Available online at www.sciencedirect.com
SCIENCE DIRECT®
Materials Research Bulletin 41 (2006) 1001–1007
Materials Research Bulletin
www.elsevier.com/locate/matresbu

High pressure neutron diffraction study of the magnetoresistive 1222-type ruthenocuprate, $RuSr_2Nd_{0.9}Y_{0.2}Ce_{0.9}Cu_2O_{10}$

S.A.J. Kimber [a], A.C. Mclaughlin [b], J.P. Attfield [a,*]

[a] *Centre for Science under Extreme Conditions, University of Edinburgh, King's Buildings, Mayfield Road, Edinburgh EH9 3JZ, United Kingdom*
[b] *Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, United Kingdom*

Received 21 December 2005; accepted 4 January 2006
Available online 2 February 2006

Abstract

The crystal structure of the 1222-type ruthenocuprate $RuSr_2Nd_{0.9}Y_{0.2}Ce_{0.9}Cu_2O_{10}$ has been studied by time-of-flight neutron diffraction at temperatures 100–160 K and pressures up to 5 GPa. The structure has tetragonal *I*4/*mmm* symmetry throughout (e.g. $a = 3.8104(2)$ Å and $c = 28.125(3)$ Å at 160 K and 5.1 GPa) with no significant distortions observed at the 140 K Ru spin ordering transition. The strongly bonded Cu–O and Ru–O network leads to a bulk modulus of 145 GPa which is high for layered cuprates, with a low anisotropy in the cell compressibility ($k_c/k_a = 1.32$). The Cu–O–Cu buckling angle and the tilting of the CuO_5 square pyramids decreases with pressure, but the in-plane rotation of the RuO_6 octahedra increases.

Keywords: A. Oxides; A. Magnetic materials; C. High pressure; C. Neutron scattering

1. Introduction

High pressure provides an unrivalled tool for tuning interatomic interactions and structure in the solid state. This paper presents results from a high pressure neutron diffraction study on the 1222-type layered ruthenocuprate $RuSr_2Nd_{0.9}Y_{0.2}Ce_{0.9}Cu_2O_{10}$. The structure (Fig. 1) is similar to that of $YBa_2Cu_3O_{7-\delta}$ with the addition of a fluorite type mixed rare earth oxide layer. Layers of corner-sharing CuO_5 square pyramids and of corner-sharing RuO_6 octahedra are present. The copper oxidation state in these materials is controlled by the trivalent rare earth/cerium ratio and by any oxygen non-stoichiometry [1].

Interest in the layered 1212- and 1222-type ruthenocuprates was stimulated by the observation of co-existing superconductivity and (ferro)magnetism in $RuSr_2Eu_{1.4}Ce_{0.6}Cu_2O_{10}$ with $T_c = 32$ K and $T_m = 122$ K [2]. Numerous studies have been performed in an attempt to elucidate the relationship between superconductivity and magnetism [3–5], which are confined to the copper oxygen layers and ruthenium oxygen layers, respectively. To date, detailed neutron diffraction experiments have been hampered as most ruthenocuprates are stabilised by the mid-series rare earths Sm, Eu, and Gd which have very high neutron absorption cross-sections. Recent results [6] on a new 1222

* Corresponding author. Tel.: +44 131 651 7229; fax: +44 131 651 7228.
E-mail address: j.p.attfield@ed.ac.uk (J.P. Attfield).

0025-5408/$ – see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.materresbull.2006.01.009

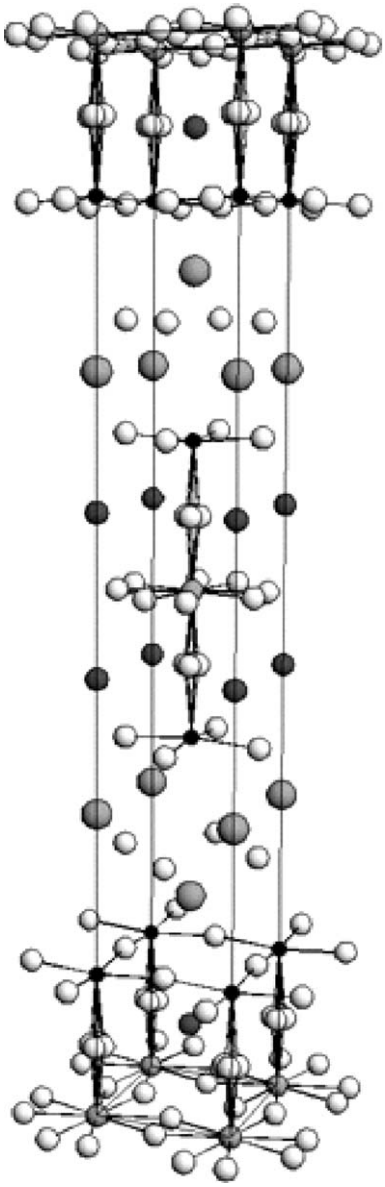

Fig. 1. The *I*4/*mmm* unit cell of $RuSr_2Nd_{0.9}Y_{0.2}Ce_{0.9}Cu_2O_{10}$, The sequence of layers (from top to centre) is $RuO(3)_2$, SrO(1), $CuO(2)_2$, R, $O(4)_2$, R, $CuO(2)_2$, SrO(1), $RuO(3)_2$.

ruthenocuprate based on non-absorbing Nd, $RuSr_2Nd_{0.9}Y_{0.2}Ce_{0.9}Cu_2O_{10}$, show antiferromagnetic ordering of ruthenium spins below $T_{Ru} = 140$ K. This is similar to the ruthenium spin ordering [7] in the related 1212 phase $RuSr_2GdCu_2O_8$. $RuSr_2Nd_{0.9}Y_{0.2}Ce_{0.9}Cu_2O_{10}$ is underdoped to just below the minimum limit for superconductivity and instead shows an ordering of copper spins below $T_{Cu} = 40$ K, this observation is very unusual for a layered cuprate with a significant (5%) hole doping. This spin ordering gives unusual magneto-transport behaviour, a copper spin reorientation at high fields is responsible for large negative magnetoresistances of up to 34% at 4 K in the related compound $RuSr_2Nd_1Y_{0.1}Ce_{0.9}Cu_2O_{10}$.

It is clear that a wide range of properties can be induced in this system by 'chemical pressure' and doping effects and this high-pressure study is part of a larger attempt to understand how subtle structural changes govern the physics of this complex group of oxides.