Abstract

Name of the Scholar: Preeti Singh

Name of the Supervisor: Prof. M.A.Wahab

Department: Physics

Title of the Thesis: "Microscopic and Structural study of Semi-Organic and KDP Crystals with different concentration and impurity content"

Aim & Objective for the present study:

1) To grow Bis Thiourea Cadmium Iodide (BTCI), L-Proline Cadmium Chloride (LPCCM), Tri Glycine Sulpahate (TGS), Potassium Dihydrogen Phosphate (KDP) single crystals by slow evaporation solution technique (SEST).
2) The above selected materials were growing under inverted microscope to unravel the precise mechanism by which the growth takes place and the role of impurities at different concentrations.
3) After successful growth, as grown crystals were subjected to different characterization like powder XRD, HRXRD, FT-IR and UV-Vis spectroscopy, TG/DTA analysis, dielectric and electrical analysis.

Summary of work

Optically transparent good quality single crystals of bis thiourea cadmium iodide (BTCI) were grown by SEST. An attempt has been made to understand the nucleation kinetics of BTCI crystals. Microscopic and Powder X-ray diffraction studies confirm the monoclinic morphology of the grown single crystal. Vibrational and thermal study confirms the cadmium coordination with thiourea in the BTCI complex. Optical study confirms that the grown crystals are highly transparent. Specific heat is found to be 54.319J/g^{o}C. A mechanical study confirms that the grown crystals are mechanically stable. DC conductivity shows its NTCR behaviour and high activation energy. Single crystal grown is free from the major structural defects, confirmed by SEM as well as dielectric study.

LPCCM compound was successfully synthesized and good quality of single crystal obtained by using SEST. We observed that the growth of the cross sectional area of a particular plane was very slow as compared to their lengths. The structure and respective values of lattice parameters, crystalline grain size, tensile strain and dislocation density were calculated using powder X-ray diffraction. The FTIR spectroscopic measurements confirmed the formation of all functional groups in the grown crystal. The optical band gap 5.6eV was determined. The chemical etching study shows the parallel striations and etch pits on the surface of the crystal with increasing

time duration. Photoluminescence study revealed that the crystal shows the prominent emission for violet radiation. The thermal study indicates towards the stability of LPCCM crystal up to its melting point of 200^0C. Improvement in the mechanical strength of the compound is required to be used in devices. Dielectric constant and loss are observed to decrease with frequency. Positive temperature coefficient behaviour is observed in LPCCM single crystal.

Optically transparent pure and L-Glutamic acid (LG) doped TGS single crystals were grown by SEST method. Powder XRD studies revealed that doping has no affect on the crystal system as well as lattice parameters and FT-Raman study confirms the same. Optical study shows increase in the conducting nature of LG doped TGS. The emission spectrum in PL indicates that PRTGS and LGTGS are efficient for absorption of ultra violet light and emission of light in violet region. Thermal study clearly indicates change in the exothermic nature of Pure TGS crystal, due to the presence of dopant. Doped TGS crystals have good and comparable SHG efficiency with KDP. SEM images show the grain which appears to be in round shape and have rock like structure. The lower hardness of the doped crystals indicates the loosening of the lattice due to the incorporation of dopant. The low value of dielectric loss and dielectric constant at higher frequency shows its utility for the fabrication of photonic, electro optics devices and high frequency response devices.

Grown crystals of pure and Mn^{2+} doped KDP are found to be transparent. The growth of the cross sectional area (mid face) of a particular crystal takes longer time to complete (because they require a large number of atoms) as compared to its edges and corners. When two or more growing crystals merge with each other, they generate defects in the form of tilt boundaries and suppress the growth of single crystals. The Powder X-ray diffraction analysis also confirms the Mn^{2+} incorporation in KDP crystal. Dye and PbI_2 doped KDP crystals with different mole concentrations were crystallized by the solution growth technique at room temperature. Dye doped KDP crystals were found to have more inclusion and less transparency as the dye concentration is increased whereas PbI_2 doped KDP crystals were found to have less inclusion and higher transparency. X-ray powder diffraction revealed that the impurities were adsorbed and distorted the crystal lattice parameters. And the crystallite size was found to be changed with doping concentration. Respective values of lattice parameters, crystalline size, and strain were calculated using powder X-ray diffraction results. Powder XRD results and microscope pictures reveal that doping affects the morphology to a certain extent but not the crystal structure.