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Title of the thesis: *"Theoretical and Experimental Studies on GaSe, Ga_3Se_4 Chalcogenide Compounds"*

ABSTRACT

GaSe has attracted the interest of both theoretical and experimental researchers due to its potential applications in making a number of devices like MOSFET, IR detectors, solar cells, etc. A systematic study of GaSe and Ga_3Se_4 is reported in this thesis.

GaSe Poly-crystal: With the help of rocking furnace, the synthesis carried out using specially designed and fabricated ampoule, at low heating/cooling rate, was found to be efficient in getting single-phase and impurity-free GaSe. Hexagonal structure with lattice parameters a = b = 3.7384 Å and c = 16.0282 Å has been confirmed by powder X-ray diffraction (XRD) analysis. The XRD patterns, corroborated with the Raman spectra, emphasizing three strong lines located at 208.89 cm^{-1}, 253.95 cm^{-1} and 306.52 cm^{-1} explain the single-phase crystalline nature of the material. The obtained crystallite size (36.77 nm) of the specimen based on XRD result is an order of magnitude smaller than the observed particle size (10 μm – 400 nm) of the images obtained using scanning electron microscope (SEM). The low values of dielectric constant and dielectric loss confirm that the specimen has low density of defects.

GaSe Single-crystal: GaSe single crystals were grown by the vertical Bridgman technique. Hexagonal structure with lattice parameters a = b = 3.74909 Å and c = 15.90698 Å has been confirmed by powder XRD analysis. Respective values of strain (3.43×10^{-4} lin^{-2} m^{-4})

and dislocation density (1.35 x 10^{14} lin m^{-2}) were calculated using powder XRD results. Moreover, the XRD results revealed the single phase crystalline nature of the specimen whereas the high resolution X-ray diffraction (HRXRD) results confirmed the good crystalline perfection of the specimen. The obtained crystallite size (102 nm) of the specimen based on XRD result was found to be comparable with the observed particle size (115 nm) of the SEM images. Dielectric constant, dielectric loss and ac. conductivity were studied over a wide range of frequencies which shows that the grown crystal behaves like a semiconductor and contains low defect density. Negative capacitance was observed in GaSe single crystals.

Ga_3Se_4 Poly-crystal: With the help of powder XRD result, it was concluded that the growth of polycrystalline Ga_3Se_4 is most favourable at elevated temperatures followed by quenching and long annealing. Dielectric constant, dielectric loss and ac conductivity were studied over a wide range of frequencies which show that Ga_3Se_4 behaves like a semiconductor and contains low defect density. Negative capacitance was observed in Ga_3Se_4.

Ga_3Se_4 Thin film: Thin films of Ga_3Se_4 were deposited on glass substrates by thermal heating method. The powder XRD analysis shows that the as-deposited films are of amorphous nature. Lower cut-off wavelength (550 nm), width of the band tails of the localized states (0.25 eV), optical band gap (2.14 eV), dispersive energy (6.75 eV), oscillator energy (2.86 eV), static refractive index (1.83), and static dielectric constant (3.35) were determined by optical measurements.

References:

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