CHAPTER - 7

SUMMARY, CONCLUSION AND FUTURE PROSPECTS

7.1 Summary and Conclusion

The following single crystals have been grown using solution growth adopting slow evaporation method for ferroelectric application.

1. Ethylenediaminium Tetrachlorozincate ($(C_2H_{10}N_2)^{2+}[ZnCl_4]^{2-}$)
2. Tetramethylammonium Tetrachlorozincate $[N(CH_3)_4]_2ZnC1_4$
3. Tetraethylammonium Tetrachlorozincate $[N(CH_3)_4]_2ZnC1_4$
4. Tetramethyl tetraethyl ammonium Tetrachlorozincate $[N(CH_3)_4]_2ZnC1_4$
5. 1-(2,3- dimethylphenyl)piperazinium Tetrachlorozincate(II) Monohydrate $[1\text{-}(2,3\text{-}(CH_3)_2C_6H_3)C_4H_{10}N_2]ZnCl_4 \cdot H_2O$
6. Bis(2-amino-6-methylpyridinium) tetrachlorozincate(II) $(C_6H_9N_2)_2[ZnCl_4]$

Stiochiometric amount of basic chemical substances are taken and used solvents suitable for the growth of single crystals which yielded the above said single crystals. In all the systems the anion tetrachlorozincate is retained with different organic cation by using appropriate cationic chemical substance in stoichiometry with the chemical substance zinc chloride adopting necessary crystal growth conditions. Well defined single crystals were identified from each slot and they were used for various characterizations necessary for confirmation and application. Single crystal XRD has been used for confirming the crystal structures of all the above mentioned single crystals and documented well. The various functional groups present in the systems grown are identified with FTIR and wherever necessary Raman studies were also used. UV- Visible studies were undertaken to study the

absorption in the entire region from which the absorption coefficients have been obtained. They gave information about the indirect bandgap nature and the Tauc plot for all the systems estimated the bandgap and revealed the insulating behaviour of all the systems. The zero value of extinction coefficient supports the insulating behaviour and it leads to the absence of imaginary dielectric function. This has promoted us to investigate the dielectric behaviour of all the systems which accounted the high value of dielectric constant in all the cases. This higher value of dielectric constant gave an indication that the materials can be tested for ferroelectric behaviour. The real dielectric constant is derived from the refractive index values. The electronic polarizability is calculated from the real part of the dielectric constant values using the Clausius-Mossotti equation in the optical frequency region. This value of polarizability also confirmed that these materials could have been good candidates for ferroelectric application. Hence we attempted to study the ferroelectric behaviour of these materials by applying electric filed and to study the polarization behaviour. The ferroelectric hysteresis loop obtained in all the cases revealed the ferroelectric behaviour of all the materials. Theoretical Penn analysis has been used for all the cases since this theory essentially uses the value of dielectric constant and the properties related to the wide bandgap semiconductor. The value of electronic polarizability obtained using this method has been compared with the one using Clausius-Mosotti equation and they agreed well. The ferroelectric behaviours among some of the single crystal materials grown have been compared and the possible explanation from the analysis of hydrogen bonding profile using theoretical means is given here in support. Finger print plots gave an evidence of reduction in the interaction between the alkyl group and anion $ZnCl_4$ with the introduction of ethyl

group as it creates disorder in the layered structure. The disorderliness and alkyl chain length substantially influence on the degree of polarizability of $TEAZnCl_4$ crystals, shows high polarizability value (1.44×10^{-22} cm^3) compared with $TMATEAZnCl_4$ (1.20×10^{-22} cm^3).

7.2 Future prospects

1. Choosing appropriate cation with tetrachlorozincate anion by testing with theoretical fingerprint analysis (hydrogen bonding estimation), single crystal of their combination can be tested for better ferroelectric property.

2. The anion can also be changed with appropriated cations and initially tested theoretically for better hydrogen bonding ability and then single crystals of their combination can be tested for definite application.

3. Mutiple cations with anion and multiple anions with cations can be tried to form single crystals which can be tested for betterment in the desired application.

4. Formation of such single crystals are difficult to harvest as the possibility of coordination of multiple cations/anions depend on the availability of coordination centre and the strength of coordination of the given cations/anions.

5. Since organic cations of pervoskite nature in many cases are responsible for the ferroelectric and related properties, chemical substances based on them can be tried.

6. Basically organic single crystals are mechanically soft, their stability and life time are short. Hence they can be prepared as thin films and tested for desired applications.

7. While preparing for organic thin films degradation on annealing and change in structure may be some of the difficulties pose problems to be solved.