Experimental report

09/02/2016

Proposal: 5-51-499 **Council:** 4/2014

Title: Spin density distribution in ferromagnetic SrRuO3

Research area: Physics

This proposal is a new proposal

Main proposer: Stefan KUNKEMOELLER

Experimental team: Stefan KUNKEMOELLER
Markus BRADEN

Local contacts: Anne STUNAULT

Samples: SrRuO3

Instrument	Requested days	Allocated days	From	To
D9	4	4	02/10/2014	06/10/2014
D3 High field >1T	8	12	06/10/2014	18/10/2014

Abstract:

We propose to study the spin-density distribution and to determine the precise crystal structure in ferromagnetic SrRuO3. SrRuO3 is the only simple ruthenate that exhibits ferromagnetic order at ambient conditions. A study of the spin-density distribution in SrRuO3 appears highly interesting in view of the general importance of ferromagnetism in ruthenates, and in view of the proposed half metallic behavior of SrRuO3.

1 Introduction

$SrRuO_3$ is the infinite-layer material of the well known Ruddlesden-Popper series of Ruthenates $Sr_{n+1}Ru_nO_{3n+1}$, which have attracted enormous interest not only due to the unconventional superconductivity in Sr_2RuO_4 [1]. Ruthenates also exhibit metamagnetic transitions, Mott insulating phases, SDW ordering arising from nesting and hidden order phases, to cite the most prominent features. The rich variety of physical phenomena in ruthenates arises from electronic correlations and spin-orbit coupling. $SrRuO_3$ is particularly interesting as it is the only simple material (otherwise one has to study three or higher-number layer members of the Ruddlesden-Popper series) that exhibits ferromagnetic order at ambient conditions. The magnetic moment of ferromagnetic $SrRuO_3$amounts up to 1.6 μ_B and the transition temperature amounts to 160 K [2]. The ferromagnetism in $SrRuO_3$ is associated with strongly anomalous behavior in various properties of this material: Thermal expansion shows an invar effect in the ferromagnetic phase [3]. Furthermore, ferromagnetism clearly interferes with the DC electronic transport yielding a linear resistivity that breaks the Ioffe rule already at 500 K [4].

2 Experimental

We could grow a large single crystal of $SrRuO_3$, from which we cut a nearly cubic peace with a mass of 220 mg. The [1,0,0] directions of the cubic cell were perpendicular to the faces of the sample and glued on the sample holder so that the magnetic field is applied in a cubic [1,0,0] direction.
In the D9 Experiment two sets of data at 10 K and 170 K were measured with 1642 and 1147 single reflections. In order to measure reflections of all possible 6 twins in that perovskite it is necessary to measure half integer reflections or to transform into the double cubic cell. During the measurement we used the Pnma cell with lattice constants of 5.4x8x5.4 Å.
In the D3 Experiment the magnetic field of 9 T was applied along a pseudo-cubic [100] direction. In total 222 Flipping ratios at 10 K and 155 Flipping rations at 200 K were measured.

Table 1: *Crystal structure of $SrRuO_3$ at 10 K and 170 K. The atomic positions are given in fractions of the unit cell, the atomic displacements are given in $\AA^2$, values in brackets indicate the error on the last digits.*

	Sr	Ru	O1	O2
10 K				
x	0.0220(2)	0	−0.0046(3)	0.2779(3)
y	0.25	0	0.25	0.02871(13)
z	−0.0036(5)	0.5	0.4460(3)	0.7220(2)
ai	1	1.014	0.962	1.044
U_{11}	0.0056(8)	0.0060(9)	0.0042(9)	0.0103(10)
U_{22}	0.0025(8)	0.0044(8)	0.0000(8)	0.0069(7)
U_{33}	0.0045(8)	0.0015(8)	0.0064(9)	0.0073(9)
U_{12}	0	0.0012(4)	0	0.0007(6)
U_{13}	0.0003(5)	0.0026(12)	0.0010(4)	0.0003(3)
U_{23}	0	−0.0003(7)	0	0.0017(5)
170 K				
x	0.0206(2)	0	−0.0031(3)	0.2789(5)
y	0.25	0	0.25	0.0299(2)
z	−0.0031(5)	0.5	0.4472(5)	0.7229(6)
ai	1	1.021	0.927	1.056
U_{11}	0.0079(8)	0.0067(11)	0.0053(12)	0.0122(9)
U_{22}	0.0037(13)	0.0117(18)	−0.0025(13)	0.0105(9)
U_{33}	0.0092(10)	0.0026(10)	0.0078(10)	0.0119(10)
U_{12}	0	0.0006(4)	0	−0.0023(10)
U_{13}	0.0002(5)	0.0033(15)	0.0004(4)	0(4)
U_{23}	0	0.0015(7)	0	0.0007(11)

3 Results

3.1 D9

The structural refinement is performed with Jana 2006. The averaging over the Friedel pairs of the D9 data recorded at 10 K yield 833 symmetrically different reflections. The R_{int} value is 2.33 %. The same for the data recorded at 170 K yield 617 symmetrically different reflections and a R_{int} value of 2.28 %. The refinements take into account six twins. Starting from the ideal cubic structure they can be obtained by doubling one lattice constant. Then the two other ones lie 45 °rotated to the prior cubic axis in one or the other direction and elongated by a factor square root two. An extinction correction of type I is applied. In table 1 the structural parameters of the refinement can be seen. The refinements yield R values of wR(all)=4.57 % for 10 K and 4.3 % for 170 K respectively. The magnetic contribution is neglected and the refinements of the twin fractions reveal non equal domain occupations.

3.2 D3

The magnetic field of 9 T was applied along a cubic 100 direction. The two twin orientations of the crystal having the long axis parallel to the magnetic field posses about two thirds of the volume of the entire crystal. The spin density is determined using

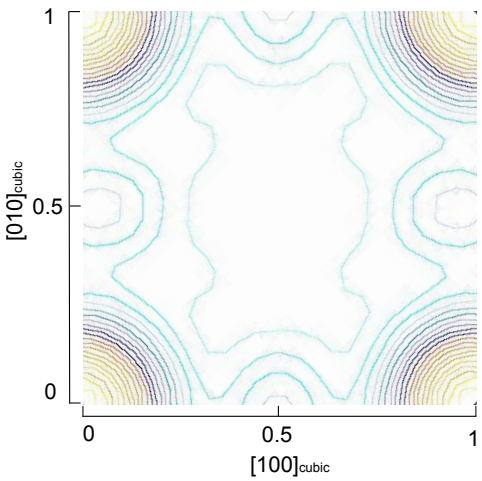

Figure 1: *Illustration of the Spin density of $SrRuO_3$. A cut through a cubic a-b-plane at c=0 is shown. The magnetic moment on the oxygen sites is clearly visible.*

the FullProf Suite. Due to the twinning of the crystal the refinements are performed in a cubic framework. So a monopol model was applied allowing magnetic moments on the ruthenium and oxygen sites. The refinements show that about one third of the total magnetic moment is on the oxygen sites and the total magnetic moment amounts to 1.50(5) μ_B at 10 K, which perfectly agrees with the 1.6 μ_B found in magnetization measurements performed at 2 K in a magnetic field of 7 T. At 200 K a total magnetic moment of 0.42(4) μ_B is found with the same distribution of moment on the ruthenium and oxygen sites as at 10 K. Figure 1 illustrates the Spin density in a drawing which is generated with the GFour program from the FullProf Suite.

References

[1] Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J. G. Bednorz, F. Lichtenberg, Nature (London) **372** (1994) 532–534. 1

[2] A. Kanbayasi, J. Phys. Soc. of Japan **41** (1976) 1876 . 1

[3] T. Kiyama et al., Phys. Rev. B **54** R756 (1996). 1

[4] L. Klein et al. Phys. Rev. Lett. **77** 2774 (1996). 1