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Studies on Selenium Rich Nano-Chalcogenides

Study of Metal-chalcogenides at nano scale is interesting in itself in addition to prospects of applications. Particular attention is being paid to size effect on physical and chemical properties. Till now, there have been only limited studies on the nanostructures of lead chalcogenides. Further investigations are required to identify the mechanism responsible for change in properties due to change in size and relative concentrations of such materials.

One of the interesting materials among the group of metal chalcogenides is lead selenides which are distinctive materials, having low band gap, quick response time, high dielectric constant and large Bohr exciton radius (46 nm) [4]. These properties of Lead selenide lead to a strong quantum confinement effect, which holds even for particles of large sizes [5]. These consequences of strong charge confinement and significant optical nonlinearity make lead selenide an ideal material for devices application such as: solar cells, sensors, thermoelectric generators and cooling units [6]. The energy band gap in lead selenide nanomaterials can be easily tailored by varying the alloy composition and by doping with different elements [7].

In this research work, we synthesized nanostructured thin films of the proposed materials. The overall objective of the research work is divided into two parts:

- (i) Synthesis of the Nanostructured materials by Thermal evaporation technique.
- (ii) Characterizations of the synthesized materials for studying their properties.

Our research work thesis is divided into eight chapters which are outlined as follows: **Chapter-1:** General background is presented. The major problems in fabricating of metal chalcogenides nanostructures are mentioned. There applications are simply introduced. The objectives and outline of the doctoral study are also presented.

Chapter-2: presents a comprehensive literature review on nanostructured metal chalcogenides, especially with respect to the effect of doping with different metals in PbSe nanochalcogenides. The fabricating method is described and some important applications of nanostructured metal chalcogenides are mentioned such as: quantum dot solar cells, thermoelectric, IR-detectors and Sensor

Chapter-3: presents the physical methods of synthesis as well as generally used characterization techniques and facilities such as: XRD, SEM, TEM, EDX, SAED, Photo-luminescence (PL) and

UV/VIS Spectroscopy, FTIR-Spectroscopy.

Chapter-4: describes the synthesis and characterizations of $(PbSe)_{100-x}Zn_x$ NPs' thin films via low cost method and studies on properties alterations due to variation of doping content and effect of laser-irradiation time.

Chapter -5: presents the synthesis of Selenium rich lead chalcogenide nanomaterials. The study of variation of Zn-doping as well as Laser irradiation time on the structural and optical properties has been carried out.

Chapter-6: presents low cost synthesis method and describes the characterizations of In doped QDs' thin films of PbSe material. We have studied the effect of Indium doping on PbSe materials for the properties study.

Chapter-7: summarizes the general conclusions of the research work.

Chapter-8: Describes the scope, applications and future plans of the research work.

Our research work comprises of synthesis of three different selenium rich nano chalcogenide materials whose *results* are summarized as follows:

(a) : We synthesized thin films $(PbSe)_{100-x}Zn_x$ thin films composed of NPs via Thermal Evaporation method. The nanoparticles of size 50 nm of $(PbSe)_{100-x}Zn_x$ samples have been synthesizd. Blue shift in the PL emission spectra has been observed on the addition of Zn. This is effect is due to decrease in band gap which is verified by calculated values of Urbach energy and dislocation density (ρ). This result is published in Thin Solid Films Journal (Ashraf, Md Tanweer, et al. "Optical studies on Zn-doped lead chalcogenide (PbSe)_{100-x}Zn_x thin films composed of nanoparticles." *Thin Solid Films* 612 (2016): 109-115)

(b) : We have synthesized $(PbSe)_{100-x}In_x$ thin films composed of QDs From HRTEM images, it has been observed that as-deposited thin film composed of cubic QDs and from TEM-Histogram, the mean particles' size and particles' density come out to be 5.25 nm and 47.8 x10¹² cm⁻² respectively. Blue shift and peak broadening effect have been observed in PL- emission spectra with increase in In concentration. This result is published in journal of Alloys and Compounds (Ashraf, Md Tanweer, et al. "Synthesis and characterization of Indium doped Lead chalcogenides (PbSe)_{100-x} In_x thin films composed of QDs." Journal of Alloys and *Compounds* 701 (2017): 850-857

(c) : We deposited $Pb_5Se_{95-x}Zn_x$ (X= 0, 2.5, 5, and 10) thin films composed of NPs From HRTEM study, we observed that as-prepared sample were contained cubic nanoparticles with average size of 20.5 nm and lattice constant of 0.38 nm; Peak broadening and blue shift behaviors were observed in PL emission spectra with the increase in dopent content and laser-irradiation time. The study of optical absorption suggested a direct band-gap which was found to be increased with increase in metallic impurity as well as laser- irradiation time. This result is published in the journal of Materials Science in Semiconductor Processing (Ashraf, Md Tanweer, et al. "Studies on selenium rich Lead Chalcogenide Pb 5 Se $_{95-x}$ Zn_x (X= 0, 2.5, 5, and 10) thin films composed of NPs." *Materials Science in Semiconductor Processing* 60 (2017): 53-59)