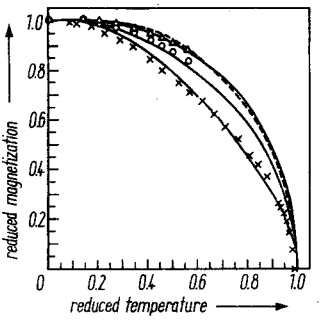

Fig.2

Fig. 1. Reduced magnetization versus reduced temperature in $NiFe_2O_4$. The full and dashed curves are for Morel exchange integrals /4/; the dashed line represents the $m_3(T)$ curve; Δ m_1, $\circ$ m_2 data /4/; $\times$ m data (this work)

Fig. 2. Reduced magnetization versus reduced temperature in $NiFe_2O_4$. The full and dashed curves are for our values of exchange integrals given in the text; the broken line represents the $m_3(T)$ curve; Δ m_1, $\circ$ m_2 data /4/; $\times$ m data (this work)

in antiferromagnets /11/), are mathematically too complex /5/ to be applied in deriving exchange parameters from experimental data in ferrimagnets.

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(Received August 9, 1978)