CHAPTER-VII

CONCLUSIONS AND SUGGESTIONS FOR FUTURE WORK

7.1 Summary and Conclusions

The aim of this work is to grow and study some amino acid and thiourea based nonlinear optical single crystals. Growth of crystals from aqueous solutions is one of the methods of crystal growth which is extremely popular in the production of many technologically important crystals that were adopted to grow the NLO crystals. Various physical properties of the crystals are studied for application point of view. This chapter summarizes the main results obtained in this work along with further studies that can be carried out in future. Amino acid based salts were synthesized by mixing L-asparagine monohydrate with Phosphoric acid, L-histidine monohydrate monohydrochloride mixed with Phosphoric acid, and 3% KCl and the samples are abbreviated as, LASP, LHMHCL, LHMHCL-3% KCl, LHP. Thiourea based salts were synthesized by mixing with sodium nitrate, and was further doped with 1% KCl, and 2% NaCl and the samples are abbreviated as BTSN, BTSN-1% KCl, BTSN-2% NaCl. Solubility studies in the temperature range 30-55 °C for all the synthesized samples were performed. It is found that solubility of the samples increases with increase in temperature. Materials having moderate to high solubility can be grown by low temperature solution growth and this method is well suited for growing amino acid and thiourea based crystals. Transparent single crystals of the synthesized salts were successfully grown by slow evaporation technique (low temperature solution growth) at room temperature (30 °C).

From XRD studies, the lattice parameters of the grown crystals have been determined and the crystals of LASP, LHMHCL, LHMHCL-3% KCl, LHP, BTSN, BTSN-1%KCl, BTSN-2%NaCl crystallize in orthorhombic structure.
The grown crystals were further characterized by recording the powder X-ray diffraction patterns and by identifying the diffraction planes. The reflections of powder XRD patterns of the grown samples were indexed using INDEXING software package.

The FTIR spectra of the samples were recorded in the range 400-4000 cm\(^{-1}\). The important functional groups such as \(\text{NH}_3^+\), OH, COO\(^-\), P=O, C-S etc of the grown crystals were identified from the spectra. The FTIR spectra confirmed the protonation of the amino group in the samples. UV-Visible transmittance spectra of the grown samples were recorded in the wavelength range 200-1100 nm. The crystals have sufficient transmission in the entire visible and near IR region. This property enables the material for optoelectronic applications. Using Tauc’s plots, the values of optical band gap of the grown crystals of this work were obtained and it is confirmed that the samples are wide band gap materials. The EDAX spectrums of the grown samples were recorded and the weight percentage of the dopant is recorded.

TG/DTA studies of the grown samples were carried out using a thermal analyzer in nitrogen atmosphere at a heating rate of 20°C/minute for a temperature range of 10-700 °C. The TG/DTA studies establish that the samples are thermally stable up to their melting points/decomposition points. The thermal stability indicates that the samples can be used for device fabrication. From dielectric studies, the dielectric behaviour of the samples was analyzed. It is observed that the values of dielectric constant and dielectric loss factor of the samples decrease with increase in frequency and increase with increase in temperature. The nature of decrease of dielectric constant and dielectric loss with frequency suggests that the crystals seem to contain domains of continuously varying relaxation times. Low value of dielectric loss indicates that the grown crystals of this work are of good quality. It was noticed
that AC conductivity increases with increase in temperature. The values of activation energy were determined and found to be low for the grown crystals. The obtained values of dielectric parameters such as dielectric constant, loss factor and AC conductivity help us to understand various electrical phenomena that are taking place in the samples.

The Kurtz powder technique was used to test the second order NLO activity and SHG measurements have shown that some of the amino acid based samples of this work are second harmonic generators and hence the samples can be useful in the fields of optical communication, optical computing, optical data processing, optical data storage. Significant wider optical transparency and lower cut-off values of the samples make them promising materials for NLO applications involving frequency doubling process and other NLO phenomena.

Micro hardness studies are carried out for the grown crystals. From the results of micro hardness studies, it is observed that the hardness number increases with the increase in load showing reverse indentation size effect. The values of work hardening coefficient for the samples have been calculated using the Meyer’s relation. From the values of work hardening coefficients, it is concluded that all the samples belong to the category of soft materials.

7.2 Suggestions for Future work

In this work, the growth of single crystals was carried out by solution method with slow evaporation technique. It is suggested that the crystals of this work can also be grown by Sankaranarayanan-Ramasamy (SR) method and gel method. A comparative study can be made on the crystals grown from solution method and gel method and their properties can be studied for the suitability for NLO applications. Doping of crystals is known to change physical and chemical properties of crystals
and attempts can be made to add various organic and inorganic dopant into the amino acid based samples. The electro-optic and piezoelectric phenomena can be carried out for the samples of this work in the future. Attempts could be made to grow bulk size crystals by estimating the growth parameters using nucleation experiments. Large size crystals are more effective for second harmonic generation devices. As already mentioned, some of the samples exhibit second harmonic efficiency showing a bright emission of green light. Hence, various NLO related studies may be carried out. Experiments may be performed to determine the nonlinear optical, electro-optic, piezoelectric coefficients and nonlinear absorption which are important parameters for NLO samples. It is suggested that laser damage threshold experiment, etching studies, SEM studies and HRXRD studies can be performed for the samples of this work in the future.