Chapter -5

Summary and Conclusions
5. SUMMARY AND CONCLUSIONS

This Chapter provides the summary of the research work carried out together with the conclusions derived.

5.1. Summary of The Work Done

There is an increasing demand for crystals of complex composition containing multiple materials. The mixed and impurity added (doped) crystals of alkali halides are found to be harder and more stable than the end member crystals and so they are more useful in their applications. Also, the development of lasers revived the interest in alkali halides as materials for optical components which led to the development of alkali halide polycrystalline material for use as optical windows. In addition, alkali halide mixed crystals find their applications in optical, opto-electronic and electronic devices. So, it becomes necessary and useful to prepare alkali halide mixed crystals (single as well as poly crystals) and characterize them by measuring their physical properties.

In the present investigation, with an aim of discovering new useful materials, an attempt was made to grow polycrystals of pure and CdS added \((\text{NaCl})_x(\text{NaBr})_{-x}(\text{NaI})_{1-y}\) crystals (for various values of \(x\) and \(y\)) by the melt method. Densities (by the flotation method) and refractive indices (by using the Gladstone’s rule) of pure \((\text{NaCl})_x(\text{NaBr})_{-x}(\text{NaI})_{1-y}\) crystals grown were determined and used for the estimation of
composition in the crystal. Atomic absorption spectroscopic measurements were made to estimate the Cd atom contents in the CdS added crystals.

X-ray powder diffraction data were collected for all the twenty crystals grown (7 pure and 7 CdS added ternary mixed crystals and 3 pure and 3 CdS added end member crystals) and the lattice parameters were determined using the available methods. Thermal parameters like Debye-Waller factor, Debye temperature, mean square amplitude of vibration, Debye temperature and mean sound velocity were determined using the X-ray powder diffraction (integrated) intensity data for all the ten pure (ternary mixed and end member) crystals.

DC and AC (with a fixed frequency of 1 kHz) electrical measurements were done at various temperatures ranging from 40 to 150°C for all the twenty crystals grown by using the parallel plate capacitor method. DC electrical conductivity (σdc), dielectric constant (εr), dielectric loss factor (tan δ), AC electrical conductivity (σac), DC activation energy (E_{dc}), AC activation energy (E_{ac}), etc were determined.

In the case of CdS added (NaCl)$_{0.7}$(NaBr)$_{0.1}$(NaI)$_{0.2}$ crystal, in all the characterization studies, the depth profile was made by making the measurements for three different samples taken from top, middle and bottom portions. In the case of all the other nineteen crystals (both pure and CdS added) sample taken from the middle portion was considered for measurements.
5.2. Conclusions Derived

All the twenty crystals (both pure and CdS added) grown in the present study are polycrystalline in nature, but are found to be compact and can be cut into required shapes and polished. The transparency of the crystals reduced and became white when they were cooled from high (melting) temperature to the low (room) temperature which could be explained as due to introduction of thermal defects and natural impurities into the crystals.

The ternary mixed crystals are found to be more hard, more stable (less deliquescent) and less transparent when compared to the end member crystals. CdS addition leads to brown colouration with significant intensity. The CdS added crystals grown are found to be more hard, more stable and less transparent when compared to the pure simple and mixed alkali halide crystals.

All the X-ray diffraction peaks could be indexed with only one f.c.c. phase for the ternary mixed crystals indicating the single phased mixed crystalline nature. This shows that a continuous series of solid solutions can be prepared with NaCl-NaBr-Nal ternary combination. The lattice parameters determined and the Cd atom contents estimated for the CdS added crystals indicate that the CdS molecules have entered into the lattices of alkali halide crystals. In addition, the CdS addition is found to change significantly the lattice parameters of both the pure and mixed alkali halide crystals.

The thermal parameters obtained in the present study for the \((\text{NaCl})_x (\text{NaBr})_y_x (\text{NaI})_{1-x}\) crystals indicate that the bulk composition has nonlinear influences on them. This is attributed to an increase in the vibrational entropy due to mixing. The
Debye temperature values obtained from the melting point, Kopp-Neumann relation extended to ternary mixed crystals and X-ray diffraction data are in essential agreement with each other. The Debye frequencies obtained lie in the infrared range. The present study indicates that the bulk composition has nonlinear influences on the thermal parameters although a continuous series of solid solutions (mixed crystals) could be made with NaCl-NaBr-Nal ternary combination.

*DC and AC electrical measurements made in the present study indicate that the electrical parameters increase with the increase in temperature. Also, the present study indicates that the bulk composition has nonlinear influences on the electrical parameters. This is attributed to the enhanced diffusion of charge carriers along dislocation and grain boundaries which are expected to be more in mixed crystals considered in the present study. Significant changes have been observed with the electrical parameters caused by the CdS addition.*

The depth profile study made on CdS added \((\text{NaCl})_{0.7}(\text{NaBr})_{0.1}(\text{NaI})_{0.2}\) crystal indicates that the dopant addition creates different layers along the crystal with increase of dopant content from the top to bottom. The crystals can be cut into thin wafers. These wafers will be highly useful for devices as each wafer will have different physical properties. The depth profile study, ultimately, indicates that a series of materials with different properties can be prepared in a single growth experiment.

*In effect, the present study indicates that the pure and CdS added alkali halide mixed crystals grown are expected to be more useful than the end member crystals.*