CHAPTER 6

SUMMARY AND SCOPE FOR FUTURE WORK

6.1 INTRODUCTION

This chapter describes the general conclusions derived from the work carried out for this thesis. While detailed and specific conclusions are discussed in the respected chapter, general conclusions would give an overall perspective of the entire investigations carried out. Briefly discussed at the end is the scope for future work.

6.2 GENERAL CONCLUSIONS

In recent years considerable attempts are being made to design and synthesize new nonlinear optical (NLO) materials with enhanced second harmonic conversion efficiencies with phasematching ability for nonlinear and electro-optic applications. In this direction a new organic NLO material, 2-amino-4-picolinium nitrophenolate nitrophenol (2A4PNN) has been synthesized and the single crystals were grown using solution growth method after analysing their solubility and nucleation. This material crystallizes in noncentrosymmetric space group of $Pna2_1$ in orthorhombic crystal system. Optical transmission spectrum showed extended transparency down to 425 nm and no absorption was seen in Nd:YAG fundamental as well as second harmonic frequencies. The grown single crystal was non-hygroscopic in ambient condition and its thermally stable upto its melting point 103.08 °C. It

is also identified as a phasematchable organic NLO material with good SHG efficiency. Since the device performance of NLO materials chiefly depends on their physical properties a number studies were carried out for 2A4PNN. These include specific heat capacity, laser damage threshold, dielectric, hardness and elastic constant, third order optical property and theoretical DFT calculations. These investigations exhibited that 2A4PNN could be a good candidate for device applications since it is physically rugged, chemically and thermally stable.

Optical quality single crystals are critically important for terahertz generation. DAST has been synthesized and the single crystals were grown using solution growth method. The slow evaporation solution technique is adopted for the growth of these crystals with methanol solvent. The challenging problem of influence of crystallization conditions on the form of resulting crystal was encountered in the case of DAST single crystals. DAST material is dissolved in methanol solution it gives mostly twin DAST crystals. In addition, DAST solution readily absorbs water molecule from atmosphere from slow evaporation technique and its transform to DAST. H_2O (centrosymmetric space group). Efforts were made to grow twin free high quality single crystals by optimizing the growth condition and it could be successfully grown by the slow evaporation method. The crystal structure confirmed that this grown crystal could indeed be DAST. The indigenously grown DAST crystals effectively generate at low frequency output (0.2-3THz).

The challenging problem of influence of crystallization conditions on the form of resulting crystal was encountered in the case of BNA single crystals. This task is invariably achieved by optimizing the growth condition. The BNA was synthesized in the laboratory and the growth of BNA crystal

was performed in selected single and mixed protic and aprotic polar solvents. Attempts were made to grow bulk BNA single crystals by using different polar protic and aprotic solvents. The solvents explored were found to influence growth rate along polar axes (except ethyl acetate grown BNA crystal). Hence it could be understood that the solvents employed for the growth could also influence growth rate, absorption of solvent molecules, morphology, optical transmission, crystal surface quality and THz efficiency. As for the adsorption of inclusions are concerned, it was observed that the interaction between the solute-solvent pairs play crucial role at the crystal-solution interface and that incorporations differ significantly along polar axes. This observation further emphasized the necessity for fruitful attempts on identifying suitable solvent(s) for the growth of crystals from solutions. The high-conversion efficiency (0.25%) and the low-frequency THz output (0.2–3 THz) make this crystal a valuable alternative to LN sources commonly used in this frequency range. Further, this systematic approach has resulted in the generation of THz waves with enhanced efficiency, which is essential to realize their potential applications in the fields such as homeland security, pharmaceutics and medicine.

Placing the OSC on a prefabricated flexible substrate during the growth could be a challenging task but, if achieved, would be a desirable approach. Thin and flexible AN single crystals were grown in a short duration using CS_2 solvent. The OFET was successfully fabricated by depositing AN single crystals on prefabricated flat and flexible substrate during the growth. The charge carrier transport of rapid grown AN single crystal was studied by means of field-effect-transistor. The attempt reported here could facilitate direct growth of other efficient organic semiconductor crystals on prefabricated flat and flexible substrates.

6.3 SCOPE FOR FEATURE WORK

On the whole, present investigated single crystals are still not fully characterized and there are avenues for future work on these crystals. The future work in continuation to the present work may be pursued as follows:

NLO crystal

- Nonlinear Co-efficient of 2A4PNN single crystal
- Phasematching angle of 2A4PNN single crystal
- Birefringence studies
- Electro-optic modulator based on 2A4PNN single crystal

Terahertz crystal

- High Quality with large size crystal for effective terahertz generation
- Identifing new NLO crystal for terahertz application

Semiconductor crystal

- Organic Light Emitting Diode based on rapid grown anthracene single crystal
- Attempts will be made to grow existing organic semiconductor materials by using rapid growth technique for OFET and OLED applications.