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Synthesis, Structure and Electric Transport Properties of Sr_3NbCrO_7

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Abstract

A new phase with the composition Sr_3NbCrO_7 has been synthesised by the standard ceramic method. X-ray diffraction studies show that the phase crystallises in the RP-type (n=2) structure with tetragonal unit cell (a = 3.994 and c=21.015 Å) in the space group I4/mmm. The electrical resistivity measurements as a function of temperature suggest that the phase is semiconductor in nature in the temperature range 100-300 K and the conduction occurs by 3D hopping mechanism.

Keywords: Sr_3NbCrO_7, RP-type, XRD studies, electrical resistivity, hopping conduction

1. Introduction

The Ruddlesden-Popper-type phases have been subject matter of intense studies for their wide range of properties. These phases are represented by the composition $A_{n+1}B_nO_{3n+1}$, where usually B-site is occupied by one or more transition metal ion(s). It has been observed that these compounds, generally, crystallise in the space group I4/mmm or Fmmm with tetragonal or orthorhombic unit cell (Battle, 2004; Shilova, 2002; Shivakumar, 2004). RP-phases exhibit electic transport properties ranging from insulator to superconductivity behaviour. The nature and the valance state of the ion/ions at the position B and oxygen content immensely influence the transport properties (Mahesh, 1996; Sharma, 1999). It has been observed that some phases with the ions like Mn^{3+} exhibit colossal magnetoresistance due to induction of mixed valance state in these ions, where I-M transition accompanied by ferromagnetism is obsereved (Gupta, 2011; Helmolt, 1993; Ramirez, 1997; Tsipis, 2007). The presence of an ion with e_g electron at the site B leads to distortion of the unit cell, also known as John-Teller effect. This phenomenon results in interesting electric transport and magnetic properties (Matsukova, 2005).

In the present paper, synthesis of a new RP-type phase with the composition Sr_3NbCrO_7 has been reported. Its crystal structure has been determined from the powder X-ray diffraction data. Electric transport property has been studied in the temperature range 10-300 K.

2. Experimental

2.1 Synthesis

Aldrich make SrO, Nb_2O_5, and Cr_2O_3 (purity 99.9%) have been used for synthesis of the new phase. The constitutent oxides, weighed corresponding to the stoichiometry Sr_3NbCrO_7, were pulverized and mixed by grinding in cyclohexane. The dried and homogenised mixture, pressed in to pellets in a hydraulic press, was heat-treated at 1348 K (with 10 degree variation) for 72 hours in the static air atmosphere. The mixture during heat-treatment was subjected to a number of intermediate grindings and pelletization for completion of the reaction.The product was pulverized for further studies.

2.2 X-ray Diffraction Studies

The powder X-ray diffraction data of the product were recored on a Rigaku Multiflux X-ray diffractometer in the 2θ range of 10-70° at the scanning speed of 1°/min. The X-ray diffraction pattern, intensity versus 2θ, is drawn in the Figure 1, while the data are given in the Table 1.

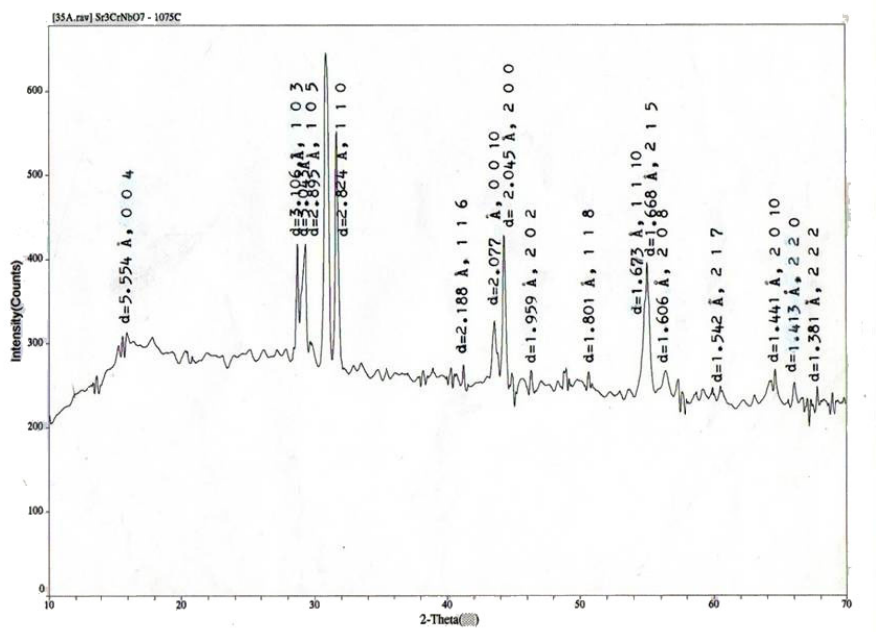

Figure 1. X-ray diffraction pattern of Sr_3NbCrO_7

2.3 Electrical Resistance Study

The electrical resistivity of thin pellet of the phase, sintered at 1200 K before use, was recorded in a Leybold closed cycle helium cryostat, using Keithley 6517 electrometer/high resistance meter. Thin copper wires were attached to the pellet using silver epoxy for the purpose of electrodes. The log ρ versus temperature (**K**) data are plotted in the Figure 2.

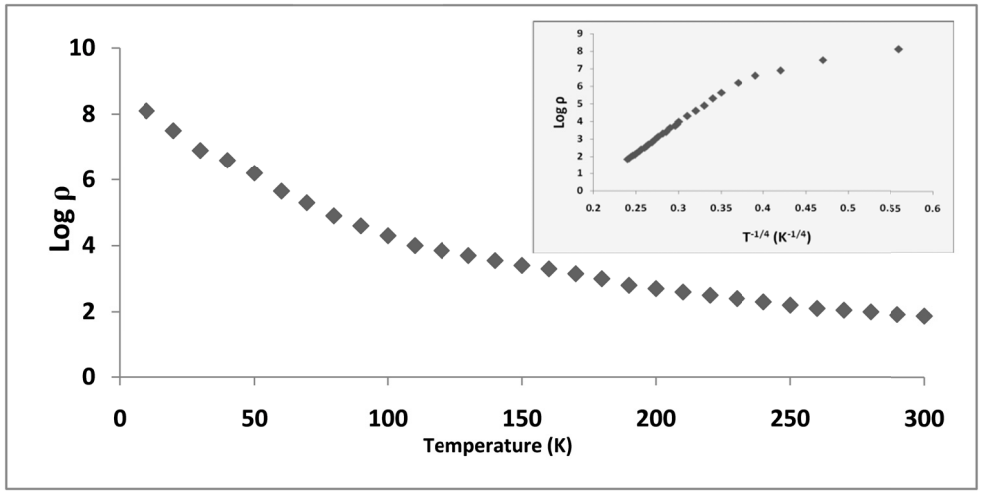

Figure 2. Log ρ versus Temperature (K), (inset) log ρ versus $T^{-1/4}$ ($K^{-1/4}$) for Sr_3NbCrO_7

3. Results and Discussion

3.1 Crystal Structure

The unit cell structural parameters of the phase were calculated from the X-ray diffraction data (Table 1). The indexing of the data shows that it crystallises in the tetragonal unit cell with a = 3.994 and c = 21.015 Å. In order to determine the crystal structure, the theoretical X-ray diffraction data were generated by the Lazy-Pulverix analysis (Yvon, 1977). The structural parameters (positional co-ordinates, occupation factors and the space group I4/mmm) of the RP-type phase $Sr_3Ti_2O_7$ (Ruddlesden & Popper, 1958; Sharma, 2005) were the basis of

the structural analysis. The positional co-ordinates and the occupancy factors applicable for $Sr_3Ti_2O_7$ were gradually varied to arrive at the best fit theoretical d-values and their intensities matching the experimental data. The theoretical X-ray diffraction data are given along with the corresponding experimental data in the Table 1. Comparison of the two sets of the values shows that except for a line at the d-value 3.043 Å, which is attributed to some impurity, there is good agreement between the experimental and the theoretical data. This is especially true when no preferential orientation factors have been taken in to consideration. The agreement shows that the newly synthesised phase has crystallised in the RP-type (n=2) structure with the composition Sr_3NbCrO_7. The composition of the phase as Sr_3NbCrO_7 is based on the chemical structure $(Sr^{2+})_3(Nb^{5+})(Cr^{3+})(O^{2-})_7$. The occupancy factors for oxygen, O_1, O_2 and O_3, (Table 2) which suggest the stoichiometry of oxygen as 7, also substantiate this composition of the phase. Using the positional co-ordinates given in the Table 2 and the space group I4/mmm, the cell structure has been drawn with the programme 'Powder' and the same is given in the Figure 3.

Table 1. Powder X-ray diffraction data of Sr_3NbCrO_7

h	K	l	d_{obs} (Å)	d_{cal} (Å)	I_{obs}	I_{cal}
0	0	4	5.554	5.254	8	2
1	0	3	3.106	3.469	35	10
--	--	--	3.043	------	35	---
1	0	5	2.895	2.895	100	100
1	1	0	2.824	2.824	76	76
1	1	6	2.188	2.198	7	13
0	0	10	2.077	2.102	20	10
2	0	0	2.045	1.997	49	47
2	0	2	1.959	1.962	7	2
1	1	8	1.801	1.924	5	15
1	1	10	1.673	1.686	30	38
2	1	5	1.668	1.644	41	38
2	0	8	1.606	1.590	6	8
2	1	7	1.542	1.535	6	6
2	0	10	1.441	1.447	11	11
2	2	0	1.413	1.412	8	13
2	2	2	1.381	1.399	6	2

Space group: I4/mmm

a = 3.994 Å; c = 21.015 Å

Table 2. Positional coordinates for Sr_3NbCrO_7

Atom	x	y	z	Occupancy
Sr(1)	0.0	0.0	0.5	1
Sr(2)	0.0	0.0	0.3105	1
Nb/Cr	0.0	0.0	0.075	1
O(1)	0.0	0.5	0.093	1
O(2)	0.0	0.0	0.1842	1
O(3)	0.0	0.0	0.0	1

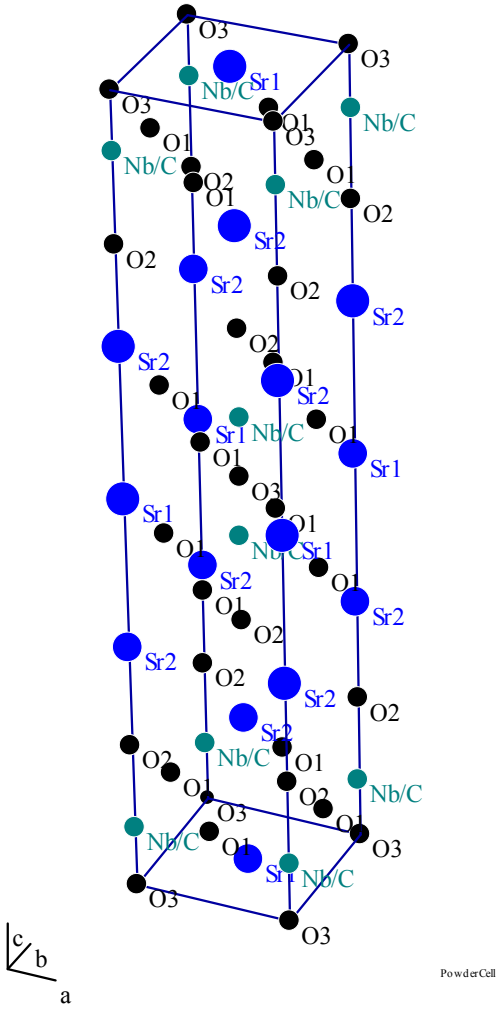

Figure 3. Unit Cell structure of Sr_3NbCrO_7

3.2 Electric Transport Properties

The log of specific resistance (log ρ) versus temperature (**K**) values are plotted in the Figure 2. The negative temperature co-efficient of resistivity and the values of the specific resistance show that the phase is semiconductor in nature. The plot of log ρ versus $T^{-1/4}$ (Figure 2, inset) is linear, except at very low temperatures, which suggests that 3D hopping mechanism governs the electronic conduction in this phase (Helmolt, 1993; Sharma, 1999). The phenomenon is attributed to superexchange coupling of electrons. There is deviation from this mechanism at temperatures below 100 K, indicating that the conditions of 3D hopping do not operate in this temperature region.

4. Conclusions

A new phase with the composition Sr_3NbCrO_7 has been synthesised by the standard ceramic method. On the basis of Lazy-Pulverix analysis of the X-ray diffraction data it is concluded that the phase crystallises in the RP-type (n = 2) structure with I4/mmm space group. The unit cell structure has been drawn. The study of electrical resistivity in the temperature range 10-300 K suggests that the compound is an electrical semiconductor and conduction above 100 K occurs through 3D hopping.

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