REFINEMENT OF THE CRYSTAL AND MAGNETIC STRUCTURE OF $PrFeO_3$ AT $T = 8$ K*

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Summary

The orthoferrite $PrFeO_3$ crystallizes according to space group *Pbnm*, and the magnetic structure is of the G_x type. Based on neutron-diffraction measurements performed at 8 K with improved resolution, the structure parameters and the ordered magnetic moment of Fe^{3+} ($\mu = \mu_x = 4.14(4)\mu_B$) were refined. The results are compared with previous room-temperature data.

1. Introduction

The crystal structures of rare earth orthoferrites were extensively investigated at room temperature by Marezio *et al.* employing single-crystal X-ray studies [1]. Neutron-diffraction measurements of the 011 and 101 reflections of $PrFeO_3$, performed by Pinto and Shaked [2], indicate G_x-type antiferromagnetic ordering of Fe^{3+} moments in the temperature range 4.2 - 293 K. The time-of-flight (TOF) neutron-diffraction study reported by Kaun *et al.* [3] supports this model in the temperature range 77 - 293 K. In a previous neutron-diffraction study of $PrFeO_3$ made at room temperature by the authors [4] the ordered magnetic moment $\mu = \mu_x = 3.73(3)\mu_B$ per Fe^{3+} ion was determined, and the orthorhombic crystal structure corresponding to space group *Pbnm* [1] was confirmed. By means of high-resolution TOF neutron data Sosnowska and Steichele [5] proved that the magnetic structure of $PrFeO_3$ is of pure G_x type at room temperature. The present experiment extends the quantitative analysis of the crystal and magnetic structures of $PrFeO_3$ to low temperatures (8 K).

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2. Experimental details and discussion

Using improved resolution (neutron wavelength, $\lambda = 1.503$ Å, from a Ge 311 monochromator and collimations $\alpha_1 = \alpha_3 = 10'$) compared with the 293 K study [4], the neutron-diffraction measurement was performed on a polycrystalline sample of $PrFeO_3$ on a two-axis spectrometer situated at the Saphir reactor, Würenlingen. Figure 1 shows the corresponding 8 K diffraction pattern. The neutron intensities were analysed by the Rietveld profile method [6] using the neutron scattering lengths $b_{Pr} = 4.45$, $b_{Fe} = 9.54$, $b_O = 5.81$ F and the neutron magnetic form factor of Fe^{3+} [7]. Good agreement of observed and calculated neutron intensities was achieved. The relevant results are summarized in Table 1. The 8 K and room-temperature structures appear to be similar. Also at 8 K, the magnetic structure is of the G_x type, and the ordered magnetic moment, μ_{Fe}, amounts to $4.14(4)\mu_B$, *i.e.*, it is reduced below the free-ion value of 5 μ_B ($S = 5/2$). These results support ref. 2 as well as the estimate of a weak Pr–Fe coupling in $PrFeO_3$ published by Pataud and Sivardière [8], which makes reorientation phase transitions improbable.

TABLE 1

Parameters of the crystal and magnetic structure of $PrFeO_3$ for space group *Pbnm*, determined by means of neutron diffraction

T (K)	8	293 [4]	293 [1]
λ (Å)	1.503(1)	2.331(2)	X-rays
a (Å)	5.486(4)	5.483(5)	5.482
b (Å)	5.591(4)	5.578(5)	5.578
c (Å)	7.783(5)	7.788(7)	7.786
B_{Pr} (Å^2)	0.5(1)	0.92(5)	
B_{Fe} (Å^2)	0.22(4)	0.92(5)	
B_O (Å^2)	0.41(4)	0.92(5)	
x_{Pr}	0.990(2)	0.984(2)	0.99097(4)
y_{Pr}	0.0450(9)	0.044(1)	0.04367(5)
x_{O1}	0.086(1)	0.084(1)	0.0817(7)
y_{O1}	0.4795(9)	0.481(1)	0.4788(9)
x_{O2}	0.7076(6)	0.7065(7)	0.7075(5)
y_{O2}	0.2925(6)	0.2908(6)	0.2919(5)
z_{O2}	0.0448(5)	0.0449(6)	0.0437(5)
μ_{Fe} (μ_B)	4.14(4)	3.73(3)	
R_{wp}	0.121	0.091	
R_{in}	0.046	0.034	0.023
R_{im}	0.033	0.017	
R_e	0.071	0.058	

T = temperature, λ = neutron wavelength, a, b, c = lattice constants, B = temperature factor, R_{wp}, R_{in}, R_{im} = agreement ratios concerning weighted profile and integrated nuclear and magnetic intensities, respectively, R_e = statistically expected R factor [6], μ = ordered magnetic moment per Fe^{3+} ion. Literature data for the room-temperature structure are added for comparison.

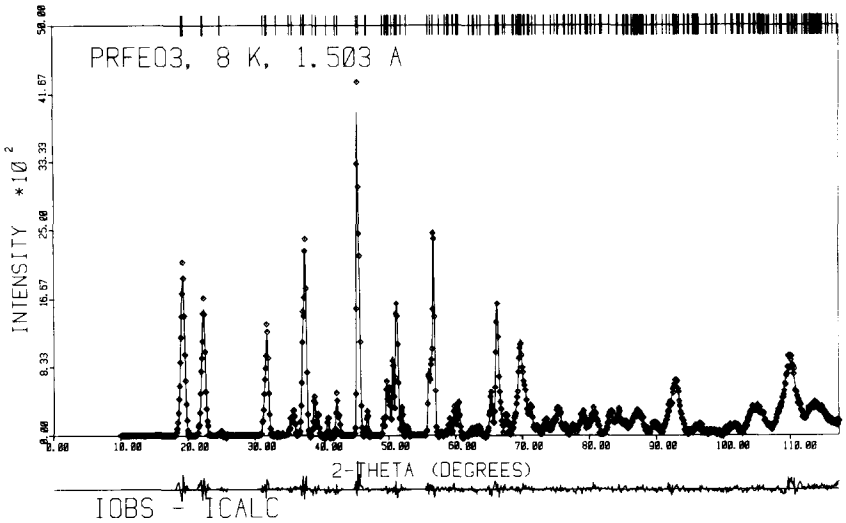

Fig. 1. Observed (points, corrected for absorption and background) and calculated (line) neutron diffraction patterns of $PrFeO_3$ at 8 K (step $\Delta 2\theta = 0.1°$).

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