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A NEUTRON DIFFRACTION DETERMINATION OF THE MAGNETIC FORM FACTOR FOR Ni^{2+} IN NiO

BY

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1. INTRODUCTION

Recently Roth (1) has shown that the intensities of the magnetic reflections from NiO decrease more slowly with scattering angle than those from MnO.

The present investigation in which a larger crystal was used extends the Ni^{2+} form factor curve to $4 \sin\theta/\lambda = .9$ and shows that the form factor is larger than would be expected from the Hartree–Fock calculations of Piper (2).

2. THEORY

The intensity of a magnetic reflection is given by

$$I = \frac{q^2 F^2}{\sin 2\theta} e^{\frac{-B}{2d^2}}$$

where

$$F = \Sigma_j \; p_j \; e^{2\pi i \underline{k} . \underline{r}_j}$$

$$p = \frac{e^2 \gamma}{mc^2} S f = 0.539 \, S f$$

S = spin quantum number

f = magnetic form factor

q^2 = $\sin^2 \alpha$

and α is the angle between the scattering vector and the magnetic moment direction.

An experimental determination of the rate of fall–off of f with θ can be made by comparing the intensities of reflections from successive orders of the same plane but an absolute form factor determination requires that the moments are allotted specific lattice directions.

The model used to determine q^2 values for the various reflections is that of Li type A (3) with each domain (defined as a region in which a particular set of (111) planes are ferromagnetic sheets) further divided into regions in which the magnetic moments have the same direction in the (111) sheets. If the assumptions are made that the vector sum of these orientations is zero and that the same number of moments within a domain have each orientation, then

$$q^2 = \frac{1}{2} (1 + \frac{(h - k + l)^2}{3(h^2 + k^2 + l^2)}$$

for moments lying in $(1\bar{1}1)$ with similar expressions for other (111) planes.

Reflection	q^2
$1\,\bar{1}\,1$	1
$\bar{1}\,1\,3$	17/32
$1\,\bar{1}\,5$	65/81
$\bar{1}\,1\,7$	89/153
$\bar{3}\,3\,1$	41/57
$3\,\bar{3}\,3$	1
$\bar{3}\,3\,5$	65/129
$3\,\bar{3}\,7$	170/171
$\bar{3}\,3\,9$	17/33
$5\,\bar{5}\,1$	137/153
$\bar{5}\,5\,3$	113/177
$5\,\bar{5}\,5$	1
$7\,\bar{7}\,7$	1
$\bar{9}\,9\,3$	41/57

In each domain F is non–zero only under the following conditions:–

Ferromagnetic Sheet	$F \neq 0$
111	h, k, l all odd, $h+k,\ k+l,\ l+h = 4n+2$
$11\bar{1}$	h, k, l all odd, $h+k,\ k-l,\ h-l = 4n+2$
$1\bar{1}1$	h, k, l all odd, $h-k,\ -k+l,\ h+l = 4n+2$
$\bar{1}11$	h, k, l all odd, $-h+k,\ k+l,\ l-h = 4n+2$

These restrictions mean that any magnetic reflection must arise only from a single domain, so that a set of reflections can be chosen which are reflections from a single domain.

3. EXPERIMENTAL

The crystal used in this work was grown by the flame fusion technique and was supplied by Dr. F.W.Harrison of the Mullard Research Laboratories, England. Its volume was 150 mm^3. The spectrometers used were the two single crystal spectrometers on BEPO and the neutron wavelength was 1.108Å . The following experiments were carried out:–

(1) The crystal was set up with [100] vertical and a series of nuclear reflections measured. The second order contamination in the monochromatic beam was found to be 0.27% by comparing the intensities at the (100) and (200) positions for $\lambda = 1.08$ Å.

(2) The crystal was set up with [110] vertical and all available nuclear and magnetic reflection measured. The ratio of the (222) nuclear and (333) magnetic intensities was measured at 0.81 Å, 1.08 Å and 1.21 Å in order to correct for extinction by the method of Bacon and Pease (4).

(3) The crystal was set up with [1$\bar{1}$0] vertical and the intensities of the (111), (11$\bar{1}$) nuclear and magnetic reflections determined.

4. RESULTS

All line intensities are in arbitrary units and are normalised to (111) nuclear = 15.0. The temperature factor was found from the nuclear reflections to be $B = 0.5 \times 10^{-16}$ cm.

The corrected nuclear and magnetic (111) intensities are given below:–

Reflection	Magnetic	Nuclear
111	9.58	15.0
11$\bar{1}$	7.07	15.0
1$\bar{1}$1	4.69	15.0
$\bar{1}$11	5.15	15.0

These results were used to give an absolute value for the (111) form factor.

The total magnetic intensity of 26.54 was corrected for lack of magnetic saturation by the factor $\frac{I_{298}}{I_o} = 0.74$

(1) and compared with the nuclear intensity of 15.0 to give $f_{111} = 0.91$.

The form factors for the other reflections were calculated from the observed intensities using $f_{111} = 0.91$ and the q^2 value calculated in section 2. The intensities of the reflections from two domains were used.

The form factor curve is shown in Fig. 1 with the calculated curve for comparison.

CONCLUSION

The experimental errors, in particular the uncertainties arising from the extinction correction do not warrant an attempt to fit a more detailed model of the magnetic movement orientations.

The higher flux from HIFAR will permit the use of a smaller crystal with a consequent decrease in the extinction correction. The fit of the experimental points shows that the present model is not unreasonable, but it will be examined with more precise data.

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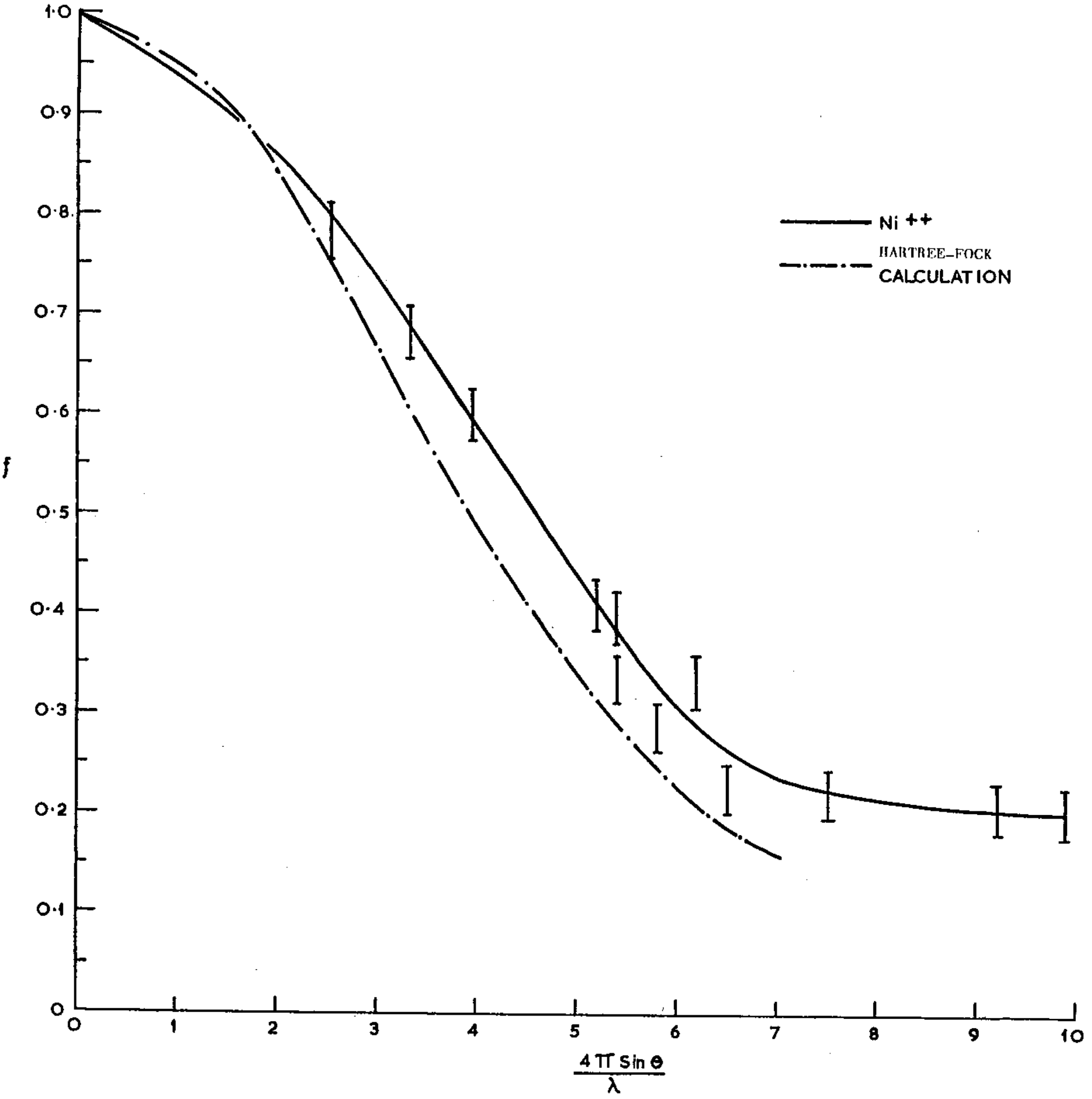

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0·1
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4 π Sin θ / λ
Ni ++
HARTREE–FOCK CALCULATION