

TABLE OF CONTENTS

CHAPTER NO.	TITLE	PAGE NO.
	ABSTRACT	v
	LIST OF TABLES	xvii
	LIST OF FIGURES	xviii
	LIST OF SYMBOLS AND ABBREVIATIONS	xxii
1	INTRODUCTION TO CRYSTAL AND CRYSTAL GROWTH TECHNIQUES	1
	1.1 INTRODUCTION TO CRYSTALS	1
	1.2 STRUCTURE OF CRYSTALS	3
	1.3 SIGNIFICANCE OF SINGLE CRYSTAL	6
	1.4 EXTERNAL APPEARANCE OF CRYSTALS	7
	1.5 EXTERNAL SYMMETRY OF CRYSTALS	8
	1.6 TYPES OF CRYSTALS	12
	1.6.1 Covalent Crystals	12
	1.6.2 Ionic Crystals	13
	1.6.3 Molecular Crystals	13
	1.6.4 Metallic Crystals	14
	1.7 INTRODUCTION TO CRYSTAL GROWTH	14
	1.8 NUCLEATION	15
	1.9 THEORY OF NUCLEATION AND GROWTH	16
	1.9.1 Nucleation	16
	1.9.2 Heterogeneous Nucleation	16
	1.9.3 Homogeneous Nucleation	17
	1.9.4 Growth Mechanisms	18

CHAPTER NO.	TITLE	PAGE NO.
1.14	OPTIMIZING SOLUTION GROWTH	40
1.14.1	Material Purification	40
1.14.2	Solvent Selection	41
1.14.3	Solubility	43
1.14.4	Solution Preparation	44
1.14.5	Seed Preparation	44
1.14.6	Agitation	45
1.14.7	Crystal Habit	45
1.14.8	Cooling Rate	46
2	NON LINEAR OPTICAL (NLO) MATERIAL & ITS APPLICATIONS	47
2.1	NON LINEAR OPTICAL (NLO) MATERIAL	47
2.2	WORKING PRINCIPLE	48
2.3	LIFETIME OF NONLINEAR CRYSTALS	52
2.4	ORGANIC CRYSTALS	54
2.4.1	Pros of Organic Crystals	55
2.4.2	Cons of Organic Crystals	56
2.5	INORGANIC CRYSTALS	56
2.5.1	Pros of Inorganic Crystals	57
2.5.2	Cons of Inorganic Crystals	57
2.6	SEMI ORGANIC CRYSTALS	57
2.6.1	Pros of Semi Organic Crystals	58
3	LITERATURE SURVEY	59
3.1	ORGANIC CRYSTALS	59
3.2	INORGANIC CRYSTALS	60
3.3	SEMI ORGANIC CRYSTALS	60

CHAPTER NO.	TITLE	PAGE NO.
3.4	NON LINEAR OPTICAL MATERIALS	61
3.5	FERRO ELECTRIC MATERIALS	62
3.6	APPLICATIONS OF FERROMAGNETIC MATERIALS	62
3.7	COMPARATIVE STUDIES	65
4	CHARACTERIZATION TECHNIQUES	72
4.1	INTRODUCTION	72
4.2	SINGLE CRYSTAL X-RAY DIFFRACTION STUDIES	74
4.2.1	Working Principle	74
4.3	POWDER X-RAY DIFFRACTION STUDIES	77
4.4	FOURIER TRANSFORM INFRARED (FTIR) ANALYSIS	81
4.5	UV-Vis-NIR SPECTROSCOPY	82
4.6	THERMAL STUDIES	83
4.7	KURTZ POWDER SHG TEST	85
4.8	DIELECTRIC STUDIES	87
4.9	MICROHARDNESS STUDIES	88
4.10	PHOTOLUMINESCENCE	91
4.10	CONCLUSION	94
5	GROWTH AND CHARACTERIZATION OF SEMI ORGANIC NONLINEAR OPTICAL L-VALINE FERRIC CHLORIDE SINGLE CRYSTAL BY SOLUTION GROWTH TECHNIQUE	95
5.1	INTRODUCTION	95
5.2	CRYSTAL GROWTH	96

CHAPTER NO.	TITLE	PAGE NO.
5.3	RESULTS AND DISCUSSION	97
5.3.1	Single Crystal X-RAY Diffraction Analysis	97
5.3.2	Powder X-Ray Diffraction	97
5.3.3	FTIR Analysis	98
5.3.4	Thermal Studies	100
5.3.5	Linear Optical Property	101
5.3.6	Micro Hardness Analysis	102
5.3.7	Photoluminescence Studies	104
5.3.8	Kurtz Powder SHG Test	104
5.3.9	Dielectric Studies	106
5.3.10	Scanning Electron Microscope Analysis	108
5.4	CONCLUSION	109
6	GROWTH AND CHARACTERIZATION OF SINGLE CRYSTAL - THIOSEMICARBAZIDE MANGANOUS ACETATE (TSMNAC)	110
6.1	GRAPHICAL ABSTRACT OF TMnAc	110
6.2	INTRODUCTION	111
6.3	EXPERIMENTAL PROCEDURE	112
6.3.1	Material Synthesis	112
6.3.2	Solubility	113
6.3.3	Characterization Techniques	114
6.4	RESULTS AND DISCUSSION	114
6.4.1	Single Crystal X-Ray Diffraction Analysis	114
6.4.2	Powder X-Ray Diffraction Analysis	115
6.4.3	Optical Absorption Analysis	115
6.4.4	Mechanical Studies	117

CHAPTER NO.	TITLE	PAGE NO.
	6.4.5 Dielectric Studies	118
	6.4.6 Antibacterial Studies	119
	6.4.7 Antifungal Studies	121
	6.4.8 SEM Studies	123
	6.4.9 Nonlinear Optical Studies	124
6.7	CONCLUSION	124
7	GROWTH, SPECTROSCOPIC, DIELECTRIC & ELECTRICAL STUDIES OF GLYCINE MANGANOUS ACETATE SINGLE CRYSTAL	126
7.1	GRAPHICAL ABSTRACT OF GLYCINE MANGANOUS ACETATE	126
7.2	INTRODUCTION	127
7.3	EXPERIMENTAL PROCEDURE	128
	7.3.1 Crystal Growth	129
	7.3.2 Characterization Techniques	129
7.4	RESULTS AND DISCUSSION	130
	7.4.1 Single Crystal XR Diffraction Analysis	130
	7.4.2 Powder X-RAY Diffraction	130
	7.4.3 Thermal Studies	131
	7.4.4 Optical Studies	132
	7.4.5 Mechanical Studies	134
	7.4.6 Dielectric Studies	137
	7.4.7 AC Conductivity Studies	140
	7.4.8 D.C. Conductivity Studies	141
	7.4.9 A.C resistivity and Conductivity	143
7.5	CONCLUSION	145

CHAPTER NO.	TITLE	PAGE NO.
8	GROWTH AND CHARACTERIZATION OF SINGLE CRYSTAL: L- HISTIDINE CADMIUM BROMIDE (LHCdBr)	146
8.1	GRAPHICAL ABSTRACT OF L–HISTIDINE CADMIUM BROMIDE	146
8.2	INTRODUCTION	147
8.3	EXPERIMENTAL PROCEDURE	148
8.4.1	Materials and Crystal Growth	148
8.4	RESULTS AND DISCUSSION	149
8.4.1	Single Crystal X-ray Diffraction	149
8.4.2	Powder X-ray Diffraction	149
8.4.3	FTIR Analysis	150
8.4.4	Linear Optical Property	151
8.4.5	Thermal Analysis	153
8.4.6	Micro Hardness Analysis	154
8.4.7	Dielectric Studies	155
8.4.8	FE-SEM Analysis	157
8.4.9	NLO Studies	158
8.5	CONCLUSION	158
9	SUMMARY	159
9.1	SUMMARY	159
9.2	SUGGESTION AND FUTURE WORK	160
	REFERENCES	162
	LIST OF PUBLICATIONS	175

LIST OF TABLES

TABLE NO.	TITLE	PAGE NO.
1.1	Flow chart of Seven Crystal system	10
2.1	Optical effects of nonlinear materials	50
2.2	Parameters for selecting a NLO crystal	52
5.1	FTIR Analysis of LVFC	100
5.2	Comparative Efficiency of LVFC	106
6.1	Antibacterial activity of TSMnAc at different concentrations (25, 50, 75, 100 $\mu\text{g/ml}$)	121
6.2	Antifungal activity of TSMnAc at different concentrations (25, 50, 75, 100 $\mu\text{g/ml}$)	123
7.1	Stiffness constant	137

LIST OF FIGURES

FIGURE NO.	TITLE	PAGE NO.
1.1	Beautiful specimens of Lapis lazuli (a) and Turquoise(b)	2
1.2	Pyrite (iron sulphide)	4
1.3	Diamond (pure carbon)	4
1.4	Periodic repetition model in Mosaic drawing	4
1.5	Periodic repetition in Military parade	5
1.6	Atomic model of an ordered material	5
1.7	Atomic model of glass	6
1.8	External appearance of a Crystal	7
1.9	Flow chart of Seven Crystal system	8
1.10	Flow chart of 32 Symmetry classes	9
1.11	A wall diagram, the petals of flower, Sides of a Butterfly	9
1.12	Diamonds - covalent crystal	12
1.13	Table salt - ionic crystal	13
1.14	Hydrogen bonds between sugar molecules make rock candy	13
1.15	Gold Nuggets -Metallic Crystals	14
1.16	Flow chart of Nucleation	16
1.17	Heterogenous Nucleation	17
1.18	Homogenous Nucleation	17
1.19	Ledge formation and Lateral Growth	18
1.20	(a)Total free energy versus cluster size (b) Nucleation rate as a function of supersaturation	20
1.21	Schematic representation of processes involved in the crystal growth	23

FIGURE NO.	TITLE	PAGE NO.
1.22	Slow evaporation method	39
2.1	Electrons in a nonlinear crystal are bound in a potential well, holding the electrons to lattice points	49
2.2	Two photons are welded together to produce a single photon with the energy of both original photons	50
3.1	Dielectric, Paraelectric & Ferroelectric Polarizations	60
3.2	Domain configuration encountered in ferro electric Crystals (1) first class (2) second class	61
3.3	A Hysteresis loop illustration the Coercive field E_c	63
4.1	Structure analysis and performance	73
4.2	Schematic diagram of Single crystal X-Ray Diffraction	75
4.3	Simple schematic diagram of PXRD	79
4.4	Schematic representation of a FTIR spectrometer	81
4.5	Schematic diagram of dual slit spectrometer	83
4.6	A block diagram of Thermogravimetric analysis	84
4.7	Schematic arrangement of the experimental setup used for measuring SHG	86
4.8	Schematic diagram of digital Vickers hardness	90
4.9	Principle of photoluminescence spectroscopy	92
4.10	Block diagram of fluorescence spectrometer	93
5.1	Grown LVFC Crystal	97
5.2	Powder XRD pattern of LVFC	98
5.3	FTIR Analysis of LVFC	99
5.4	TG/DTA curve of LVFC	101
5.5	Absorption spectrum of LVFC	102
5.6	LVFC as a function of applied load	103
5.7	Photoluminescence spectrum of LVFC	105
5.8	Variation of Dielectric constant Vs Frequency	108
5.9	Scanning electron Microscope picture of LVFC	108
6.1	Grown Crystal of TSMnAc	113

FIGURE NO.	TITLE	PAGE NO.
6.2	Solubility curve of TSMnAc	113
6.3	Powder XRD pattern of TSMnAc	114
6.4	Absorption Spectra of TSMnAc	116
6.5	Transmission Spectra of TSMnAc	116
6.6	Variation of Hardness with Load P	118
6.7	Variation of Dielectric constant with applied frequency	119
6.8	(a) Zone of Inhibition of TSMnAc in E.coli (b) Zone of Inhibition of TSMnAc in E.coli (c) Zone of Inhibition of TSMnAc in S.Aureus (d) Zone of Inhibition of TSMnAc in Shigella	120
6.9	(a) Zone of Inhibition of TSMnAc in A.niger (b) Zone of Inhibition of TSMnAc in A. clavatus (c) Zone of Inhibition of TSMnAc in Candida albicans	122
6.10	SEM images of TSMnAc	123
7.1	As grown crystal of GMnAc	129
7.2	Powder XRD Pattern of GMnAc	131
7.3	DSC curve of GMnAc	131
7.4	Absorption spectra of GMnAc	132
7.5	Transmission spectra of GMnAc	133
7.6	Plot of $(ah\nu)^2$ vs Photon energy of GMnAc	134
7.7	Plot of load p vs. hardness number	135
7.8	Plot of Log d Vs Log P	137
7.9	Variation of Dielectric constant Vs Log Frequency	138
7.10	Variation of Dielectric Loss Vs Frequency	139
7.11	Variation of Dielectric constant Vs Temperature	139
7.12	Temperature variation of A.c. Conductivity	140
7.13	Plot of Log σ_{ac} Vs. $1000/T$	141
7.14	Plot of Voltage (V) Vs Current (A)	142

FIGURE NO.	TITLE	PAGE NO.
7.15	Variation of $\ln(\sigma) T$ vs. $(1000/T)$	142
7.16	Variation of Frequency Vs Resistivity	143
7.17	Variation of Conductivity with frequency	144
7.18	Variation in Current with Temperature	144
8.1	Grown crystal of LHCdBr Crystal	148
8.2	PXRD graph of LHCdBr	149
8.3	FTIR Analysis of LHCdBr	150
8.4	Absorption Spectrum of LHCdBr	152
8.5	Transmission Spectrum of LHCdBr	153
8.6	Thermal Analysis of LHCdBr	154
8.7	Relation between Vickers hardness number vs load	155
8.8	Variation of Dielectric constant with applied frequency	156
8.9	FE-SEM analysis of LHCdBr	157

LIST OF SYMBOLS AND ABBREVIATIONS

A_α	-	Absorbance
α	-	Absorption coefficient
\AA	-	Angstrom
P	-	Applied load
A	-	Area of the sample
α_1	-	Change in absorption
$\Delta\alpha$	-	Change in absorption coefficient
Δn	-	Change in index of refraction
Q	-	Charge
J	-	Current density in the material
ρ	-	Density of molecule
d	-	Diagonal length
ϵ_r	-	Dielectric constant,
DSC	-	Differential Scanning Calorimetry
DTA	-	Differential Thermal Analysis
θ	-	Diffraction angle
2θ	-	Diffraction angle
χ_{eff}	-	Effective susceptibility
C11	-	Elastic stiffness constant
E	-	Electric field strength (V/m)
d	-	Electric flux density (C/m),
σ_e	-	Electrical conductivity
α_e	-	Electronic polarizability
Eg	-	Energy band gap

F	-	Force
FTIR	-	Fourier Transform Infrared
γ	-	Frequency of electromagnetic wave
β	-	Full width half maximum
ϵ_i	-	Imaginary dielectric constant
Z	-	Impedance
n	-	Index of refraction
I	-	Irradiance(power per unit area)
L	-	Length of the sample
α_0	-	Linear absorption
$\chi^{(1)}$	-	Linear or first order susceptibility
α_p	-	Linear polarisability
H	-	Magnetic field strength (A/m)
K	-	Material constant
μ	-	Molecular polarization
$\Delta\Phi$	-	On axis phase shift
C_p	-	Parallel plate capacitance
I_0	-	Peak intensity
ϵ_0	-	Permittivity of free space
ϵ	-	Permittivity of the material
PL	-	Photoluminescence
E	-	Photon energy
h	-	Planck's constant
ϵ_{re}	-	Real dielectric constant
R	-	Resistance
τ	-	Response time
SEM	-	Scanning Electron Microscope
SHG	-	Second Harmonic Generation
$\chi^{(2)}$	-	Second order nonlinear optical susceptibilities

C_s	-	Specific heat capacity of solids (J/Kg.K)
C	-	Speed of electromagnetic wave
dn/dT	-	Temperature coefficient of therefractive index
TGA	-	ThemoGravimetric Analysis
k	-	Thermal conductivity (W/m K)
α_d	-	Thermal diffusivity of the sample
D	-	Thickness of the sample
$\chi^{(3)}$	-	Third order nonlinear optical susceptibilities
E_{gc}	-	Transition energy
T	-	Transmittance
UV/Vis	-	Ultraviolet Visible Spectroscopy
Hv	-	Vickers micro hardness
λ	-	Wavelength
XRD	-	X-Ray Diffraction
σ_y	-	Yield strength