5. SUMMARY, CONCLUSIONS AND FUTURE SCOPE

In this Chapter we provide here a summary of the present research work along with the conclusions derived. Some suggestions for future work are also provided.

5.1 Summary and Conclusions

Crystal growth and characterization is an expanding field in materials science which is identified as a thrust area of research. Artificial crystals are grown everyday and now we are more concerned to discover new materials for the purpose of industrial and academic uses. Recent investigations for materials having better optical nonlinearity with chemical flexibility and mechanical properties have resulted in the preparation of semiorganic materials which are used as nonlinear optical (NLO) devices in practice.

Nonlinear optical (NLO) materials have a significant impact on laser technology, electro-optic modulation, optical communication and optical storage technology. Metal complexes of polarisable ligands are currently explored for their nonlinear optical properties. These have been commonly referred to as semiorganics, as their physical and chemical properties set them apart from the usual organic and inorganic materials. The search for new frequency conversion materials over the past decade has led to the discovery of many semiorganic materials. Semiorganics share advantages of both organic and inorganic materials, which include extended transparency, high optical nonlinearity, good mechanical hardness and chemical inertia.
Single crystals of zinc tris(thiourea) sulphate is an efficient semiorganic nonlinear optical material for second harmonic generation. It has a high damage resistance and low UV cut-off of about 290 nm which makes it suitable for frequency conversion of high power lasers. ZTS is less hygroscopic and crystallizes in orthorhombic structure with space group Pca2\(_1\) (point group mm2). The Second Harmonic Generation (SHG), laser-induced damage threshold, thermal properties and hardness of ZTS crystals are reported to be better when compared to other nonlinear materials.

In the present research work, we have made an attempt to grown Zinc – Magnesium Tris(thiourea) Sulphate (ZMTS) single crystals for various molar concentrations of Zinc Sulphate and Magnesium Sulphate. The ZMTS crystals were grown from aqueous solutions by slow evaporation technique. Morphological changes have been observed when ZTS crystals mixed with magnesium sulphate.

The lattice parameters of the grown crystals have been determined by X-ray diffraction technique. The grown crystals were characterized by recording the powder X-ray diffraction patterns and by identifying the diffraction planes. The external appearance of the grown crystals is found to be different when magnesium content increases. Except MTS all the other crystals belong to orthorhombic system and the lattice parameters are found to be in line with those of ZTS crystals. The MTS crystals belong to monoclinic system. Atomic absorption studies reveal the presence of Zn and Mg in ZTS crystals. The flotation method was employed for the precise determination of density. From the measurements of density, it is concluded that density of Mg mixed ZTS crystals increases with increase in the concentration of dopants.
Microhardness studies have been carried out for all the grown crystals. It is observed that microhardness number increases with the applied load for ZMTS crystals. For all the samples of this work, the work hardening coefficients have been calculated. From the values of work hardening coefficients, it is concluded that ZMTS crystals belong to the category of soft materials.

The FT-IR spectra have been recorded in the range 400-4000 cm\(^{-1}\) for all the samples. The important functional groups associated with the crystals and their respective absorption bands/peaks have been identified and assigned. ZMTS crystals observed that there is broadening, narrowing of shift of absorption peaks/bands in the FTIR spectra. The UV-Visible spectra show that the materials have wide optical transparency in the entire visible region. The cut-off wavelength found for all the sample crystals. The Second Harmonic Generation (SHG) was confirmed by Kurtz powder method for all the grown sample crystals.

TGA and DTA studies have been carried out for all the samples of this work. From these thermal studies, it is observed that all the grown crystals have decomposition between 239 ºC and 730 ºC. From TGA/DTA studies, it is concluded that there is no water of crystallization in the lattice of ZMTS crystals. Due to the more hardness, good thermal stability and good transparency, ZMTS crystals may be a better alternative for ZTS crystals in technological, industrial and academic uses.

The capacitance and dielectric loss factor (\text{tan} \delta) measurements were carried out using a Precision LCR meter (Agilent 4284A) with a frequency of \(10^2\text{-}10^6\) Hz at room temperature (30ºC) along the a- direction and at different temperatures ranging from 40-120ºC using the conventional parallel plate capacitor method for all the
eleven grown crystals. DC electrical conductivities were measured by two-probe method at various temperatures ranging from 40-120ºC along a- direction. From electrical studies, it is observed that the values of dielectric constant ($\varepsilon_r$), dielectric loss (tan $\delta$), AC conductivity ($\sigma_{ac}$) and DC conductivity ($\sigma_{dc}$) of ZMTS crystals increase with the increase of temperature and with the increase of concentration of Mg$^{2+}$ ions. The increase in the values of electrical parameters is attributed to the presence of charged concentration in the lattice of ZMTS crystals. Activation energies were also determined for both DC and AC conduction processes taking place in the ZMTS crystals.

5.2 Suggestions for Future Work

Development of technology in the near past has stimulated the importance of discovering new materials. With an interest to discover new materials, in the present investigations, Zinc - Magnesium Tris(thiourea) Sulphate ($\text{Zn}_x\text{Mg}_{1-x}[(\text{CS (NH}_2)_2]_3\text{SO}_4$) different molar concentrations, (x = 0.0 to 1.0 in steps of 0.1) total of 11 samples grown by slow evaporation technique at room temperature. ZTS crystals are NLO materials which find applications in SHG, opto-electronics and optical communications. In the future, much interest will be shown to discover new NLO crystals by doing research on crystal growth in our laboratory.

Scientific research on crystal growth and characterization is normally constituted by the following:

(i) Nucleation and growth of crystals and

(ii) Structural and physical characterization.
Technological research on crystal growth and characterization is normally constituted by the following:

(i) Growth of large crystals and
(ii) Fabrication of devices with the grown crystals.

The present research work (reported in this thesis) is of scientific nature only and not technological. Several investigations have been made in the present research work and several useful results have been obtained. However, the present study indicates that several more investigations have to be carried out in the future to understand the full potential of these new mixed crystals.

As the grown ZMTS crystals are found to be more stable, harder, and wide optical transparency, their applications in device fabrication and electro-optic modulation are expected to bring good results in the future. The electrical measurements (AC and DC) may be extended to lower temperatures for both the pure ZTS and ZMTS crystals considered in the present study.

In the present study, Zinc - Magnesium Tris(thiourea) Sulphate (Zn$_x$Mg$_{1-x}$[(CS(NH$_2$)$_2$)$_3$]SO$_4$) with different molar concentrations, total of 11 samples grown. In the future, the study may be extended by considering the left out evaporation of Zn$^{2+}$ and Mg$^{2+}$.

Large single crystals may be grown.

The effect of organic and inorganic impurities on these mixed crystals may be carried out.