S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

Publications, Seminars and Conferences Attended

S.No	Date	Name of the Lecturer	Event in which participated	Institute which organized the event
1.	27-02-2023	Sri K Venkanna	National seminar	Andhra Loyala college
2.	22-02-2023	Sri K Venkanna	International seminar	Andhra Loyala college
3.	25-03-2023	Sri K Venkanna	National Conference	Vignan university
4.	03-03-2023	Sri K Venkanna	National Seminar	GDC(W), Srikakulam
5.	01-02-2020	Sri K Venkanna	National Conference	GDC(W), Srikakulam
6.	14-12-2022	Sri K Venkanna	National Science academia workshop	M R College, Vizianagaram
7.	19-12-2014	Sri P S Jaggarao	National Seminar	Dr V S K GDC
8.	05-02-2015	Sri P S Jaggarao	National Level Workshop	Department of nuclear physics, AU
9.	06-07-2015	Sri P S Jaggarao	UGC Workshop	Dr V S K GDC
10	10-10-2015	Sri P S Jaggarao	AP GCGTA Workshop	Andhra university
11	04-08-1992	Sri P S Jaggarao	Dielectric and Resistive properties of lanthanum doped Ba $Cu_{1/3}$ $Ta_{2/3}$ O_3	Indian journal of pure and applied physics
12	10-04-1994	Sri P S Jaggarao	Dielectric and conductivity properties of lanthanum modified strontium copper niobate	Journal of material science letters
13.	30-06-2021	Sri B Nageswara Rao	https://doi.org/10.1016/j.matpr.2021.06.301	Materials Today
14.	12-07-2021	Sri B Nageswara Rao	https://doi.org/10.1016/j.matpr.2021.07.122	Materials Today

Head of the Department
Department of Physics
S.G.A. Govt. Degree College
Yellamanchili-531055
ANAKAPALLI District

Principal
S.G.A. Govt. Degree College
Yellamanchili-531 055
Anakapalli District. (A.P.)

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

Sri K Venkanna , Lecturer in Physics Presented Paper in “National seminar” held at Andhra Loyala college, organized by department of Physics Vijayawada dated: 27-02-2023.

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

National Conference on

Recent Trends in Smart Materials and Applications

NCRTSMA – 2023

on 27th & 28th February 2023

Organized by

DEPARTMENT OF PHYSICS

ANDHRA LOYOLA COLLEGE (AUTONOMOUS), VIJAYAWADA-8

IN COLLABORATION WITH

INDIAN ASSOCIATION OF PHYSICS TEACHERS (IAPT)

CERTIFICATE

This is to certify that ~~Prof.~~ /~~Dr.~~ /Mr. /~~Ms.~~ K. Venkanna

of SGA GDC, Yellamanchi University / College / Organisation has presented a Paper / participated / delivered an Invited Talk in the National Conference on 'Recent Trends in Smart Materials and Applications' NCRTSMA-2023 held at Andhra Loyola College (Autonomous), Vijayawada, on 27th and 28th February 2023.

Title of the Paper / Invited Talk: first principle studies on novel CuCrMnAl quaternary Heusler alloy for thermoelectric applications

Dr. Ch. Srinivasa Rao, Organising Secretary

Dr. T. Srikumar, Convener

Sri. P. Srinivasa Sastry, Head, Dept of Physics

Fr. Dr. G.A.P. Kishore, S.J., Principal

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

Sri K Venkanna , Lecturer in Physics Presented Paper in “International seminar” held at Andhra Loyala college, organized by Department of Electronics, Vijayawada dated: 22-02-2023.

Proceedings of ICESET – 2023

First Principle Studies on Novel Ru_2TiMn Heusler Alloy for Thermoelectric Properties

Karumuri Venkanna[1*], Ch Prashanth[1], Dr P Rambabu[2] and Dr J Krishnamurthy[1]
[1]Department of Physics, School of Sciences, National Institute of Technology, Andhra Pradesh, India
*Department of Physics, SGA Government Degree College, Yellamanchili, Andhra Prasesh, India.
[2]Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur, India.
**Corresponding author: karumuri.venkanna@gmail.com*

Abstract
We report the structural stability, electronic, magnetic, thermodynamic and thermoelectric properties of novel Ru_2TiMn Heusler alloys using first principle studies based on density functional theory (DFT). With the reports of martensitic phase transformation from cubic to tetragonal structural phase in this series of samples, Ru_2TiMn alloy is found to be stable in tetragonal phase at c/a ratio 0.92, fitted with Birch-Murnaghan equation of state. The observed negative formation energy making it the alloy is physically synthesizable. Further non-zero density of states (DOS) in both spin-up and spin-down channels near to Fermi energy with no energy gap proves its metallic character. Absence of imaginary frequencies in phonon dispersion spectrum confirms the dynamical stability of the compound. Integration of DOS indicates the magnetic moment of a compound and estimated magnetic moment is $3.025\mu_B$. It is observed that major contribution for magnetic moment is coming from Mn atoms. The calculations of different thermodynamic properties such as entropy, free energy and specific heat at constant volume (C_V) of Ru_2TiMn alloy are performed by varying the temperature from 0 K to 2000 K. To estimate thermoelectric properties of Ru_2TiMn alloy as a function of chemical potential, we have used the BoltzTrap code based on the Boltzmann model via Boltzmann transport equation. The figure of merit (zT) is very large as calculated thermal conductivity is low and Seebeck coefficient is large value of about 100 μV/K, shows that our Ru_2TiMn alloy can be used for powerful thermoelectric devices.

Key words: Heusler alloy, martensitic phase, thermoelectric materials, dynamical stability

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

ANDHRA LOYOLA COLLEGE

(AUTONOMOUS)

Vijayawada - 520 008, Andhra Pradesh, India

Accredited at A+ Grade with CGPA of 3.66 in III Cycle by NAAC

All India 94th Rank NIRF 2022, MoE, Govt. of India, Selected under Star College Scheme by DST - FIST Govt. of India

SSRN

Proceedings Hosted on SSRN.com

ELSEVIER

Certificate of Presentation

International Conference on

Emerging Trends in Science, Engineering and Technology (ICESET-2023)

This is to certify that ~~Dr.~~ / Mr. / ~~Ms.~~ KARUMURI VENKANNA

has participated / presented a paper on First Principle Studies on Novel Ru_2TiMn Heusler Alloy for Thermoelectric Properties in the Three Day 'International Conference on Emerging Trends in Science, Engineering and Technology' (ICESET-2023) conducted by the department of Electronics at Andhra Loyola College in association with SOLETE (Society for Learning Technologies), 20 - 22 February, 2023.

Mr. N. Lakshmikanth
Organising Committee Member

Dr. B. Balaji Bhanu
Organising Secretary

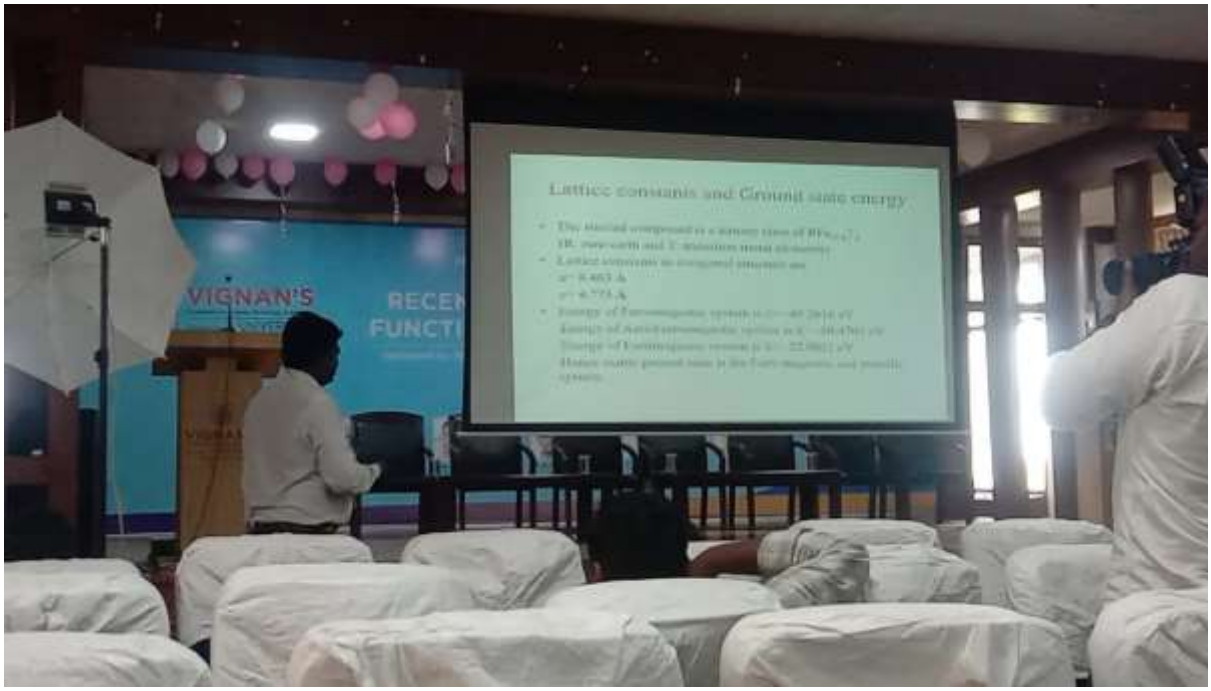
Rev. Fr. Dr. G. A. P. Kishore, S. J.
Principal and Chairman

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS



Sri K Venkanna , Lecturer in Physics Presented Paper in “National Conference” held at Vignan university, organized by Department of Physics (BS), Guntur dated: 25-03-2023.

First principle studies on Iron rich permanent magnetic compound $YFe_{10}Cr_2$

Karumuri Venkanna[1,2], Ch Prashanth[1], Dr P Rambabu[3] and Dr J Krishnamurthy[1]

[1]*Department of Physics, School of Sciences, National Institute of Technology, Andhra Pradesh, India*
[2]*Department of Physics, SGA Government Degree College, Yellamanchili, Andhra Pradesh, India.*
[3]*Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur, India.*

**Corresponding author: karumuri.venkanna@gmail.com*

Abstract

We report on electrical, magnetic, thermoelectric and thermodynamic properties of iron rich, permanent magnetic compound $YFe_{10}Cr_2$ using first principles calculations. The studied compound is a ternary class of $RFe_{12-x}T_x$[1] (R: rare-earth and T: transition metal elements) family. For all the theoretical calculations, we have taken practically reported lattice constants in tetragonal structure as a= 8.463 Å and c= 4.775 Å. From the density functional theory (DFT) studies, it is proved that the ground state of the compound is ferrimagnetic with metallic states through the structural optimization and spin density of states plots. The calculated magnetic moment of the compound is found to ~16.7μ_B is matches well to the experimental value of 16.7μ_B[2,3]. It is observed from the spin density of states that the major contribution for the magnetic moment is from Fe-3d orbital states. The absence of negative phonons in a phonon dispersion spectrum suggest that the studied compound is dynamically stable. We have calculated exchange interaction constants (J_{ij}) using Green's function formalism as implemented in SPRKKR package. Using these interaction constants, it is estimated magnetic transition temperature as T_C = 623 *K*, using mean field approximation which is close to the experimental value T_C = 510 *K*. Further, to characterize the thermoelectric property, it is estimated the figure of merits are 0.4 % and 1.1 % at 1000 *K* and 2000 *K*, respectively.

Keywords

Iron rich permanent magnetic, Mean field approximation, Exchange interactions, Magnetic and thermoelectric properties.

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

Sri K Venkanna , Lecturer in Physics Attended a “National Seminar” held at GDC(W), Srikakulam dated: 03-03-2023.

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

S.G.A.GOVERNMENT DEGREE COLLEGE

(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

UGC Sponsored National Conference

FCHIARF-2020

CERTIFICATE

This is to certify that Prof./Dr./Mr./ Ms. K. Venkanna - GDC(M) SKLM has participated/presented a paper on Emerging Global Scenario of Higher Education in Two Day National conference on " Future Challenges of Higher Educaiton Institutes in Assessment Accreditation and Ranking Framework Methodologies" (FCHIARF-2020) organized by IQAC, Governement College for Women(A), Srikakulam on 31st January & 1st February 2020.

Convener
FCHIARF-2020

Principal
GDCW(A)-Srikakulam

Sri K Venkanna , Lecturer in Physics Attended a “National Conference” held at GDC(W), Srikakulam dated: 01-02-2020.

S.G.A.GOVERNMENT DEGREE COLLEGE

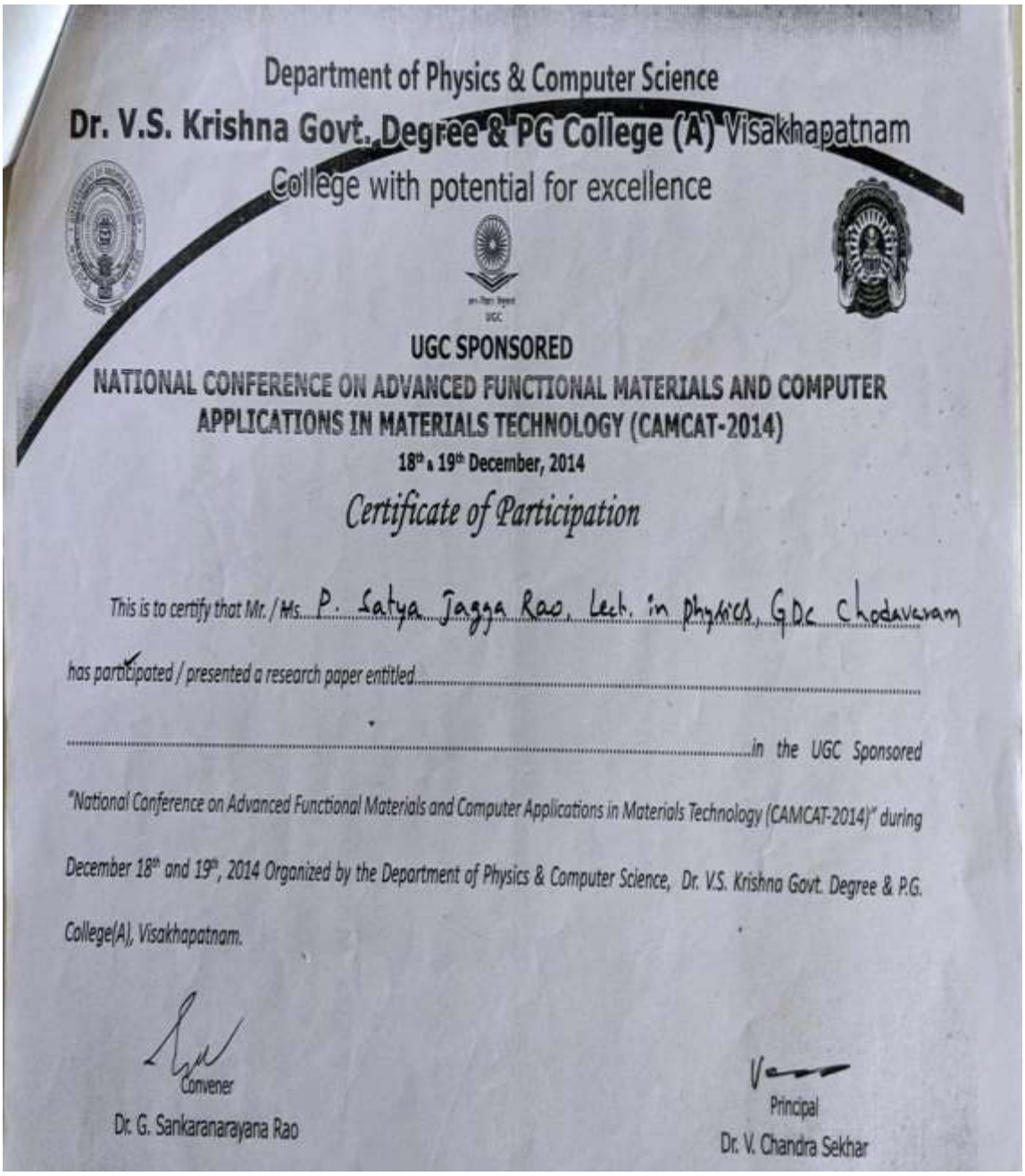
(Re-accredited by NAAC with 'A' Grade, Affiliated to Andhra University)

YELLAMANCHILI - 531055, ANDHRA PRADESH

DEPARTMENT OF PHYSICS

Sri K Venkanna , Lecturer in Physics Attended a “National Science academia workshop” held at M R College, Vizianagaram dated: 14-12-2022.

DEPARTMENT OF PHYSICS



Department of Physics & Computer Science

Dr. V.S. Krishna Govt. Degree & PG College (A) Visakhapatnam

College with potential for excellence

UGC SPONSORED

NATIONAL CONFERENCE ON ADVANCED FUNCTIONAL MATERIALS AND COMPUTER APPLICATIONS IN MATERIALS TECHNOLOGY (CAMCAT-2014)

18th & 19th December, 2014

Certificate of Participation

This is to certify that Mr. / Ms. P. Satya Jagga Rao Lect. in Physics, GDC Chodavaram

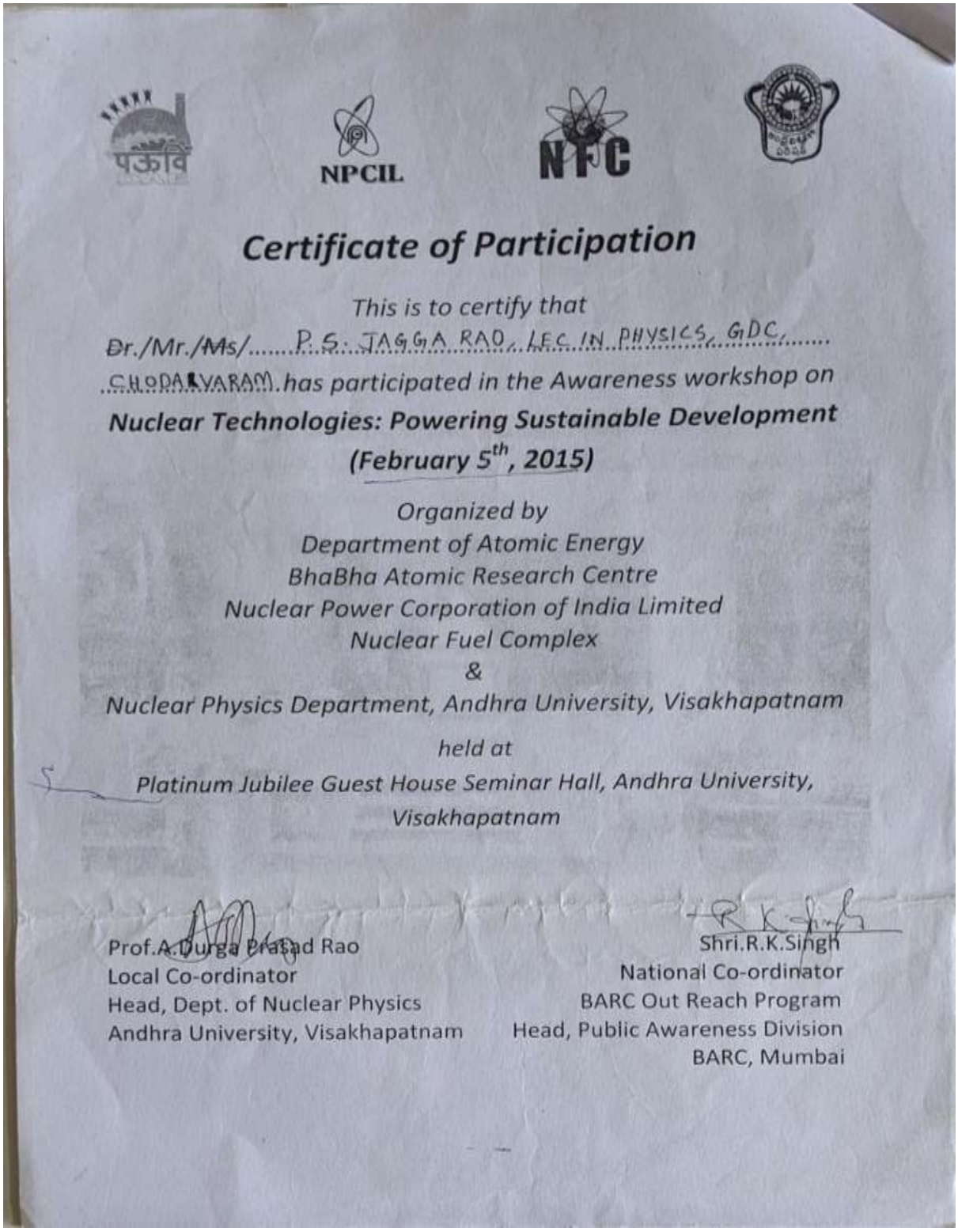
has participated / presented a research paper entitled.....

.....in the UGC Sponsored "National Conference on Advanced Functional Materials and Computer Applications in Materials Technology (CAMCAT-2014)" during December 18th and 19th, 2014 Organized by the Department of Physics & Computer Science, Dr. V.S. Krishna Govt. Degree & P.G. College(A), Visakhapatnam.

Convener
Dr. G. Sankaranarayana Rao

Principal
Dr. V. Chandra Sekhar

Sri P S Jaggarao, Lecturer in Physics participated in “National Seminar” held at Dr V S K GDC, Visakhapatnam dated: 19-12-2014



NPCIL

NFC

Certificate of Participation

This is to certify that

Dr./Mr./Ms/..... P.S. JAGGA RAO, LEC IN PHYSICS, GDC, ...
CHODAVARAM. has participated in the Awareness workshop on

Nuclear Technologies: Powering Sustainable Development

(February 5th, 2015)

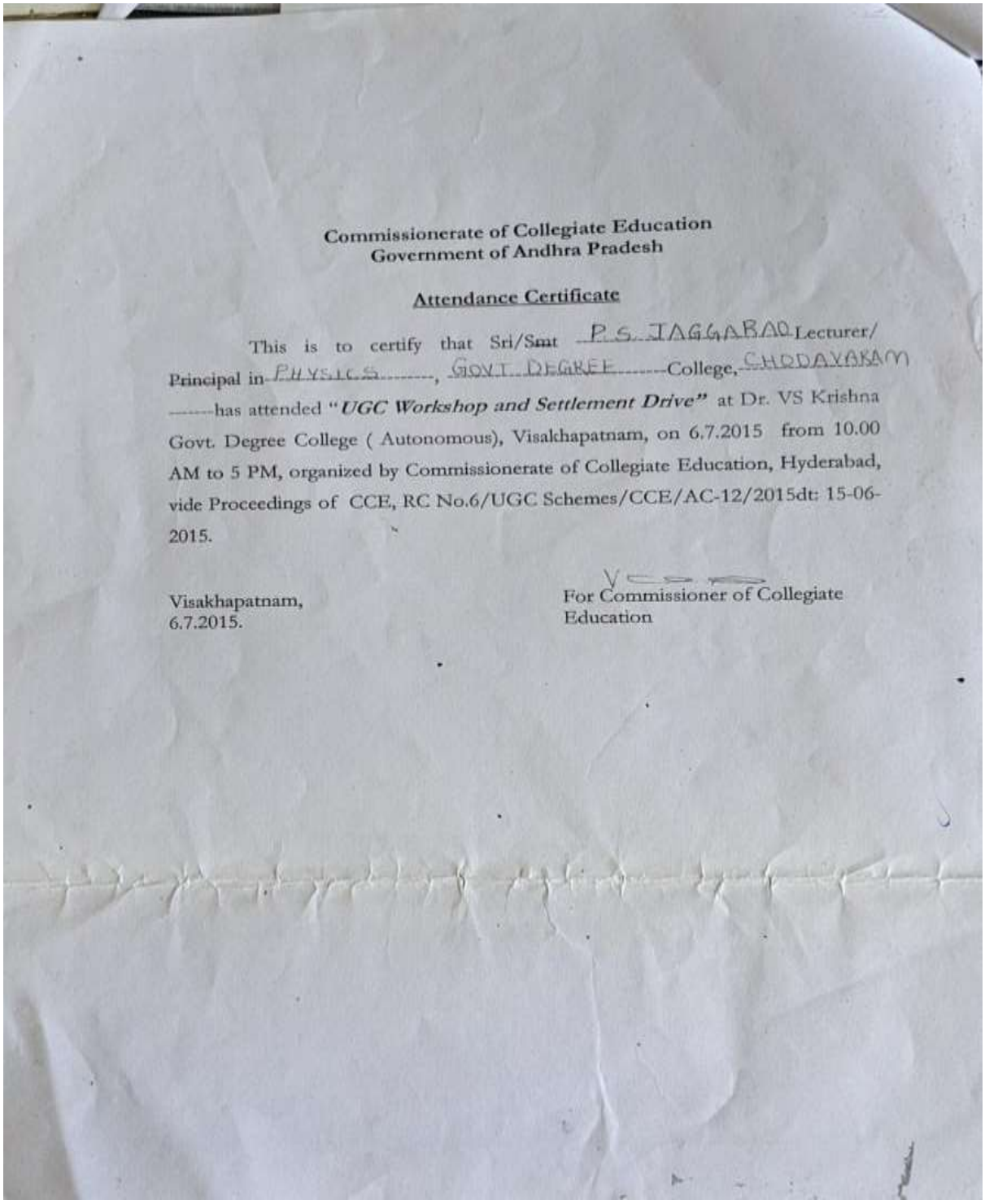
Organized by
Department of Atomic Energy
BhaBha Atomic Research Centre
Nuclear Power Corporation of India Limited
Nuclear Fuel Complex
&
Nuclear Physics Department, Andhra University, Visakhapatnam

held at
Platinum Jubilee Guest House Seminar Hall, Andhra University, Visakhapatnam

Prof.A.Durga Prasad Rao
Local Co-ordinator
Head, Dept. of Nuclear Physics
Andhra University, Visakhapatnam

Shri.R.K.Singh
National Co-ordinator
BARC Out Reach Program
Head, Public Awareness Division
BARC, Mumbai

Sri P S Jaggarao, Lecturer in Physics participated in “National Level Workshop” held at Andhra university, Organized by Department of Nuclear Physics, Visakhapatnam dated: 05-02-2015.



Commissionerate of Collegiate Education
Government of Andhra Pradesh

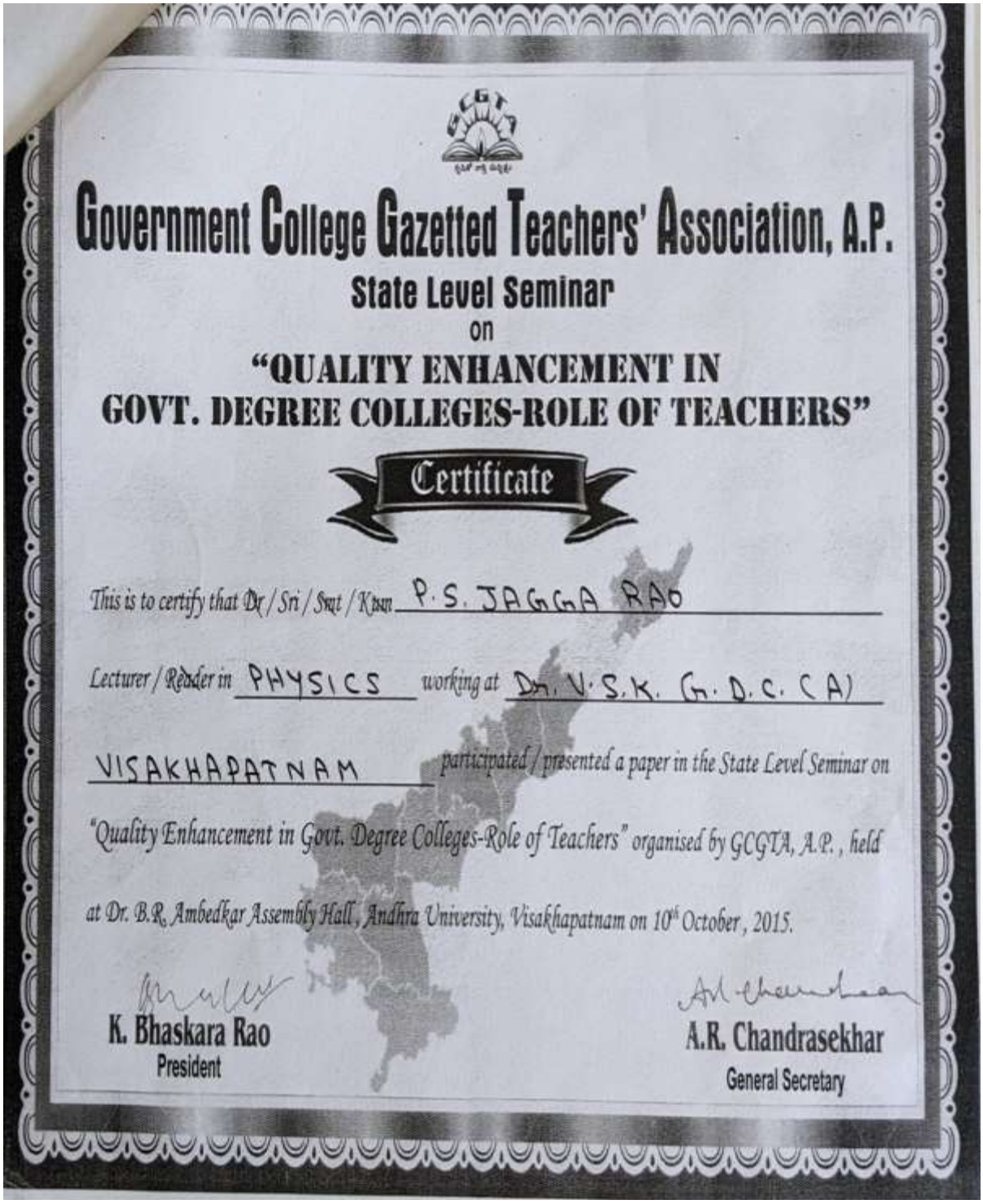
Attendance Certificate

This is to certify that Sri/Smt P.S. JAGGARAO Lecturer/ Principal in PHYSICS, GOVT. DEGREE College, CHODAVARAM has attended "*UGC Workshop and Settlement Drive*" at Dr. VS Krishna Govt. Degree College (Autonomous), Visakhapatnam, on 6.7.2015 from 10.00 AM to 5 PM, organized by Commissionerate of Collegiate Education, Hyderabad, vide Proceedings of CCE, RC No.6/UGC Schemes/CCE/AC-12/2015dt: 15-06-2015.

Visakhapatnam,
6.7.2015.

For Commissioner of Collegiate Education

Sri P S Jaggarao, Lecturer in Physics participated in "UGC Workshop" held at Dr V S K Government degree college, Visakhapatnam dated: 06-07-2015.



Government College Gazetted Teachers' Association, A.P.

State Level Seminar

on

"QUALITY ENHANCEMENT IN GOVT. DEGREE COLLEGES-ROLE OF TEACHERS"

Certificate

This is to certify that Dr / Sri / Smt / Kum P. S. JAGGA RAO

Lecturer / Reader in PHYSICS working at Dr. V. S. K. G. D. C. (A) VISAKHAPATNAM participated / presented a paper in the State Level Seminar on "Quality Enhancement in Govt. Degree Colleges-Role of Teachers" organised by GCGTA, A.P., held at Dr. B.R. Ambedkar Assembly Hall, Andhra University, Visakhapatnam on 10th October, 2015.

K. Bhaskara Rao
President

A.R. Chandrasekhar
General Secretary

Sri P S Jaggarao, Lecturer in Physics participated in "AP GCGTA Workshop" held at Andhra university, Visakhapatnam dated: 10-10-2015.

Full length papers presented by Sri P S Jaggarao-Paper-1

Indian Journal of Pure & Applied Physics
Vol. 31, January 1993, pp. 43-47

Dielectric and resistivity properties of lanthanum doped $Ba(Cu_{1/3}Ta_{2/3})O_3$ and $Ba(Cu_{1/3}Nb_{2/3})O_3$

K Sambasiva Rao, P S Jagga Rao & K Rama Rao
Department of Physics, Andhra University, Visakhapatnam 530 003
and
A V Prasada Rao, A Isaac Robin & R P Tandon*
School of Chemistry, Andhra University, Visakhapatnam 530 003

Received 27 April 1992; revised received 4 August 1992

A series of samples of the systems $Ba_{1-2x}La_{2x}(Cu_{1/3}Ta_{2/3})O_3$ and $Ba_{1-3x}La_{2x}(Cu_{1/3}Nb_{2/3})O_3$ where $x = 0.000, 0.025, 0.050, 0.075$ and 0.100 have been prepared by the usual ceramic technique. X-ray diffraction data indicated that they are of tetragonal symmetry. Dielectric properties of $Ba(Cu_{1/3}Ta_{2/3})O_3$ (BCT) revealed a diffused phase transition. Curie temperatures obtained from dielectric measurements were compared with differential thermal analysis studies. Doping of lanthanum in BCT and $Ba(Cu_{1/3}Nb_{2/3})O_3$ (BCN) decreased the curie temperatures of BCT and BCN. DC resistivity studies in modified and unmodified BCT and BCN indicated a positive temperature coefficient (PTC) behaviour.

1 Introduction

The discovery of barium titanate as ferroelectric material stimulated a further search and creation of perovskite-type and oxygen-octahedra ferroelectrics. Time has shown barium titanate appears as "a parent" of a huge family of ferro and antiferroelectrics with perovskite-type crystal structure. Perovskite-type ferroelectrics are found to be outstanding materials in view of their device applications, e.g. $BaTiO_3$, lead zirconate titanate (PZT). Some copper containing perovskites $Ba(Cu_{1/3}Ta_{2/3})O_3$ and $Ba(Cu_{1/3}Nb_{2/3})O_3$ have been synthesised by Kapyshev *et al.*[1], Blasse[2] and Venevtsev[3], respectively. Also, they were reported to be ferroelectric having high curie temperatures of 470 and 380°C respectively, with tetragonal symmetry. Literature survey revealed that no further experimental investigations have been made on these materials. Systematic dielectric and resistivity studies have been made on these materials for the first time by the present authors.

Present paper describes preparation, dielectric and resistivity studies on lanthanum modified barium copper tantalate (BCT) and barium copper niobate (BCN) systems.

2 Material Preparation

The constituent raw materials, $BaCO_3$, CuO, Ta_2O_5, Nb_2O_5 and La_2O_3 of reagent grade have been weighed in required proportion to give the following compositions:

1.	$Ba(Cu_{1/3}Ta_{2/3})O_3$	BCT
2.	$Ba_{0.925}La_{0.05}(Cu_{1/3}Ta_{2/3})O_3$	0.05 La-BCT
3.	$Ba_{0.850}La_{0.10}(Cu_{1/3}Ta_{2/3})O_3$	0.10 La-BCT
4.	$Ba_{0.775}La_{0.15}(Cu_{1/3}Ta_{2/3})O_3$	0.15 La-BCT
5.	$Ba_{0.700}La_{0.20}(Cu_{1/3}Ta_{2/3})O_3$	0.20 La-BCT
6.	$Ba(Cu_{1/3}Nb_{2/3})O_3$	BCN
7.	$Ba_{0.925}La_{0.05}(Cu_{1/3}Nb_{2/3})O_3$	0.05 La-BCN
8.	$Ba_{0.850}La_{0.10}(Cu_{1/3}Nb_{2/3})O_3$	0.10 La-BCN
9.	$Ba_{0.775}La_{0.15}(Cu_{1/3}Nb_{2/3})O_3$	0.15 La-BCN
10.	$Ba_{0.700}La_{0.20}(Cu_{1/3}Nb_{2/3})O_3$	0.20 La-BCN

Ceramic samples have been prepared by the usual sintering technique. Actual procedure adopted for the preparation of materials is depicted in Fig. 1.

3 Experimental Techniques

The dielectric measurements were carried out at 1 kHz using DIGITAL LCR METER TYPE VLCR 6. The temperature is monitored by a Cr-Al thermocouple. The dc resistivity was measured by two-probe method using Keithley Model 614 Electrometer.

Powder X-ray diffraction (XRD) patterns of these materials have been obtained with the diffractometer at RSIC, Nagpur University, Nagpur.

*National Physical Laboratory, New Delhi 110 012

Weighing ($BaCO_3$, CuO, Ta_2O_5, Nb_2O_5, La_2O_3)

Mixing (in alcohol, 4 hr)

Drying

Calcination (950°C / 4 hr twice)

Mixing with binder (5% PVA)

Pressing pellets (dia. = 15 mm, t = 1.1 mm for BCT)
(dia. = 14 mm, t = 1.7 mm for BCN)

Binder burn out (450°C / 1 hr)

Firing (1200°C / 4 hr)

Polishing (3 μm Al_2O_3 powder)

Electroding (air dry silver paste cured at 1400°C / 1 hr)

Fig. 1 – Procedure for sample preparation

4 Results and Discussion

4.1 *Dielectric properties*

The X-ray diffraction studies in the above materials, labelled 1-10, showed single-phase final product with tetragonal symmetry throughout the unmodified and modified compositions. The lattice parameters a and c as computed from the XRD data are shown in Table 1, which are in good agreement with the values reported in literature for BCT and BCN[3].

Dielectric constant as a function of temperature has been measured at 1 kHz in the temeprature range between room temperature and 450°C. For dielectric and resistivity measurements silver coated disc samples having dimensions around 1.1 mm thickness and 15 mm diameter of BCT, 14 mm diameter and 1.7 mm thickness of BCN cured at 400°C for one hour are used.

Fig. 2 illustrates the variation of dielectric constant with temperature for BCT and lanthanum modified BCT. A maximum dielectric constant of 179 was obtained for BCT at 319°C indicating its curie temperature. The observed curie temperature is much below the value of 470°C reported by Venevtsev[3].

Differential thermal analysis studies have been made on BCT and the curie temperature is obtained from the peak temperature of exotherm (T_D). The sample BCT exhibited 300.1°C as the curie temperature. However, the curie temperature obtained from the dielectric measurement is 319°C. A typical DTA trace has been shown in Fig. 3. Similarly, in the case of 0.05 La-BCT the curie temperature obtained from the dielectric measurement is 270°C, while the value obtained from DTA is 297.3°C.

Table 1 – Lattice parameters of La-modified BCT and BCN

S.No.	Composition	a(Å)	c(Å)
1.	BCN	4.0804	4.1397
2.	0.05 La-BCN	4.0424	4.1853
3.	0.10 La-BCN	4.0611	4.1639
4.	0.15 La-BCN	4.0756	4.1695
5.	0.20 La-BCN	4.0533	4.1307
6.	BCT	4.025	4.2359
7.	0.05 La-BCT	4.0156	4.2147
8.	0.10 La-BCT	4.0416	4.1618
9.	0.15 La-BCT	4.0260	4.1980
10.	0.20 La-BCT	4.0350	4.1800

As the concentration of lanthanum in BCT increases, the curie temperature decreases from 319 to 199°C and the peak dielectric constant increases with lanthanum content except for 0.20 La-BCT (Fig. 2). Similar behaviour has been ob-

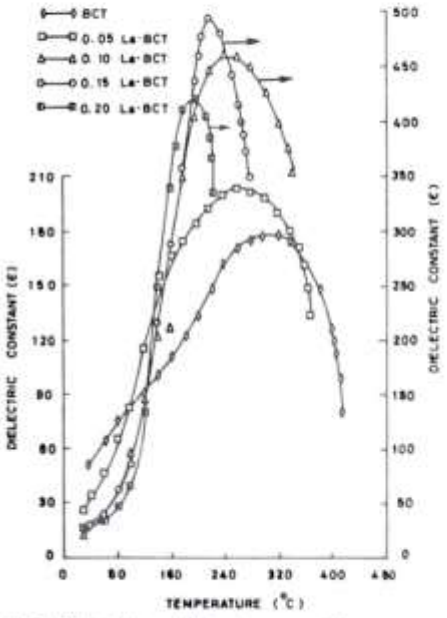


Fig. 2 – The variation of dielectric constant with temeprature for modified and unmodified BCT

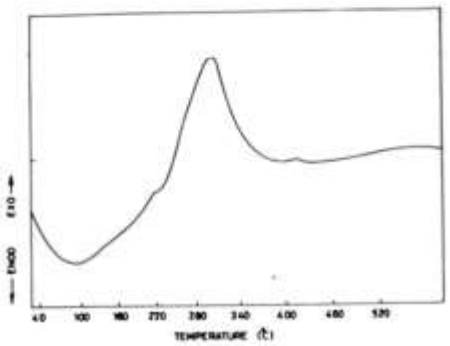


Fig. 3 – DTA trace of BCT

served in different perovskite systems, for example lead zinc niobate-lead titanate-barium titanate[4] system, barium titanate zirconate[5] and lanthanum doped lead titanate systems[6].

Further, it is evident that a diffused phase transition (DPT) is observed in the compositions from 1 to 5. In para region i.e., above T_c and equation[7] of the following form has been obeyed:

$$\frac{1}{\varepsilon} = \frac{1}{\varepsilon_{T_c}} + \frac{(T - T_c)^2}{2\varepsilon_{T_c}\delta^2}$$

where ε_{T_c} and δ are maximum dielectric constant and intensity of diffusivity, respectively. The δ values for compositions 1-5 were computed to be 70, 73, 73.5, 52 and 40 K respectively, which indicate a decrease in diffusivity with increase in lanthanum concentration in BCT.

The dielectric constant as a function of temperature in BCN and lanthanum doped BCN has been shown in Fig. 4. It is clear that at 400°C a maximum dielectric constant is observed in unmodified barium copper niobate. This transition temperature is very much nearer to the value of 380°C reported on BCN by Venevtsev[3]. The transition temperatures noted from the DTA traces in case of BCN and 0.05 La-BCN are 426.3 and 289°C, respectively. Though the transition temperatures T_c and T_D for both the systems BCT and BCN reflect the same trend, they do not coincide exactly. The reason for this discrepancy is under investigation.

It can be noticed from Fig. 4 that lanthanum modification in BCN facilitated a decrease in curie temperature from 400 to 193°C and an increase in peak dielectric constant. Similar behaviour has been observed in different perovskite

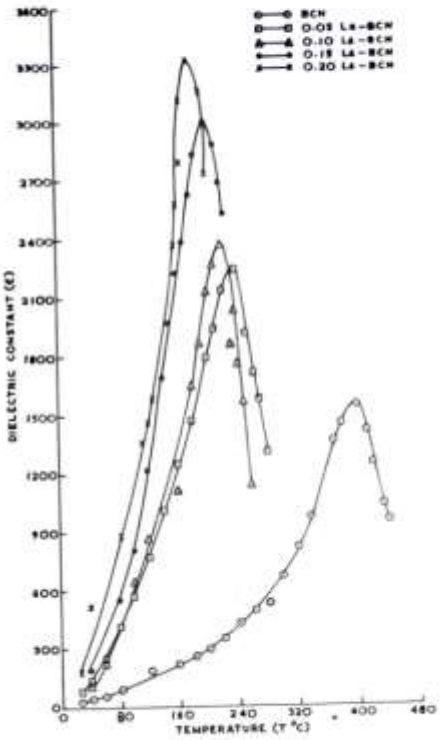


Fig. 4 – The variation of dielectric constant with temperature for modified and unmodified BCN

systems like barium strontium titanate and barium calcium titanate[8]. Curie-Weiss law has been obeyed in the para region of the compositions, 6 to 10, and the curie constants have been computed for all the compositions. Curie constant of the order of 10^5 K has been observed in all the five materials.

In both the systems BCT and BCN, the decrease in curie temperature with increase of lanthanum may be attributed to the decrease in polarizability of A-site cations (for example $\alpha(Ba^{2+}) = 1.55 \times 10^{-24}$ cm^3, while $\alpha(La^{3+}) = 1.04 \times 10^{-24}$ cm^3). Under these circumstances the dipoles at the large cation site interact weakly with those at the Ta^{5+} and Nb^{5+} sites in BCT and BCN, respectively, resulting in a decrease of T_c. Similar phenomenon has been reported for the systems $(Na_{1/2}La_{1/2})Pb_{1-x}TiO_3$ and $(Li_{1/3}La_{2/3})Pb_{1-x}TiO_3$ [Refs 9, 10].

Table 2 – Dielectric, DTA and resistivity data of lanthanum doped BCT and BCN

Composition	Curie temp.		ϵ_{RT}	ϵ_{T_c}	Δ, °C	$\rho_{RT} \times 10^8$ Ω-cm	$\rho_T \times 10^8$ Ω-cm	T, °C	E_a (eV)	
	T_c, °C	T_D, °C							+ ve	− ve
BCT	319	300.1	42	779	70.0	4.80	11.90	75	0.11	0.11
0.05 La-BCT	270	297.3	28	203	73.0	2.30	7.13	60	0.17	0.12
0.10 La-BCT	244	–	23	462	73.5	0.16	3.97	55	0.21	0.12
0.15 La-BCT	221	–	23	493	52.0	0.47	1.76	55	0.27	0.26
0.20 La-BCT	199	–	26	423	40.0	0.25	0.88	55	0.15	0.14
					$C \times 10^5$ K					
BCN	400	426.3	42	1531	0.8	0.36	5.02	68	0.12	0.11
0.05 La-BCN	242	289.8	48	2279	1.5	0.19	0.38	60	0.21	0.21
0.10 La-BCN	226	–	52	2357	1.2	0.21	0.29	50	0.04	0.05
0.15 La-BCN	216	–	57	3167	1.8	0.18	0.23	50	0.02	0.06
0.20 La-BCN	193	–	56	3317	32.0	0.14	0.18	50	0.08	0.07

The room temperature and peak temperature dielectric constants, ϵ_{RT}, ϵ_{Tc} respectively, curie temperatures obtained from both dielectric measurements (T_c) and DTA (T_D), the intensity of diffusivity (δ) and curie constants (C) for pure and La-modified BCT and BCN samples are given in Table 2.

4.2 DC Resistivity Properties

Variation of dc resistivity with temperature in unmodified and modified BCT and BCN has been studied in the temperature range from room temperature to 230°C by applying a small voltage of 10 V. The dc resistivity versus temperature for the two systems is depicted in Figs 5 and 6.

It is obvious from these figures that an anomalous behaviour is evident in both the systems. That is, there is an initial increase of resistivity to a maximum at a particular temperature, followed by a gradual decrease. This type of positive temperature coefficient (PTC) anomalous behaviour in ferroelectrics can be explained by Heywang[11] model when the temperature corresponding to the maximum resistivity coincides with their respective T_c values. But, in the present study the temperatures corresponding to the maximum resistivity are well below their respective T_c values in unmodified and modified BCT as well as in BCN. One of the reasons for this behaviour may be due to the vacancy of barium sites in BCT and BCN as a result of aliovalent lanthanum doping in place of Ba^{2+}. However, this type of behaviour

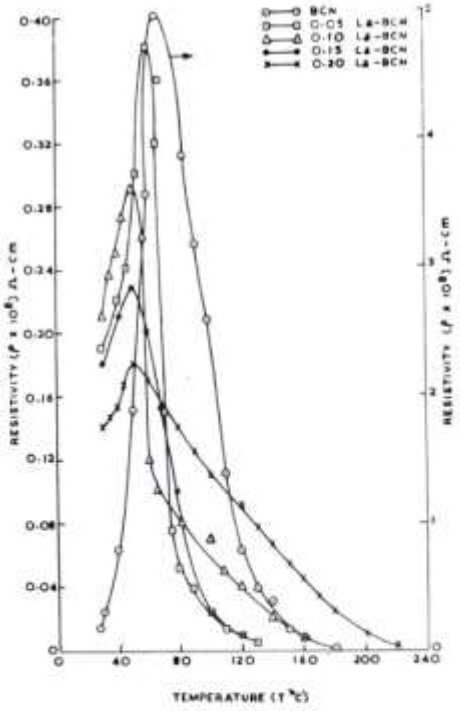


Fig. 5 – DC resistivity versus temperature for modified and unmodified BCT

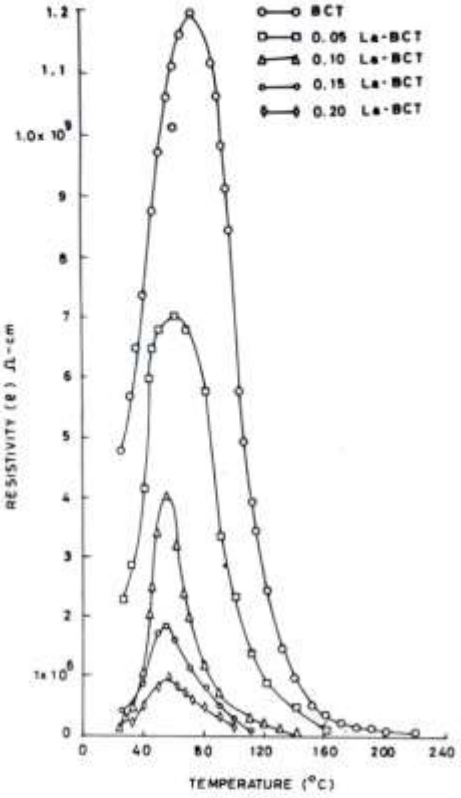


Fig. 6 – DC resistivity versus temperature for modified and unmodified BCN

has also been observed in other systems such as Dy-doped barium sodium niobate ceramics[12]. The room temperature resistivity (ρ_{RT}) and peak resistivity (ρ_T) are found to decrease with the increase in lanthanum concentration in BCT. All these curves show resistivity maximum at a certain range of temperature, which is a property of a semiconducting material and doping of lanthanum either in BCT or in BCN did not alter this behaviour.

The variation of resistivity (ρ) with temperature (T) in BCT and BCN obeys the equation.

$$\rho = \rho_0 \exp(E_a/kT)$$

where E_a is the activation energy, k is the Boltzmann constant and ρ_0 is a constant. The values of E_a in both the regions of all the compositions have been computed from the above equation and tabulated in Table 2, along with ρ_{RT}, ρ_T and temperature of maximum resistivity (T, °C).

5 Conclusions

In view of the above observations, it is concluded that, the systems BCT and BCN are monophasic and tetragonal. Substitution of lanthanum in BCT as well as in BCN to an extent of $x = 0.100$ in $Ba_{1-3x}La_{2x}(Cu_{1/3}Ta_{2/3})O_3$ and $Ba_{1-3x}La_{2x}(Cu_{1/3}Nb_{2/3})O_3$ did not alter the crystal structure. Nevertheless progressive addition of lanthanum caused a decrease in T_c with a simultaneous increase in peak dielectric constant. BCT and La-modified BCT samples exhibited diffused phase transition. Both the compositions of BCT and BCN showed resistivity maxima with a PTCR behaviour. Addition of lanthanum did not show any significant effect on the conductivity properties of BCT and BCN.

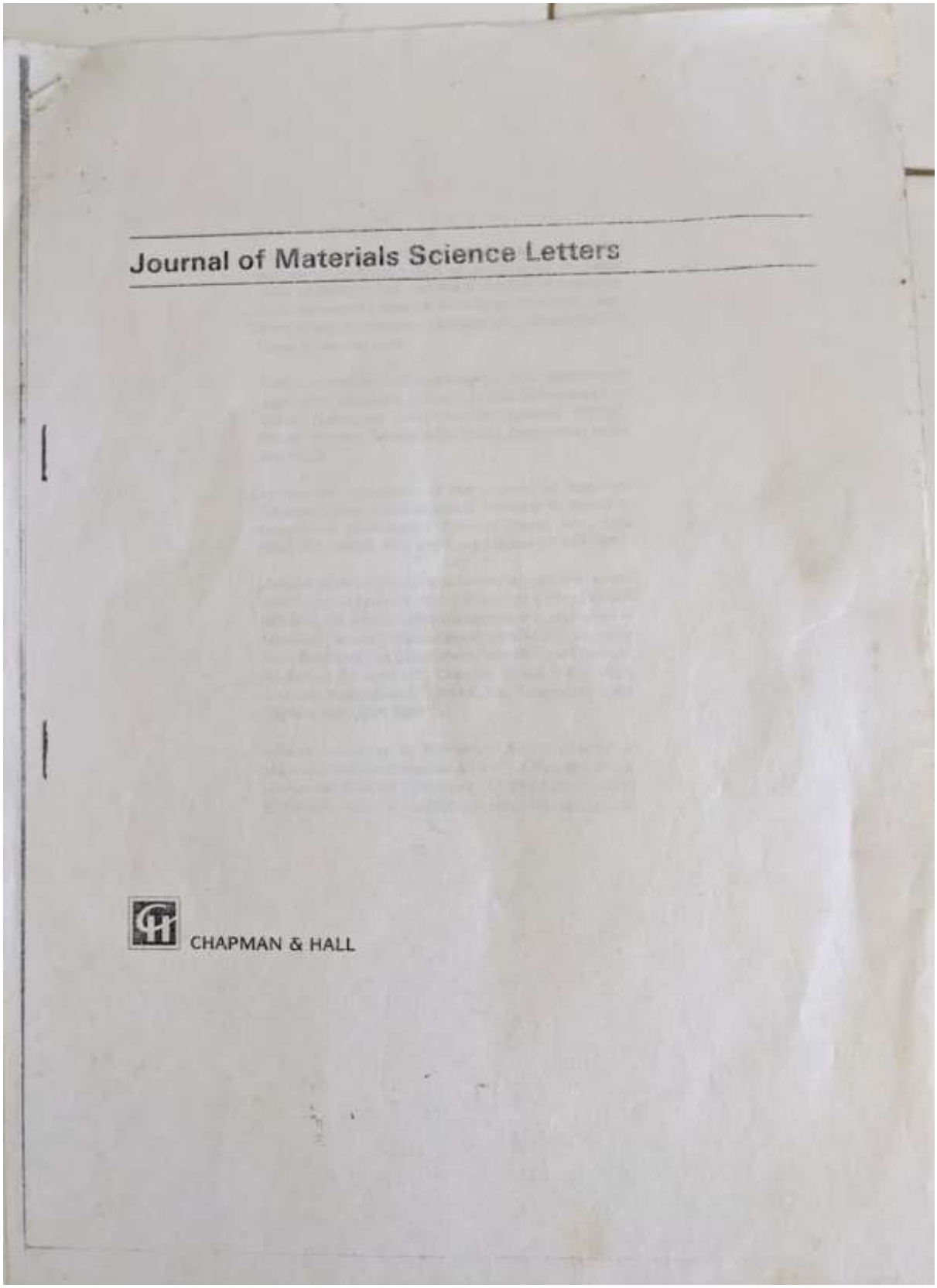
Acknowledgement

One of the authors (KSR) is grateful to CSIR, New Delhi, for their financial support.

References

1 Kapyshev A G, Ivanova V V & Venevtsev Yu N, *Dokl Akad Nauk SSSR*, 167 (1966) 56.
2 Blasse G, *J Inorg Nucl Chem*, 27 (1965) 393.
3 Venevtsev Yu N, *Mat Res Bull*, 6 (1971) 1085-96.
4 Halliyal A, Kumar U, Newnham R E & Cross L E, *J Am Ceram Soc*, 69 (1986) 119.
5 Hennings D, Schnell A & Simon G, *J Am Ceram Soc*, 65 (1982) 539.
6 Keizer K & Burggraaf A J, *Ferroelectrics (GB)*, 14 (1976) 671.
7 Uchino K & Nomura S, *Ferroelectrics Lett Sect. (GB)*, 44 (1982) 55.
8 Chavan S H & Kulkarni P G, *Ind J Phys*, 60A (1986) 124.
9 Sakata K, Masuda Y & Ohara G, *Rec Electr Commun Engg Conversazione*, 48 (1964) 135.
10 Vara Prasad A M, Shashimohan A L, Biswas A B & Chakrabarty D K, *Phys Status Sol (A)*, 44 (1977) 787.
11 Heywang W, *Solid State Elect.*, 3 (1961) 51; Angew Z, *Phys*, 16 (1963) 1.
12 Subba Rao P S V & Sambasiva Rao K, *Ferroelectrics (GB)*, 102 (1990) 183.

Full length papers presented by Sri P S Jaggarao-Paper-2



Journal of Materials Science Letters is an international publication reporting recent advances in all the major fields of investigation into the properties of materials. Short communications on metallurgy, ceramics, polymers, electrical materials, biomaterials, composites and fibres appear regularly.

Technical articles of full page length, or over, appearing in *Journal of Materials Science Letters* are indexed in *British Technology Index, Current Contents, INSPEC, Pascal, Science Citation Index (USA), Engineering Index* and *ASCA*.

Letters for submission to the Journal of Materials Science Letters should be sent to Professor W. Bonfield, Department of Materials Science, Queen Mary and Westfield College, Mile End Road, London E1 4NS, UK.

Journal of Materials Science Letters is published semi-monthly by Chapman & Hall, 2-6 Boundary Row, London SE1 8HN, UK, as a combined subscription with *Journal of Materials Science*. Subscription details are available from: Subscriptions Department, International Thomson Publishing Services Ltd., Cheriton House, North Way, Andover, Hampshire SP10 5BE, UK. Telephone: 0264 332424, Fax: 0264 333471.

Editorial enquiries to: Publisher's Editor, Journal of Materials Science, Chapman & Hall, 2-6 Boundary Row, London SE1 8HN, UK. Telephone: 071 865 0066; Fax: 071 522 9624; email: journal@chali.mhs.compuserve.com.

JOURNAL OF MATERIALS SCIENCE LETTERS 13 (1994) 253–255

Dielectric and conductivity properties of lanthanum-modified strontium copper niobate

K. SAMBASIVA RAO, P. S. JAGGA RAO, K. RAMA RAO
Solid State Physics Laboratories, Physics Department, Andhra University, Visakhapatnam 530 003, India

A. V. PRASADA RAO, A. I. ROBIN
School of Chemistry, Andhra University, Visakhapatnam 530 003, India

R. P. TANDON
National Physical Laboratory, New Delhi 110 012, India

A number of compounds with perovskite structure exhibit ferroelectricity. Barium titanate, one of the important ferroelectric materials for device applications [1], has a relatively low Curie temperature (T_c) of 120 °C. In order to alter the Curie point to higher or lower temperatures, solid solutions are usually formed by judicious selection of suitable substituents either in Ba or in Ti sites. For instance, modest amounts of Pb^{2+} in $BaTiO_3$ raise its T_c whereas Sr^{2+} for Ba or Zr for Ti lowers the T_c [2–4]. Investigations on the synthesis of new perovskite-type compounds led to the unravelling of many compositions [5–7], some of which, particularly copper-containing Perovskites [6], were found to exhibit higher Curie temperatures in the range 300–1200 °C. Since the ferroelectric phase transition is connected with the electron–phonon interaction which takes place in the presence of the Jahn–Teller pseudo-effect, this is very pronounced in compounds containing bivalent copper of $3d^9$ electron configuration. Strontium copper niobate [$Sr(Cu_{1/3}Nb_{2/3})O_3$ (SCN)] crystallizes in a tetragonal symmetry with lattice parameters $a = 0.3944$ nm and $c = 0.4074$ nm, and is also reported to be a ferroelectric material with Curie temperature of 390 °C [6]. No further studies on SCN have appeared in the literature. In this letter we report the synthesis, characterization and the effect of partial substitution of lanthanum on the dielectric and conductivity properties of SCN.

Samples of SCN and lanthanum-incorporated strontium copper niobate (La-SCN) were prepared by the usual ceramic method with $SrCO_3$, CuO, Nb_2O_5 and La_2O_3 of AR grade purity as starting materials. Stoichiometric quantities of these materials are taken to yield the compositions $(Sr_{1-x}La_{2x/3})(Cu_{1/3}Nb_{2/3})O_3$ with $x = 0.0$, 0.075, 0.150, 0.225 and 0.300. The physical mixtures were dry ground into fine powders and these were further mixed thoroughly in presence of alcohol to improve the homogeneity. The mixtures were calcined twice at 950 °C for 4 h. The calcined samples were pressed into pellets with 5% poly(vinyl acid) as binder using a pressure of 4.5 tonne $in.^{-2}$ (68 MPa). The pelletized samples were sintered at 1200 °C for 6 h. The phase identification was followed by X-ray diffraction (XRD) using Cu K_α radiation. The dielectric measurements were done at 1 kHz using a capacitance bridge, digital LCR meter (type VLCR6). D.c. resistivity measurements on these samples were performed by the two-probe method with a ECIL electrometer amplifier (type EA815) using a d.c. voltage of 10 V. Silver-coated pellets were used for the above studies.

From the XRD data, SCN and La-SCN samples were found to be monophasic and tetragonal in symmetry in accordance with earlier reports [6, 7]. The lattice parameters for these samples are given in Table I. As can be seen from the XRD data in Table I, substitution of La for Sr seems to promote the tetragonal distortion.

Fig. 1 shows the temperature (T) dependence of the dielectric constant (ε) of SCN and La-SCN samples. As can be seen, increased substitution of Sr^{2+} by La^{3+} resulted in a reduction of the Curie temperature, from 345 to 245 °C, with an increase in peak dielectric constant from 255 to 1439. Furthermore, higher polarization (α) of La might be responsible for the enhanced dielectric constant [$\alpha(Sr^{2+}) = 0.86$ and $\alpha(La^{3+} = 1.08)$]. Similar behaviour was reported for other systems [8] such as $Ba(Ti_{1-x}Zr_x)O_3$. Since the maximum value of ε at the Curie point T_c in an ideal ferroelectric crystal can be described by the Curie–Weiss law, $\varepsilon = C/(T - T_c)$ for $T > T_c$. The Curie constant (C) can be obtained from the temperature dependence of ε at $T > T_c$. The estimated Curie constants for these samples are given in Table II, together with the respective Curie temperatures, room-temperature dielectric constant (ε_{RT}) and peak dielectric constant (ε_{TC}).

Fig. 2 shows the variation of resistivity (ρ) with temperature for SCN and La-SCN. These samples show resistivity maxima at temperatures (ρ_T) which

TABLE I Lattice parameters of the SCN and La-SCN samples

Sample	a (nm)	c (nm)	c/a
$Sr(Cu_{1/3}Nb_{2/3})O_3$	0.392 63	0.411 81	1.046
$(Sr_{0.85}La_{0.10})(Cu_{1/3}Nb_{2/3})O_3$	0.392 85	0.412 28	1.049
$(Sr_{0.85}La_{0.10})(Cu_{1/3}Nb_{2/3})O_3$	0.385 39	0.420 58	1.091
$(Sr_{0.775}La_{0.15})(Cu_{1/3}Nb_{2/3})O_3$	0.386 29	0.423 15	1.095
$(Sr_{0.70}La_{0.20})(Cu_{1/3}Nb_{2/3})O_3$	0.381 06	0.420 25	1.102

0261-8028