- 1. Name: S. Jemima Balaselvi Juliana, M.Sc., Ph.D, PGDCA
- 2. Designation: Associate Professor in Chemistry
- 3. Institution: The American College, Madurai
- 4. Email: jemimabalaselvijuliana@americancollege.edu.in
- 5. Mobile: 9443976827
- 6. Area of Specialisation:

Teaching – Inorganic Chemistry (Solid State, Coordination) Research – Material Science, Instrumentation

- 7. Teaching Experience: 17 yrs
- 8. Research Experience: 21 yrs
- 9. International Publications: 8
- 10. Conference papers: 18
- 11. Program Organised: 11
- 12. M.Phil students guided: 3



A. GENERAL INFORMATION	Curriculum Vitae
a) Name	: S. Jemima Balaselvi Juliana
b) Address (Residential)	: 5, Periyar Street, Thiru Kannan Nagar Thirupalai, Madurai – 17
c) Designation	: Associate Professor in Chemistry The American College, Madurai
d) Date of Birth	: 24-11-1974
e) Area of specialization	: Inorganic Chemistry

### B. ACADEMIC QUALIFICATION

Exam Passed	<b>Board/University</b>	Subject/Year	Grade
High School	Board of Matriculation Examination, TN	1990	75% (I)
Higher Secondary	Board of Higher Secondary Examination, TN	Phy, Chem, Bio, Math- 1992	88.67%
Bachelor's degree	Madurai Kamaraj University	Chemistry - 1992-1995	84.4% (I-D)
Master's degree	Madurai Kamaraj University	Chemistry - 1995-1997	83% (I)
Ph.D	Madras University	Chemistry/Material Science- 2005	
PGDCA	Manonmaniam Sundaranar University	1997-1998	83% (I)
GATE 1997			83.7 percentile

### C. RESEARCH EXPERIENCE & TRAINING

RESEARCH	TITLE OFWORK/THESIS	UNIVERSITY WHERE
STAGE		THE WORK WAS
		CARRIED OUT
Ph.D	Studies on Magnesium diboride and related	Materials Science Division,
	systems	Indira Gandhi Center for
		Atomic Research
		Kalpakkam.

Research guidance M.Phil	1. Synthesis and characterization of metal oxides	Post Graduate & Research Department of Chemistry The American College Madurai
	2. Mixed ligand complexes of Cu(II) and Ni(II) with Aspirin, Salbutamol and Amino acids – Preparation, Characterisation and Antibacterial studies	Post Graduate & Research Department of Chemistry The American College Madurai
	3. Synthesis, Spectral Characterisation and Antibacterial studies of Mixed ligand complexes of Cu(II) and Ni(II) with Aspirin, Salbutamol and Sulphur containing Amino acids	Post Graduate & Research Department of Chemistry The American College Madurai
Training	<ol> <li>Acquired skill in programming using Labview &amp; Matlab</li> <li>Got trained in the instrumentation of low temperature measurement viz., 4K-300K of resistivity and TEP</li> </ol>	

### D. RESEARCH PROJECTS CARRIED OUT

Title of the Project	Name of funding	Duration	Remarks
	agency		
Minor Project	UGC	2007-2009	Dr. Bosco Bharathy –
Synthesis of Pristine and Substituted			Principal investigator
MgB <sub>2</sub> thinfilms through			Dr. S. Jemima –
electrochemical deposition.			coinvestigator
			Project completed

### E. TEACHING EXPERIENCE

Courses taught	Name of Institution	Duration
1. UG (B.Sc.,)	The American College, Madurai-2	From 13-Sept-2004 till date
2. PG (M.Sc.,)	The American College, Madurai-2	From 13-Sept-2004 till date
3. M.Phil	The American College, Madurai-2	From June-2008 till date

### **List of Publications**

### **Papers Published in International Journals:**

- 1. Metal insulator transition in Fe<sub>2</sub>VAl<sub>1-x</sub>Si<sub>x</sub> **S.Jemima**, Awadhesh Mani, A.Bharathi, Nithya Ravindran, Y.Hariharan, Journal of Alloys and Compounds 326 (2001) 18 3-187.
- Carbon solubility and superconductivity in MgB<sub>2</sub> A.Bharathi, S.Jemima Balaselvi, S.Kalavathi, G.L.N.Reddy, V.Sankara Sastry, Y.Hariharan, T.S.Radhakrishnan – Physica C 370 (2002) 211-218.
- 3. Synthesis and search for superconductivity in LiBC– A.Bharathi, **S.Jemima Balaselvi**, M.Premila, T.N.Sairam, G.L.N.Reddy, C.S.Sundar, Y.Hariharan, Solid State Communication124 (2002) 423-428.
- 4. Superconductivity in MgB<sub>2</sub> : Phonon modes and influence of carbon doping A.Bharathi, Y.Hariharan, **S.Jemima Balaselvi**, C.S.Sundar, Sadhana Vol 28, Parts 1&2, February/April 2003, 263-272.
- 5. Peculiarities in the carbon substitution of MgB<sub>2</sub> **S.Jemima Balaselvi**, N.Gayathri, A.Bharathi, V.Sankara Sastry, Y.Hariharan, Physica C 407 (2004) 31-38.
- Stoichiometric carbon substitution in MgB<sub>2</sub> S.Jemima Balaselvi, N.Gayathri, A.Bharathi, V.S.Sastry, Y.Hariharan, Superconductor Science and Technology, 17(12) (2004) 1401.
- Study of Phytoconstituents and antibacterial activity of *Kappaphycus alvarezii* N. Jennifer Michellin Kiruba, M. Andrew Pradeep, S. Jemima Balaselvi Juliana, International Journal of Current Microbiology and Applied Sciences, ISSN: 2319-7706 4(5) (2015) 1209-1217.
- Physical characterization and kinetics studies of Zn(II) biosorption by Morganella morganii ACZ05 – D. Ramya, A. Joseph Thatheyus, S. Jemima Balaselvi Juliana, N. Jennifer Michellin Kiruba, A. Deborah Gnana Selvam, Water Science & Technology, ISSN 0273-1223, E-ISSN 1996-9732, 85(4) (2022), 970-986, https://doi.org/10.2166/wst.2022.031.

### Papers presented in Conferences:

- Carbon solubility and it's effect on superconductivity in MgB<sub>2</sub> S.Jemima Balaselvi, A.Bharathi, S.Kalavathi, G.L.N.Reddy, V.Sankara Sastry, Y.Hariharan, T.S.Radhakrishnan, Solid State Physics (India), 44 (2001) 359.
- Study of Boron Intercalation in Mg<sub>2</sub>Si S.Jemima Balaselvi, A.Bharathi, G.L.N.Reddy, V.Sankara Sastry, Y.Hariharan, T.S.Radhakrishnan, Solid State Physics (India), 44 (2001) 105.

- Effect of 4d transition metal substitution in MgB<sub>2</sub> S.Kalavathi, A.Bharathi, S.Jemima Balaselvi, G.L.N.Reddy, V.Sankara Sastry, Y.Hariharan, T.S.Radhakrishnan, Solid State Physics (India), 44 (2001) 357.
- 4. Effect of electron and hole doping on the superconducting and normal state properties of MgB<sub>2</sub> **S.Jemima Balaselvi**, A.Bharathi, V.Sankara Sastry, G.L.N.Reddy, Y.Hariharan, Solid State Physics (India), Vol 45, (2002) 383.
- 5. Labview automation of low temperature resistivity measurements A.Bharathi, S.Jemima Balaselvi, Y.Hariharan, Solid State Physics (India), Vol 45, (2002) 167.
- Virtual instrument based automation for low temperature resistivity experiments J.Jayapandian, R.Mallika, S.Jemima Balaselvi, A.Bharathi – Journal of the Instrument Society of India, Vol 33, (2003) 176.
- Raman Studies in MgB<sub>2-x</sub>C<sub>x</sub>, T. Sakuntala, S.K. Deb, A. Bharathi, S.Jemima Balaselvi, C. S. Sundar, Y.Hariharan, Solid State Physics (India), Vol 46, (2003).
- 8. Transport studies in Na<sub>x</sub>CoO<sub>2</sub> **S.Jemima Balaselvi**, N.Gayathri, A.Bharathi, V.Sankara Sastry, Y.Hariharan, Solid State Physics (India), Vol 46, (2003).
- 9. Positron annihilation studies in Na<sub>x</sub>CoO<sub>2</sub>– R.Rajaraman, A.Bharathi, **S.Jemima Balaselvi**, C.S.Sundar, Solid State Physics (India), Vol 46, 2003.
- Electrochemical studies on the deposition of metal, P. Silviya Reeta, J.R. Bosco Bharathy, S. Jemima Balaselvi, Frontier Areas in Chemistry, UGC sponsored National seminar, March 1-2, 2007, Thiagarajar College, Madurai-9
- 11. Installation and profiling of a tubular furnace, P. Silviya Reeta, **S. Jemima Balaselvi**, Frontier Areas in Chemistry, UGC sponsored National seminar, March 1-2, 2007, Thiagarajar College, Madurai-9
- Electrochemical deposition and characterization of the Li-B-C ternary phase, J. Nimitha, S. Sudha, S. Jemima Balaselvi, NSFAC, Jan 10-11, 2008, The American College, Madurai-2
- Electrochemical deposition and characterization of the Mg-B binary phase, S. Sudha, J. Nimitha, S. Jemima Balaselvi, NSFAC, Jan 10-11, 2008, The American College, Madurai-2
- 14. Synthesis, spectral characterisation and biological activity of copper complexes of anti inflammatory drug aspirin and amino acids, C. Suchitra, D. Ponpriya, S.Jemima Balaselvi, DRDO sponsored National workshop on Recent Trends in Inorganic Materials, March 15-16, 2012, National Engineering College, Kovilpatti.
- 15. Synthesis and characterisation of copper oxide nano particles from copper acetyl acetonate precursor and a capping agent, K. Santhiya Esther, M. Preethi, S. Jemima Balaselvi, ICNEEC, Dec 11-12, 2015, Madurai Kamaraj University, Madurai-21.

- Synthesis and characterisation of 12-heteropolyacids of tungsten and molybdenum, V. Sakthi, K.Keerthana, S. Jemima Balaselvi, International conference on Modern Trends in Chemistry, MTC-25, February 23, 2018 Vivegananda College, Thiruvedagam, ISBN 978-81-933998-6-6.
- Stability studies of MolybdoCopper<sup>II</sup> borate in aqueous medium by UV-Vis spectroscopy, V. Sakthi, S. Jemima Balaselvi, International Conference on Frontier Areas in Chemistry, July 17-19, 2018, American College, Madurai-2.
- Synthesis and Characterisation of Cu<sup>II</sup> incorporated Molybdoborate, N. R. Sivaram, G.M. Ranjitha Banu, S. Jemima Balaselvi, SERB sponsored National seminar on Emerging Trends in Bioinorganic and Pharmaceutical Chemistry (ETBPC-2019), February 27-28, 2019, VHNSN College (Autonomous), Virudhunagar.

### Work shop / Symposium attended:

- 1. SERC School on Precision Physical Measurements and Measurement Science, National Physical Laboratory, New Delhi, 4-23<sup>rd</sup> December 2000.
- Workshop on Enhancing Personal Excellence in Classroom Communication Skills of College Teachers, Christ College, Center for Education Beyond Curriculum, Bangalore, 5-7<sup>th</sup> October 2006.
- Workshop on Gender Awareness for Career Women, The American College, Madurai, 11 & 12 January 2007.
- 4. National Seminar on Sexual Harassment of Women at Work Place, All India Institute for Human Values and Resource Development, AIACHE, New Delhi, 25 & 26 August 2017.
- 5. National conference on Quality Enhancement and Sustenance in Higher Education sponsored by NAAC, IQAC The American College, Madurai, 6 March 2020.

### **Programs Organised**

- National Seminar on Frontier Areas in Chemistry (NSFAC), at The American College, Madurai, 10<sup>th</sup>- 11<sup>th</sup> January 2008.
- National workshop on "Applications of Nano Particle, Materials & Sensors" sponsored by DST, CSIR, UGC & DRDO, at The American College, Madurai, 7<sup>th</sup> – 8<sup>th</sup> December 2012.
- International Conference on Frontier Areas in Chemistry (ICFAC-2018), at The American College, Madurai, 17<sup>th</sup>- 19<sup>th</sup> July 2018.
- 4. International Conference on Frontier Areas in Chemistry (ICFAC-2019), at The American College, Madurai, 5<sup>th</sup> July 2019
- INSPIRE Internship Science Camp sponsored by Department of Science and Technology, New Delhi at The American College, Madurai, 15<sup>th</sup> – 9<sup>th</sup> January 2020.

- 6. Webinar on "Electroanalytical Techniques", at AMERICAN COLLEGE CENTRAL INSTRUMENTATION CENTRE (ACCIC), 24-06-2020.
- 7. Webinar on "Spectroscopic Techniques", at AMERICAN COLLEGE CENTRAL INSTRUMENTATION CENTRE (ACCIC), 07-07-2020.
- 8. Webinar on "Spectroscopic Techniques-II", at AMERICAN COLLEGE CENTRAL INSTRUMENTATION CENTRE (ACCIC), 08-07-2020.
- 9. Webinar on "Analytical Techniques", at AMERICAN COLLEGE CENTRAL INSTRUMENTATION CENTRE (ACCIC), 09-07-2020.
- Practical Workshop 1 on Molecular Techniques in Life Sciences, at AMERICAN COLLEGE CENTRAL INSTRUMENTATION CENTRE (ACCIC), 20<sup>th</sup> & 21<sup>st</sup> April 2021.
- Three days Online workshop on Xray Diffraction, at AMERICAN COLLEGE CENTRAL INSTRUMENTATION CENTRE (ACCIC), 30<sup>th</sup>-31<sup>st</sup> July & 2<sup>nd</sup> August 2021.

### Talk presented

- 1. Presented a talk on "An Introduction to Material Science", American College Chemistry Webinar Series 1, 16-05-2020.
- Resource person for the topic "Coordination Chemistry", Faculty Development Program on Nuances in Chemistry Teaching, sponsored by Department of Biotechnology, Ministry of Science & Technology, New Delhi, India and organised by Department of Chemistry, St. Mary's College (Autonomous), Thoothukudi, 23-06-2021.

### **Book edited**

1. A Laboratory Manual, Proceedings of the Practical Workshop – 1 on Molecular Techniques in Life Sciences, ISBN 978-93-80368-40-2.

### MOOC

1. Completed the 12 weeks NPTEL online course "Inorganic Chemistry of Life: Principles and Perspectives", Jul-Oct 2018 conducted by IIT Bombay.

### **Orientation/Refresher Courses**

- 1. Completed the UGC sponsored Orientation course from 09-02-2011 to 08-03-2011 and obtained A grade, Academic Staff College, Madurai Kamaraj University, Madurai.
- Completed the UGC sponsored Refresher course in Current Trends in Chemistry from 12-07-2012 to 01-08-2012 and obtained A grade, Academic Staff College, Madurai Kamaraj University, Madurai.
- Completed the UGC sponsored Refresher course in Recent Trends in Environmental Studies (ID) from 11-03-2016 to 31-03-2016 and obtained A grade, Academic Staff College, Madurai Kamaraj University, Madurai.
- Completed the two-week online Faculty Development Program (equivalent to Refresher course) on "Chemistry The catalyst for change" from 14 28 July 2021 and obtained A+ grade, Teaching Learning Centre, Ramanujan College, University of Delhi, in

collaboration with Department of Chemistry, Miranda House, University of Delhi, under the aegis of Ministry of Education, Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching.



FACULTY OFSCIENCE

2005 ஆம் ஆண்டில் சென்னைப் பல்கலைக்கழகத்தில் ஆய்வு நிகழ்த்தி
வழங்கிய ஆய்வேட்டுக்காக முனைவர் பட்டம் பெறத் தகுதியுடையவர் என்று தக்க
தேற் ாகளால் சான்றளிக்கப்பட்டு ஜெமிமா பாலசெல்வி ஜிலியானா எஸ்
ான் கொணைவர் பட்டம் அளிக்கப்படுகிறது என்று சென்னைப் பல்கலைக்கழகப் பேரவை
அறி க்கிறது.
ு என் நனப் பல்கலைக்கழக இலச்சினையுடன், சென்னையில் 2006 ஆம் ஆண்டு
ுமார்ச் திங்கள் 30 ஆம் நாள் அளிக்கப்பட்டது.
The Senate of the University of Madras hereby makes known that
JEMIMA BALASELVI JULIANA S has been confetted the
DEGREE OF DOCTOR OF PHILOSOPHY
he having been certified by duly appointed examiners to be qualified to ree we the same in the year 2005
Len under the seal of the University of Madras, at Chennai this D <sup>th</sup> day of March 2006
Title of the Thesis :

(Chemistry - Materials Science) Inter-disciplinary

பதிவாளர் Registrar



(Sd-----) S.P.THYAGARAJAN

துணை வேந்தர் Vice-Chancellor

		ana a	rai	08.03.20		Vice-Chancellor
ILC STAFF COLLEGE	durai Kamaraj University (University with Potential for Excellence) NSORED ORIENTATION COUNT	ATE OF PARTICIPATION Dr.(Mrs), S.Jemima Balaselvi Juliana	American College, Madurai	09.02.2011 ta		Registrar 12
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University Grants Commission ACADEMIC STAFF COLLEGE	Madurai Kamaraj University (University with Potential for Excellence) UGC SPONSORED REFRESHER COURSE	CERTIFICATE OF PARTICIPATION	d. Dr. S. Jemima Salaselvi Juliana Assistant Protector of Chemistry	The American College (Äutonomous), Madurai -2	esher Caurse in	01.08.2012 ta		Smuning Brann
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## HUMAN RESOURCE DEVELOPMENT CENTRE **University Grants Commission**

(Formerly Academic Staff College)

## Madurai Kamaraj University

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Dr. S. Jemima statevi Juliana This is to certify that

Assistant Professor of Chemistry

\*

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The American College, Madurai – 625 002

Environmental Studies (ID) "Recent Trends in Environmental Studies" participated in the Refresher Course in ..... on the theme .....

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Director

**Course Co-ordinator** 

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Date : 31.03.2016

Madurai.

Sulizeet: Chemistry Grade:







Indian Institute of Technology Bombay

**Jul-Oct 2018** 

(12 week course)

Head CDEEP & NPTEL Coordinator Prof. Sridhar lyer

IIT Bombay

Inorganic Chumistry of Life: **Principles and Perspectives** 

S. JEMIMA BALASELVI JULIANA

This certificate is awarded to

for successfully completing the course

**NPTEL** Online Certification

Elite

(Funded by the Ministry of HRD, Govt. of India)

with a consolidated score of **60** %

Online Assignments |24.18/25| Proctored Exam | 35.5/75

Total number of candidates certified in this course: **12** 



Teaching Learning Centre, Ramanujan College

University of Delhi

In collaboration with

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**University of Delhi** 

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PANDIT MADAN MOHAN MALAVIYA NATIONAL MISSION ON TEACHERS AND TEACHING

This is to certify that

### Dr. S. Jemima Balaselvi Juliana

of

### Department of Chemistry, The American College, Madurai-625002

has successfully completed online TWO - WEEK FACULTY DEVELOPMENT PROGRAMME (equivalent to Refresher Course) on

### "Chemistry - The Catalyst for Change"

from 14 – 28 July, 2021 and obtained Grade <u>A+</u>.



Blockchain Hash: 0x1966185367468ddad94ed755944c2979b53d5cd63a53d3e4cf0088de4108dc21

Prof. S. P. Aggarwal (Principal & Director) TLC, Ramanujan College

Dr. Ashish Kumar Shukla (Convener) Ramanujan College





Dr. Mallika Pathak (Convener) Miranda House



Journal of Alloys and Compounds 326 (2001) 183-187

ALLOYS AND COMPOUNDS

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### Metal insulator transition in $\text{Fe}_2\text{VAl}_{1-x}\text{Si}_x$

S. Jemima, Awadhesh Mani, A. Bharathi\*, Nithya Ravindran, Y. Hariharan

Materials Science Division, Indira Gandhi Centre for Atomic Research; Kalpakkam 603-102, Tamil Nadu, India

Received 3 July 2000; accepted 18 October 2000

### Abstract

Resistivity and ac susceptibility measurements have been carried out in the 4.2 to 300 K temperature range for several samples in the series Fe<sub>2</sub>VAl<sub>1</sub> [Si] for  $0 \le x \le 1$ . All samples crystallise in the DO<sub>3</sub> structure, with the lattice parameter showing a systematic linear decrease with Si substitution. The magnitude of the room-temperature resistivity, which is 3.4 mΩ cm for Fe<sub>2</sub>VAl, decreases drastically even for 1% Si substitution. The temperature-dependent resistivity shows a negative temperature co-efficient for Fe<sub>2</sub>VAl, which turns positive for samples with  $x \ge 0.05$ . The ac susceptibility measurements show that Fe<sub>2</sub>VAl is non-magnetic, while they indicate the formation of a ferrimagnetic phase for x = 0.04, with  $T_2 \le 4$  K. The results are discussed in the light of currently known models of the electronic structure of these systems. (6) 2001 Elsevier Science B.V. All rights reserved.

Keywords. Ac susceptibility: Resistivity, Ferrimagnetism

### 1. Introduction

The recently reported electronic properties of Fe NAI are unusual, for example the resistivity increases by a factor of 6-8 as the sample is cooled from 400 to 0.3 K [1,2], characteristic of a non-metal, and the sample remains non-magnetic up to to 2 K. The similarity of these properties to that of FeSi suggests that Fe, VAl could be yet another Kondo insulator [3], involving 3d electrons. Unlike for FeSi, NMR spectroscopy [4] and photoemission spectroscopy [1] indicate the presence of a finite density of electron states at the Fermi level and imply that Fe<sub>2</sub>VAl is a low carrier density semi-metal. Optical reflectivity data show the presence of a pseudogap 0.1-0.2 eV in magnitude with a small, albeit finite, density of states inside the gap [5]. Further, these results reiterate that the gap is not temperature dependent unlike that seen in Kondo insulators [6]. Low temperature specific heat measurements show a maximum in the C/T versus  $T^2$  plot and a large  $\gamma$ , which is characteristic of heavy fermion metallic systems [1,2,7]. Band structure calculations indicate that the system could

be a low carrier density semi-metal, having a deep pseudogap with  $E_1$  in the middle of the gap [8,9]. Although most experimental facts can be consistently explained using the results from band structure, the negative temperature coefficient of the resistivity and the intriguing low temperature specific heat results are not easily understood. Several conjectures have been put forward to understand this: spin-glass behaviour at low temperature arising as a consequence of the presence of Fe clusters due to Fe/V anti-site disorder [8] which could give rise to anomalous electron scattering resulting in an increase in resistivity with decreasing temperature. Alternatively, the negative temperature coefficient of the resistivity is thought to arise due to excitonic correlations between electrons and holes residing at V and Fe sites [9], inhibiting charge transport. Yet another reason envisaged for the negative temperature coefficient of the resistivity is that the electron transport behaviour could be due to the detailed shape of the density of states near the pseudogap [9]. The physical properties of isostructural  $Fe_2VSi$  are less controversial [10,11], being metallic with an antiferromagnetic transition at 120 K [11]. Here we investigate the  $Fe_{1}VAl_{1}$ , Si, system with a view to studying the evolution of the ground state of Fe, VAI as it systematically evolves from Fe<sub>3</sub>VSi by Al substitution on the Si site. The

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### Carbon solubility and superconductivity in $MgB_2$

A. Bharathi \*, S. Jemima Balaselvi, S. Kalavathi, G.L.N. Reddy,
 V. Sankara Sastry, Y. Hariharan, T.S. Radhakrishnan

Materials Science Division, Indira Gandhi Centre for Atomic Research, Kalpakkam 603102, India

Received 1 February 2002; accepted 12 February 2002

### Abstract

Successful replacement of B by C in the series  $MgB_{2-x}C_x$  for values of x upto 0.3 is reported. Resistivity and ac susceptibility measurements have been carried out in the samples. Solubility of carbon, inferred from the observed change in the lattice parameter with carbon content indicates that carbon substitutes upto x = 0.30 into the  $MgB_2$  lattice. The superconducting transition temperature,  $T_c$  measured both by zero resistivity and the onset of the diamagnetic signal shows a systematic decrease with increase in carbon content upto x = 0.30, beyond which the volume fraction decreases drastically. The temperature dependence of resistivity in the normal state fits to the Bloch–Gruneisen formula for all the carbon compositions studied. The Debye temperature,  $\theta_D$ , extracted from the fit, is seen to decrease with carbon content from 900 to 525 K, whereas the electron–phonon interaction parameter,  $\lambda$ , obtained from the MgB<sub>2</sub> to 0.9 in the McMillan equation using the measured  $T_c$  and  $\theta_D$ , is seen to increase monotonically from 0.8 in MgB<sub>2</sub> to 0.9 in the x = 0.50 sample. The ratio of the resistivities between 300 and 40 K versus  $T_c$  is seen to follow the Testardi correlation for the C substituted samples. The decrease in  $T_c$  is argued to mainly arise due to large decrease in  $\theta_D$  with C concentration and a decrease in the hole density of states at  $N(E_F)$ . © 2002 Elsevier Science B.V. All rights reserved.

Keywords: MgB<sub>2</sub>; Transport properties; Transition temperature variations

### 1. Introduction

The recent discovery of superconductivity at 39 K in MgB<sub>2</sub> has initiated a flurry of activity aimed at understanding the origin of the large  $T_c$  [1]. Several experimental studies, notably the isotope effect [2] and the pressure dependence [3] of  $T_c$  point to the fact that superconductivity in this system is largely governed by the conventional electron-phonon mechanism and that the high  $T_c$ 

\* Corresponding author.

is a consequence of the large hole density of states arising from the sigma bands of boron and high phonon frequency arising on account of the low mass [4–6]. There have been several theoretical predictions of an increase in  $T_c$  by chemical substitutions at the Mg and B sublattice [6,7]. There have been experimental reports of substituting Mg by Al [8,9], Li [10,11], Si [10], 3d transition metals [12–14] and recently 4d transition metals [15]. Almost all substitutions have led to a decrease in  $T_c$ , with an exception of Zn [14], which shows no change even for 30% substitution. Our study has shown that ~5% substitution of Nb [15] at the Mg site, in MgB<sub>2</sub>, results in a small albeit definite

E-mail address: bharathi@igcar.ernet.in (A. Bharathi).

<sup>0921-4534/02/\$ -</sup> see front matter © 2002 Elsevier Science B.V. All rights reserved. PII: S0921-4534(02)01139-5

Supercond. Sci. Technol. 17 (2004) 1401-1405

### Stoichiometric carbon substitution in MgB<sub>2</sub>

### S Jemima Balaselvi, N Gayathri, A Bharathi<sup>1</sup>, V S Sastry and Y Hariharan

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### Abstract

Carbon has been substituted into the MgB<sub>2</sub> lattice, forming the series Mg(B<sub>1-x</sub>C<sub>x</sub>)<sub>2</sub>, by heat treatments in sealed Ta tubes starting with elemental constituents. The superconducting transition temperature,  $T_{\rm C}$ , was measured by diamagnetic susceptibility. The superconducting transitions are sharp and the x-ray diffraction on the samples show only trace amounts of impurity phases. The C fraction that substitutes the B atoms into the MgB<sub>2</sub> lattice, as determined from the now well established correlation between the 'a' lattice parameter and x in Mg(B<sub>1-x</sub>C<sub>x</sub>)<sub>2</sub> is found to be very close to the targeted values. The temperature dependence of the normalized resistance is similar to that seen in C doped MgB<sub>2</sub> single crystals along the *ab* plane.  $R_n/R(300 \text{ K})$ , where  $R_n$  is the resistance just above  $T_{\rm C}$ , increases with x.

### 1. Introduction

Ever since the discovery of superconductivity in MgB<sub>2</sub> [1] three years ago, many experiments have been carried out which has brought about a good understanding of the physics underlying these materials [2]. From the materials point of view MgB2 stands alone like an island. Chemical substitutions at specific crystallographic sites that lead to a variety and richness in the high temperature superconductors is not easily possible in MgB<sub>2</sub> [3]. The interest in chemical substitution of this material is still alive as the  $H_{C2}(0)$  of pristine MgB<sub>2</sub> is small  $\sim 15$  T [4] and the critical current density is strongly depressed at low magnetic fields. It is possible to enhance  $H_{C2}(0)$ , by chemical substitution, but in MgB<sub>2</sub>, the presence of two superconducting gaps arising from two bands with different dimensionality and equal density of states at the Fermi level, does not make the choice of the right substituent that straightforward [5]. Substitutions aimed at enhancing  $H_{C2}(0)$ should not lead to inter-band scattering which could bring about a reduction in  $T_{\rm C}$  in a two gap scenario. Of all the chemical substitutions that have been undertaken, Al and C substitutions have been successful both in polycrystalline [6-10] and single crystalline forms [11–13], and both of them

have resulted in a decrease in  $T_{\rm C}$ . One of the plausible reasons for a reduction in  $T_{\rm C}$  due to Al substitution is believed to arise from increased inter-band scattering, making it an unsuitable substituent to enhance  $H_{\rm C2}(0)$  [14]. In fact it has been recently observed in single crystalline Mg<sub>1-x</sub>Al<sub>x</sub>B<sub>2</sub> that Al substitution leads to a reduction in  $H_{\rm C2}(0)$  [15].

On the other hand, recent experiments that have substituted carbon into MgB2 using B4C as the precursor have shown that a carbon fraction of  $x \sim 0.12$  substitutes into the  $Mg(B_{1-x}C_x)_2$  lattice and that the  $H_{C2}(0)$  can be increased to 25–30 T [16]. In single crystalline samples the  $H_{\rm irr}$  is shown to increase for small C content [17]. For x = 0.01to 0.035 made in polycrystalline form on tungsten wires, it has been shown that the  $H_{C2}(0)$  increases with C content to 32 T [10]. There is thus a clear need to device a method for fabrication of  $Mg(B_{1-x}C_x)_2$  for a wide range of C content and therefore optimize  $H_{C2}(0)$  and  $T_{C}$ . Even though the B<sub>4</sub>C route of synthesis has yielded a high  $H_{C2}(0)$ , it is not possible to obtain a systematic variation in the C concentration and hence optimize  $H_{C2}(0)$ . Further, as mentioned above, in this method of synthesis, a maximum C fraction of x = 0.12 has been attained, with the remaining C forming impurity phases, namely  $Mg_2C_3$  and  $MgB_2C_2$ . In the wire samples prepared by chemical vapour deposition of B-C onto the tungsten wires,

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### Synthesis and search for superconductivity in LiBC

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### Abstract

Following the recent theoretical prediction of superconductivity in hole doped LiBC by Rosner et al. [Phys. Rev. Lett. 88 (2002) 127001], we have attempted to synthesize Li deficient  $\text{Li}_x \text{BC}(x = 1, 0.8, 0.6 \text{ and } 0.4)$  and looked for superconductivity in this system. Our synthesis procedure, following the recipe for MgB<sub>2</sub>, involves reaction of elemental components in a Ta crucible at 900 °C under 50 bar of argon pressure. X-ray diffraction measurements indicate the formation of  $P6_3/mmc$  structure up to x = 0.6. However, no diamagnetic signal or zero resistance, corresponding to the superconducting transition, were observed in the temperature range of 4–300 K. This is possibly related to the presence of disorder in the B–C stacking; evidence for which is suggested from a study of the vibrational modes of  $\text{Li}_x \text{BC}$  through infrared spectroscopy. © 2002 Elsevier Science Ltd. All rights reserved.

*PACS*: 74.10. + v; 74.70. - b; 78.30. - j; 61.10. - i

Keywords: A. Superconductors; B. Chemical synthesis; E. X-ray diffraction; E. Resistivity; E. Infrared spectroscopy; D. Phonons

### 1. Introduction

Since the discovery of superconductivity in  $MgB_2$  [2,3] there has been a serious effort to unravel the mechanism of superconductivity in this compound [4]. This high  $T_c$  in MgB<sub>2</sub>, is believed to arise due to strong electron-phonon coupling of the holes in the  $\sigma$  band with the bond stretching  $E_{2g}$  modes in the B planes [5]. Electronic band structure calculations [5] also show that the hole density of states is two-dimensional in character, the energy dependence is flat below  $E_{\rm F}$ , but falls off above suggesting that the density of states at  $E_{\rm F}$ ,  $N(E_{\rm F})$ , is not expected to change with hole doping, whereas it will decrease with electron doping. Attempts to increase  $T_c$  in MgB<sub>2</sub> by chemical substitution have not thus far been successful.  $T_{\rm c}$  is observed to decrease by electron [6,7] doping, as seen in Al and C substitution experiments. By the substitution of Li, which corresponds to hole doping [8]  $T_c$  remains constant. Whereas by Be substitution, which also results in hole doping [9],  $T_c$  shows a precipitous decrease [10], which is understood in terms of

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a decrease in the electron-phonon coupling strength [11]. It therefore appears that the route to increase  $T_{\rm c}$  is to increase the electron-phonon coupling strength with the hole concentration remaining fixed at least at the MgB<sub>2</sub> value. Along these lines [11] it was suggested that the  $CuB_{2-x}C_x$ system would be a likely candidate for high  $T_c$ , with Cu substitution resulting in the right magnitude of  $N(E_{\rm F})$ , but with an increased electron-phonon coupling due to the C substitution of the B layers. Experimental verification of these ideas has been hampered by the lack of solubility of Cu in MgB<sub>2</sub> and the fact that the CuB<sub>2-x</sub>C<sub>x</sub> compound does not form. The  $T_c$  in other iso-structural di-borides viz. ZrB<sub>2</sub> [12], TaB<sub>2</sub> [13] and MoB<sub>2</sub> stabilized with 4% Zr [14] have been disappointingly low. This is rationalized, based on their electronic structure [15,16], to arise because the 4d electrons of the transition metals span the Fermi level and that the  $\sigma$  bonding electrons of B are  $\sim 2-4$  eV below  $E_{\rm F}$ .

Recently band structure calculations [1], have suggested a possibility of the occurrence of superconductivity in an iso-structural compound LiBC. The electron count in LiBC is identical to that in MgB<sub>2</sub> with Li providing one electron less than Mg, and the replacement of B with C, providing the extra electron. Stoichiometric LiBC is a large gap semiconductor [1,17], and it has been reported [1,17] that

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### Superconductivity in MgB<sub>2</sub>: Phonon modes and influence of carbon doping

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**Abstract.** Following a brief overview, results of our investigations on phonon modes in MgB<sub>2</sub>, and superconducting transition in carbon doped MgB<sub>2</sub> are presented. The superconducting transition temperature in MgB<sub>2-x</sub>C<sub>x</sub> as obtained from susceptibility and resistivity measurements is observed to decrease systematically from 39.4 K for x = 0 to 26 K for x = 0.5. It is shown the changes in lattice volume, as obtained from x-ray diffraction measurements, can account only partially for the observed decrease in  $T_c$ . The observed variation of  $T_c$  with carbon content is seen to correlate with the Debye temperatures, obtained from an analysis of the resistivity data.

Investigation of the phonon modes in MgB<sub>2</sub>, through infrared absorption measurements indicate three modes at 410, 475 and 560 cm<sup>-1</sup>. The former two are associated with the infrared active modes, and the third component is associated with the Raman mode, that gets activated due to disorder. A study of the temperature dependence of these modes indicates no changes across the superconducting transition. The mode at 560 cm<sup>-1</sup> shows a significant hardening and a corresponding decrease in linewidth, with the lowering of temperature, that can been accounted in terms of anharmonicity.

**Keywords.** Superconductivity;  $MgB_2$ ; carbon-doping; susceptibility; resistivity; infrared spectroscopy.

### 1. Introduction and overview

The serendipitous discovery of superconductivity at 39K in the binary intermetallic  $MgB_2$  by Nagamutsu *et al* (2001) has initiated a flurry of activity. In a short period of time extensive studies (for a review, see Buzea & Yamashita 2000) have been carried out on the normal state and superconducting properties, which include the determination of the superconducting gap, coherence length, penetration depth and critical fields. Theoretical calculations (An & Pickett 2001; Kong *et al* 2001; Kortus *et al* 2001) indicate that superconductivity in this system can be understood in the framework of electron–phonon interaction. Initial evidence for the importance of electron–phonon interaction was provided by the experiments on boron isotope effect (Bud'ko *et al* 2001) MgB<sub>2</sub> has been syntheised in a variety of forms such as thin films



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### Peculiarities in the carbon substitution of $MgB_2$

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### Abstract

To examine the role of kinetics on C substitution into MgB<sub>2</sub>, heat treatments at 900 °C on stoichiometric quantities of Mg, B and C forming the MgB<sub>2-x</sub> $C_x$  series, have been carried out for various times and for different carbon fractions, under an external Ar pressure of 50 Bar. The variation in the superconducting transition temperatures on account of C incorporation into the MgB<sub>2</sub> matrix has been measured using the onset of diamagnetism and the appearance of zero resistance using the a.c. susceptibility and resistivity measurements carried out in the 4-300 K temperature range. The phase purity of the samples and the lattice parameters have been measured by XRD measurements. The microstructure has been characterized by scanning electron microscope observations. The heat treatments carried out on  $MgB_{2-x}C_x$  for a nominal composition of x = 0.3, indicate that for shorter periods, the superconducting transitions are broad, and with increase in the heat treatment time the transition widths narrow and the onset of diamagnetism shifts to higher temperature reaching a value of 35 K at 50 h. The *a*-lattice parameter shows a corresponding increase with heat treatment time and also attains a constant value between the 24 and 50 h treatments. These results reveal that the extent of carbon substituted into the  $MgB_2$  matrix at shorter times is large whereas for longer annealing times the matrix is depleted in carbon content, with carbon content in the superconducting volume becoming more uniform. These prolonged heat treatments were carried out for several nominal compositions of carbon and the measured  $T_{\rm C}$  decreases to less than 20 K for large carbon contents. The  $T_{\rm C}$  versus *a*-lattice parameter obtained from this work, shows a correlation in agreement with similar measurements on single crystals.

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*PACS:* 74.70.Ad; 74.62.Dh; 74.25.-q *Keywords:* MgB<sub>2</sub>; Carbon doping; Transition temperature variations

### 1. Introduction

The study of the superconductivity in  $MgB_2$  has been extensive ever since its serendipitous discovery by Nagamatsu et al. [1]. The nature of superconductivity is fairly well understood in pristine MgB<sub>2</sub> [2], arising from strong electron phonon interaction in the 2D,  $\sigma$  band, which is induced into the 3D,  $\pi$  band, resulting in the now well established, two gap superconductivity. The volatile nature of Mg and the associated difficulty in the synthesis of the material poses difficulties in the

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### **Original Research Article**

### Study of Phytoconstituents and antibacterial activity of Kappaphycus alvarezii

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### ABSTRACT

Keywords

Antibacterial Activity, bioactive, quinones, sterols and isoflavonols The aim of this investigation was to analyse the antimicrobial activity of Kappaphycus alvarezii and to study its bioactive compounds. The crude extracts of Kappaphycus alvarezii extracted in ethanol and chloroform was subjected to preliminary phytochemical estimation. Its activity against gram positive and negative bacterial strains of Escherichia coli, Staphylococcus aureus, Proteus mirabilis, Streptococcus pneumoniae, Pseudomonas aeruginosa, Vibrio cholerae, and Bacillus subtilis was also investigated. The compounds present were confirmed using HPLC and the functional groups were identified using FT-IR. Phytochemical analysis tested positive for the presence of flavonoids, cardiac glycosides, sterols and quinones. FTIR analysis of the EtOH and CHCl<sub>3</sub> extracts of Kappaphycus alvarezii showed similar peaks corresponding to functional groups such as amines (-NH<sub>2</sub>), alcohols (-OH) and carboxyl (-C=O) groups. The qualitative HPLC fingerprint profile of both extracts showed prospective peaks at lower R<sub>f</sub> values indicating the major presence of quinones. The results show that, the presence of bioactive quinones, sterols and isoflavonols, lead to active inhibition of microbial growth in a dose-dependent manner.

### Introduction

According to WHO report and fact sheet (last updated on April 2014), the causes of antimicrobial resistance (AMR) are several, namely selective pressure, mutation, gene transfer, societal pressures, inappropriate drug use, inadequate diagnostics, hospital use and agricultural use of drugs. The impact of AMR on society and economy is sky-high. It raises the death rate due to common infections, twice than normal and the low awareness among general public is not helping the already deteriorating situation.

Due to unavailability of treatment to resistant forms of microbes, the health care costs and the economic burden on public will further spike specifically in third world countries. In 2050, about 10 million deaths are expected to be due to AMR, which will dominate every other cause of mortality like cancer, road accidents and diabetes. The draft global action plan developed by the World Health Organization to combat antimicrobial resistance (to be submitted to the Sixty-eighth World Health Assembly in May 2015) sets out five strategic objectives.

### Water Science & Technology



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### Physical characterization and kinetic studies of Zn (II) biosorption by Morganella morganii ACZ05

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### ABSTRACT

Through this investigation, we establish the mechanism and physical characterization of zinc (II) sequestration by *Morganella morganii* ACZ05 strain, which was isolated and characterized from soil polluted by effluents from electroplating industries. As far as we know, there is very little literature concerning zinc biosorption using an environmental strain of *M. morganii*. The SEM analysis shows the dark porous gaps in the aggregated cell-matrix of test bacterial biomass which is inferred as water channels usually seen in biofilms, as compared to metal-unexposed control. *M. morganii* is not known to produce biofilms unless in the rare nosocomial conditions. Here, SEM analysis shows the production of biofilms after exposure to zinc (II) at 500 ppm, which has not been previously reported. EDX analysis of bacterial biomass also specified the sorption of zinc (II) by the bacterial cells and the presence of new peaks for zinc in contrast to control. Both XRD and FTIR analysis observations strongly implicate the potential of physical adsorption as a mechanism for heavy metal resistance. Analysis of the cell surface by Atomic force microscopy and examination of the topography revealed cell aggregation occurs during biofilm production after zinc biosorption. Unlike other reports, regular models such as Langmuir isotherm and Freundlich isotherm were found insufficient to explain the physisorption of zinc (II) metal ions on complex multicomponent adsorbents such as the exopolymeric surface of the bacterial cells. However, adsorption kinetics of zinc (II) to the bacterial biomass was most effectively elucidated by a pseudo-second-order kinetic model, suggesting a certain kind of chemisorption that requires further study.

Key words: Biosorption, Freundlich, Langmuir, M. morganii ACZ05, SEM/EDX, zinc II)

### HIGHLIGHTS

- XRD and FTIR potential of physical adsorption as a mechanism for heavy metal resistance.
- SEM-EDX and AFM morphological changes were observed after metal addition.
- The isotherm studies fit of pseudo-second order for biosorption experimental data suggests the involvement of cellular mechanisms for the activity of binding sites of metal ions and other chemical sorption processes.
- Biosorption, chemisorption,



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