



Crystal and magnetic structure of the YSrCuFeO_{5+y} compound

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Abstract

We studied the crystal and magnetic structure of the oxygen deficient perovskite YSrCuFeO_{5+y} . The structure was refined from neutron powder diffraction data by assuming both substitutional and displacement disorder. Three-dimensional (3D) antiferromagnetism with $T_N = 400 \pm 10$ K occurs and all the magnetic peaks were indexed with two propagation vectors $\mathbf{k}_1 = [\frac{1}{2} \frac{1}{2} \frac{1}{2}]$ and $\mathbf{k}_2 = [\frac{1}{2} \frac{1}{2} 1]$ from 300 down to 2 K.

Keywords: Antiferromagnetism; Perovskite compounds; Powder diffraction; Rietveld refinement

1. Introduction

YBaCuFeO_5 has a tetragonal structure similar to that of $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ but with the chain levels absent [1]. ^{57}Fe Mossbauer spectroscopy revealed a single Fe site typical of Fe^{+3} ($S = \frac{5}{2}$) with the Fe moments antiferromagnetically ordered ($T_N = 442$ K) [2]. The substitution of Y with other rare earths leads to a variation in T_N , probably due to the different amount of extra oxygen incorporated for each rare earth within the Y layer. In this work, we focus on the structural and magnetic properties of YSrCuFeO_{5+y} and report the results of a neutron powder diffraction (NPD) study in the temperature range 2–300 K.

2. Experimental methods

The synthesis procedure of an YSrCuFeO_5 sample along with a detailed study of the structure and of the magnetic properties (by means of Mossbauer spectroscopy) will be published elsewhere.

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NPD experiments were performed in the flat-cone E2 and E6 focusing single crystal diffractometers of the reactor BERII in Berlin. The $(3 \frac{1}{2} 1)$ reflection of a Ge monochromator with $\lambda \approx 1.2$ Å and the $(0 0 2)$ reflection of a pyrolytic graphite monochromator with $\lambda \approx 2.4$ Å were used.

3. Results and discussion

The major question of a structural study is to decide which is the more appropriate space group. For YSrCuFeO_5 the X-ray powder diffraction data certainly cannot decide between the P4mm (model I) and P4/mmm space groups (model II when $z_{\text{Cu}} = z_{\text{Fe}}$, model III when $z_{\text{Cu}} \neq z_{\text{Fe}}$). The NPD patterns were refined using the FULLPROF program [3]. The obtained lattice parameters at 2 K are $a = 3.8317(1)$ Å and $c = 7.6076(4)$ Å, while R_B is lower for model II (5.42%) than for models I and III (6.48% and 6.52%, respectively).

Since the amount of extra oxygen is very small, we cannot prove its presence by NPD. However, there is indirect evidence from Mössbauer spectroscopy for both YSrCuFeO_5 and PrBaCuFeO_5 [4]

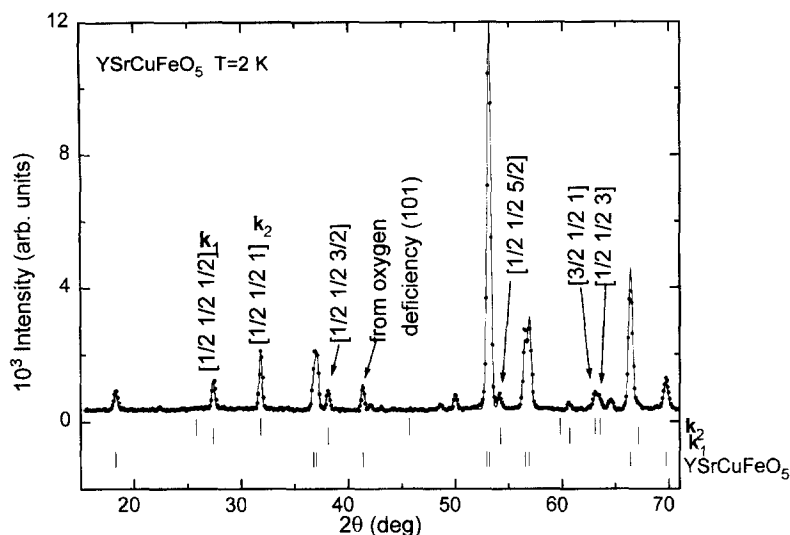


Fig. 1. The refined YSrCuFeO_{5+y} pattern at 2 K. k_1 and k_2 denote reflections from different propagation vectors.

that $\sim 15\%$ of Fe is in octahedral coordination. Moreover, in oxygen saturated PrBaCuFeO_5 the location of the extra oxygen was proved with NPD [4].

Fig. 1 shows the refined NPD pattern at 2 K. In addition to the nuclear structure peaks, there are peaks, whose intensity decreases with increasing temperature and are therefore attributed to anti-ferromagnetic ordering. Mössbauer spectroscopy determined T_N to be 400 ± 10 K. These peaks were indexed with superlattice indices $(h_1/2, k_1/2, l_1/2)$ and $(h_2/2, k_2/2, l_2)$, where $h_1, k_1, h_2, k_2, l_1, l_2$ are odd integers (like in PrBaCuFeO_5 [4]). The former family of reflections comes from a spin arrangement with propagation vector (PV) $k_1 = [\frac{1}{2} \frac{1}{2} \frac{1}{2}]$, i.e. the unit cell is doubled along all three axes. The latter comes from a spin arrangement with PV $k_2 = [\frac{1}{2} \frac{1}{2} 1]$, i.e. the unit cell is doubled only along the a - and b -axis.

The observed reflections can be interpreted either as an *incoherent mixture of domains* with different PVs and with the same ordered moment, but occupying different volumes or by a *canted spin configuration* which is the vector sum of two collinear magnetic structures with different ordered moments but occupying the same volume [5].

The expression of the magnetic structure factor for a magnetic unit cell with cell constants $a_M = b_M = \sqrt{2}a_N$ and $c_M = c_N$ (corresponding to k_2) points out that the absence of the $\ell = 0$ peak means that $p_A = -p_B$, where A and B are the (Cu, Fe) layers above and below the Y layer. This occurs only when layers A and B are equivalent. Due to the small number of magnetic reflections, we had to consider the magnetic ions at the $z = 0.25$ position and represent them by a mean magnetic moment. This assumption corresponds to model II. Regarding k_1 , it can be either $p_A = p_B$ or $p_A = -p_B$, but our data cannot distinguish between them. Thus, there are the possible collinear magnetic models for k_1 and one for k_2 (Fig. 2).

For the canted structure model, the ordered moments per ion at 2 K are $S[k_1] = 1.5(1)\mu_B + 0.2(5)z\mu_B$ ($R_B = 2\%$) and $S[k_2] = 1.6(1)y\mu_B$ ($R_B = 5.6\%$). Thus, the magnetic moment is nearly perpendicular to the c -axis. $S[k_1]$ is equal to 1.4, 1.2 and $1.0\mu_B$, while $S[k_2]$ is equal to 1.6, 1.2 and $1.0\mu_B$ at 100, 200 and 300 K, respectively. For the model with the incoherent mixture of domains and with the two PVs having the same moment ($S \approx 2\mu_B$), the two domains k_1 and k_2 represent 41% and 59%, respectively, of the total crystal volume at 2 K.

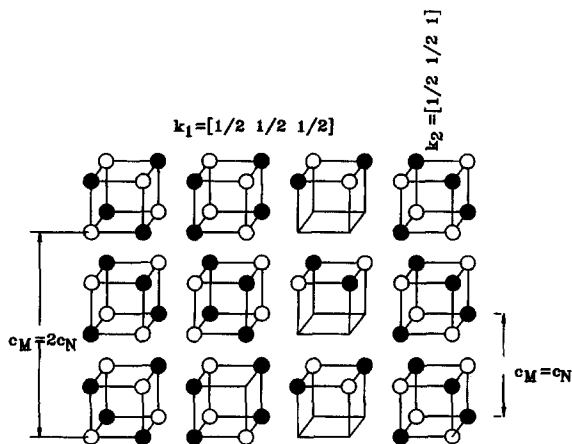


Fig. 2. The possible magnetic structures for k_1 and k_2 . Filled and open circles are for spin-up and spin-down, respectively.

The existence of two PVs cannot be explained by some kind of interactions between (Cu, Fe) and the rare-earth ions (Y or Pr), because in YSrCuFeO_5 , Y^{3+} unlike Pr^{3+} , does not carry a magnetic moment.

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