

Characterization of Nanostructure Lead selenide (PbSe) thin films

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Abstract: With reduction in size, novel electrical, mechanical, chemical, magnetic, and optical properties can be introduced. The resulting structure is then called a low-dimensional structure (or system). The confinement of particles, usually electrons or holes, to a low-dimensional structure leads to a dramatic change in their behavior and to the manifestation of size effects that usually fall into the category of quantum-size effects. The low dimensional materials exhibit new physicochemical properties not shown by the corresponding large-scale structures of the same composition. Nanostructures constitute a bridge between molecules and bulk materials. Suitable control of the properties and responses of nanostructures can lead to new devices and technologies. Lead selenide thin films were successfully prepared varying pH by chemical bath deposition technique on glass substrates. The variations were found to affect thickness of the deposited films. The structural and electrical properties of the films were found to be thickness dependent. The X-ray diffraction studies revealed that all films had FCC crystal structure with a (111) preferred orientation. Optical studies indicated that the band gap decreased with increasing thickness of the films. The electrical conductivity decreases with thickness while the dielectric constant increases with thickness.

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Introduction:

The most significant nanostructures required to design nano-electronic devices are Quantum Wells, Quantum Wires and Quantum Dots. They are the basic building blocks of nano-electronic devices. In nano-electronics also we are going to control the transfer of electrons. A standard quantum well layer can be patterned with photolithography or perhaps electron-beam lithography, and etched to leave a free standing strip of quantum well material; the latter may or may not be filled in with an overgrowth of the barrier material (in this case, Ga (1-x)Alx Quantum dots can again be formed by further lithography and etching, e.g. if a quantum well sample is etched to leave pillars rather than wires, then a charge carrier can become confined in all three dimensions, The high extinction coefficient of a quantum dot makes it perfect for optical uses. Quantum dots of very high quality can be ideal for applications in optical encoding and multiplexing due to their narrow emission spectra and wide excitation profiles. A particle cannot escape from the quantum well $0 \leq z \leq L$ and loses no energy on colliding with its walls $z=0$ and $z=L$. In real systems, this confinement is due to electrostatic potentials (generated by external electrodes, doping, strain, impurities, etc.), the presence of interfaces between different materials (e.g., in core-shell nanocrystals), the presence of surfaces (e.g., semiconductor nanocrystals), or a combination of these agents. Motion of the particle in the other two directions (i.e., in the x y plane) inside the quantum well is free. It is

generally accepted that quantum confinement of electrons by the potential wells of Nano meter-sized structures provides one of the most powerful and versatile means to control the electrical, optical, magnetic, and thermoelectric properties of solid state functional materials.

Properties Of Q-Dots:-The optical properties of Q-dots change with size. The basic phenomena can be understood by considering the uncertainty relation between position and momentum for free and confined particles. For a free particle, momentum can be precisely defined whereas the uncertainty in position increases. For a confined particle, the uncertainty in position decreases while momentum uncertainty increases. Color of emitted light is depends on size of Q-dot. Operated at different wavelength by varying dot size and composition. Color of the emitted light is shifted from red to blue when the size of the Q-dot is made smaller. Emission of Q-dot is highly tunable since the size of the Q-dot may be set when it is made, its conductive properties may be carefully controlled. Q-dots naturally produced monochromatic light. The larger the dot, the redder (lower energy) its fluorescent spectrum. Conversely, smaller dots emit bluer (higher energy) light. The coloration is directly related to the energy level of the quantum dot [1]. Larger Q-dots have more energy levels which are also more closely spaced. This allows the quantum dot to absorb photons containing less energy i.e. those closer to the red end of the spectrum. The high extinction coefficient of a quantum dot makes it perfect for optical uses.

Quantum dots of very high quality can be ideal for applications in optical encoding and multiplexing due

to their narrow emission spectra and wide excitation profiles.

Diffraction peaks are associated with planes of atoms

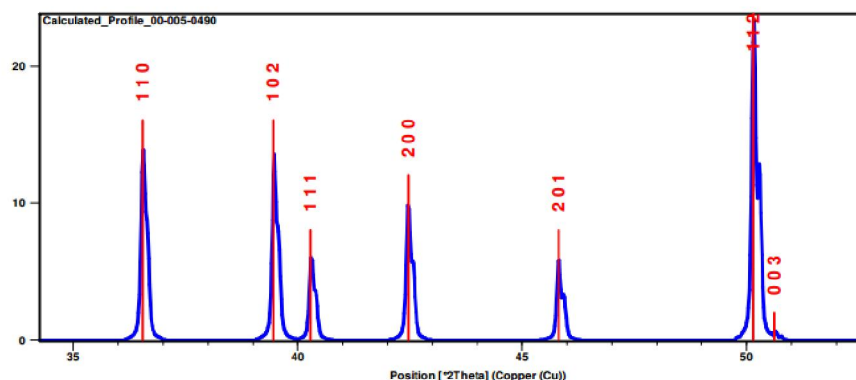


Figure: 1 Diffraction peaks of Cu

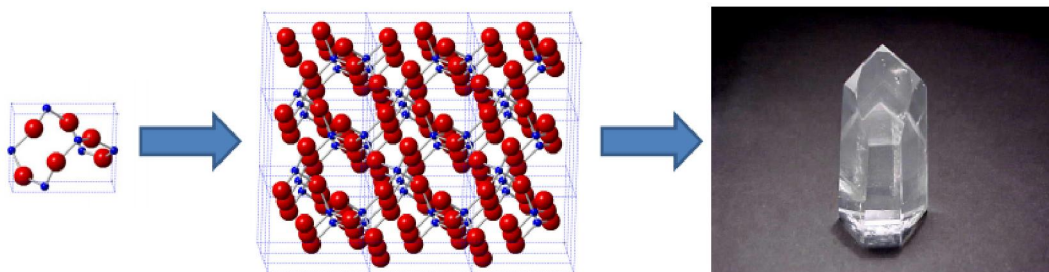
Quantum dot light emitting diodes (QD-LED) and ‘QD-White LED’ are very useful when producing the displays for electronic devices due to the fact that they emit light in highly specific Gaussian distributions. QD-LED displays can render colors very accurately and use much less power than traditional displays. Quantum dot photo-detectors (QDPs) can be produced from traditional single-crystalline semiconductors or solution-processed. Solution-processed QDPs are ideal for the integration of several substrates and for use in integrated circuits. These colloidal QDPs find use in machine vision, surveillance, spectroscopy, and industrial inspection. Quantum dot solar cells are much more efficient and cost-effective when compared to their silicon solar cells counterparts. Quantum dot solar cells can be produced using simple chemical reactions and can help to save manufacturing costs as a result [2]. The latest generation of quantum dots has great potential for use in biological analysis applications. They are widely used to study intracellular processes, tumors targeting, in vivo observation of cell trafficking, diagnostics and cellular imaging at high resolutions. Quantum dots can target specific cells or proteins using peptides, antibodies or ligands and then observed in order to study the target protein or the behavior of the cells. Quantum dots have paved the way for powerful ‘supercomputers’ known as quantum computers. Quantum computers operate and store information using quantum bits or ‘qubits’, which can exist in two states – both on and off simultaneously. This remarkable phenomenon enables information processing speeds and memory capacity to both be greatly improved when compared to conventional computers. Quantum dot (QD) semiconductors have unique optical and electrical properties that make them

promising for use in many applications, such as high-performance field-effect transistors (FETs) and solar cells. Quantum dots are particles with quantum confinement in three dimensions, resulting in a quantized density of states. One effect of such quantization is a size-tunable semiconductor band gap. As the QD continues to get smaller with respect to the material’s exciton Bohr radius, the band gap widens. Such freedom allows a chemist to choose synthetic conditions to grow a QD with the optimal band gap for a given device application. Lead (II) chalcogenide (PbX, X = S, Se, Te) quantum dots have shown particular promise for use in photovoltaic applications. The large exciton Bohr radii for the lead chalcogenides QDs allows for particularly strong confinement when compared to other QDs of similar sizes. Metal chalcogenides thin films even their compounds have been of interest due their semiconducting nature and considerable application in the field of electronics and electro-optical devices. Based on this concept, intensive research has been performed in the past to study the fabrication and characterization of these thin films. Thus, the interest for Lead Selenide (PbSe) semi conducting thin films was motivated by its application in solar cell technology. In the literature, a number of methods for the preparation of PbSe thin films were reported. A number of methods for the preparation of PbSe thin films have been reported, but chemical bath deposition is found to be attractive due to the low cost method of fabrication. Lead Selenide (PbSe) thin films are important materials for applications such as IR detector photographic plates, and photo resistors [3, 4]. Lead Selenide film is used as a target material in infrared sensor, grating, lenses and various optoelectronic devices [5]. PbSe thin films have a

direct band gap of 1.30 eV at room temperature. The possible applications of the material in solar device technology will also be determined. Nanostructured semiconductor materials feature excellent next generation photovoltaic application. Among this class of materials the most impressive results have been obtained from low dimensional PbSe such as PbSe QDs or NCs. To date, PbSe QDs arguably the best choice to generate multiple excitations from single absorbed photon and fast hot electron transfer from active layer to counter electrode. However, in most of the works, synthesis of PbSe QDs is based on chemical method of preparation.

The unit cell is the basic repeating unit that defines the crystal structure. – The unit cell contains the maximum symmetry that uniquely defines the crystal structure. – The unit cell might contain more than one molecule: for example, the quartz unit cell contains 3 complete molecules of SiO₂.

The crystal system describes the shape of the unit cell. The lattice parameters describe the size of the unit cell. The unit cell repeats in all dimensions to fill space and produce the macroscopic grains or crystals of the material.



XRD OF PbSe:

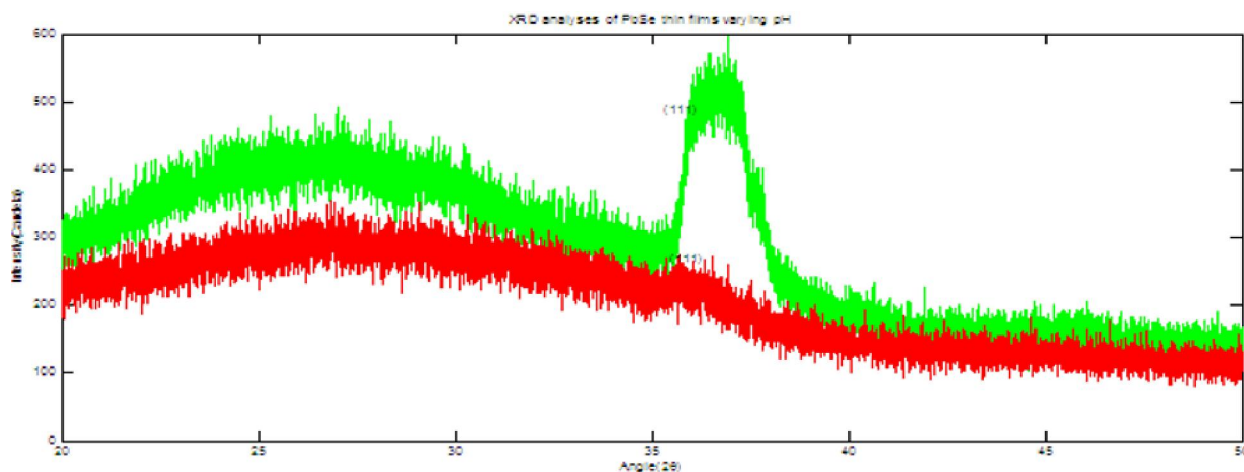


Figure:2 XRD OF 2ml (green) and 4ml (red) PbSe thin films

The XRD diffraction patterns of CBD PbSe thin films deposited for 2ml and 4ml (EDTA) are presented in Fig.2. Phase identification was then made from an analysis of intensity of peak versus 2θ . The PbSe deposited with 2ml (EDTA) ethylenediaminetetraacetic acid peaks at 36.02° which gives rise to a structure with lattice constant $a = 4.315\text{\AA}$ and (111) preferred orientation. The peak for 4ml deposition was observed at 36.49° with lattice constant $a=4.261\text{\AA}$.

The diffraction peak was observed to become much broader with increasing pH values and tends to disappear for higher pH values. Similar effect was observed in previous study by [6]. As the pH of chemical bath increased, the diffraction peak intensity decreased as shown in Fig. 11. It can be seen that the crystal structure of the films was affected strongly by the pH values of the chemical bath. The low intensity peak observed in the XRD pattern of the 4ml sample under study shows that the film is nanocrystalline [7].

The structural parameters of the PbSe thin film are shown in Table. It reveals that lattice constant, the crystal size of the film and the dislocation density increases with film thickness, but micro strain decreases with the increased film thickness. Since the dislocation density and strain are the manifestation of dislocation network in the films, the decrease in the strain of the material indicates the formation of higher quality films. This effect had also been noted by [8] in previous work. This may be due to the decrease in imperfections and dislocations of the films with increasing film thickness.

Calculations

The theoretical considerations of the optical and electrical properties of the films are as discussed in [9-18].

From the XRD analysis of the inter-planer distance (d) and lattice constants (a) as were calculated. The crystallite (grain) size (D), dislocation density and the micro strain (ε) were also calculated using the expressions below:

1. Grain size (D) was calculated using Scherer's formula

$$D = K\lambda / \beta \cos\theta \dots\dots\dots 1$$

where λ is wavelength of x-ray,
β is FWHM (full width half maximum),
θ is the diffraction angle and

K is 0.9 which varies with (h, k, l) and crystallite shape.

2. The lattice constant (a) was calculated with:

$$a = d (h^2 + k^2 + l^2)^{1/2} \dots\dots\dots 2$$

3. Micro strain: It is the root mean square of the variations in the lattice parameters across the individual crystallites, usually across microscopic distances.

$$(\epsilon) = \beta \cos\theta / 4 \dots\dots\dots 3$$

4. Non Uniform Strain:

Peak broadening may not only come from the size effect, but can also be due to strain in the particles. One way to separate the stress due to particle size from that due to stress is by the Williamson-Hall expression (8) where η is the strain in the particles which is a dimensionless quantity. For non uniform strain the formula is given below

$$\beta \cos(\theta) = \frac{k\lambda}{d} + \eta \sin(\theta) \dots\dots\dots 4$$

Where, d is partical size This method demand good data for both high and low angle reflexes. But it is difficult to get reliable data for the FWHM for both the peaks at low and high angles. So that the result comes from this is not accurate.

5. Average strain calculated by using

$$\epsilon = \beta / 4 \tan\theta \dots\dots\dots 5$$

Table: Structure Parameter Of Pbse Thin Flim

SAM- PLE	(h,K,l)	FWHM (B)	2θ (deg)	PARTI-CAL SIZE (D) (nm)	d (inter-planar spacing) (Å)	a (lattice constant) (Å)	NON STRAIN (η) (10 ⁻⁴)	UNIFORM	AVERAGE	Micro-strain
									STRAIN	ε (10 ⁻³)
2ml	(1,1,1)	0.422	36.02	3.451	2.49	4.315	-9.9337		0.3245	0.1002
4ml	(1,1,1)	0.9216	36.49	1.584	0.921	4.216	-4.0000		0.6990	0.2188

Conclusion

Lead selenide thin films were successfully prepared varying pH by chemical bath deposition technique on glass substrates. The variations were found to affect thickness of the deposited films. The structural and electrical properties of the films were found to be thickness dependent. The X-ray diffraction studies revealed that all films had FCC crystal structure with a (111) preferred orientation. Optical studies indicated that the band gap decreased with increasing thickness of the films. The electrical conductivity decreases with thickness while the dielectric constant increases with thickness.

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