Optical Properties and Band Offsets of CdS/PbS Superlattice.

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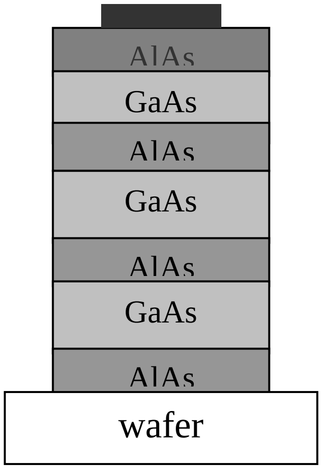
ABSTRACT

CdS/PbS superlattice has been fabricated using the chemical bath deposition method. We report optical investigations of Cds/PbS system to provide measurement of the band offset. Our results yield a valance band offset of 0.2eV. Our results also show the band alignment to be normal, making it a type 1 superlattice. We also report other optical properties, which include: Transmittance, reflectance, optical conductivity, dielectric constant, refractive index, extinction coefficient, etc.

(Keywords: chemical bath deposition, type 1 superlattice, semiconductor, optical properties)

INTRODUCTION

Semiconductor superlattices (SL), which were proposed by Esaki and Tsu [1970] about forty years ago, constituted as shown in the figure below, are structures consisting of alternating layers of two different semiconductor materials, for example AlAs/GaAs, ZnS/CdS, $GaAs/GaAs_{1-x}P_x$, Ge/GaAs, etc.



Semiconductor Superlattice

Two kinds of superlattices are envisioned (Smith D.L, 1990), namely:

(a) **Compositional Superlattice:** This type of superlattice consists of alternating layer of two different semiconductors. The thickness of the individual layers is between a few angstroms and a few hundred angstroms. The composition variation modulates the electronic potential on a length scale shorter than an electron mean free path (Esaki and Chang, 1976). The two materials possess different bandgaps. These lead to discontinuities in both the conduction and valence band.

(b) Doping Superlattices: This type of superlattice consists of alternating n- and p- type layers of a single semiconductor. The electric fields generated by dopant modulate the electronic potential. More recently, superlattices in which both the composition and doping are modulated have been considered (Dohler, 1985).

In fact, first approximation semiconductor superlattices can be considered as a series of quantum well separated by potential barriers and coupled through resonant tunneling interaction. Due to this coupling, the discrete energy levels, which would corresponds to isolated and non-interacting quantum wells, broaden in the Z-direction perpendicular to the plane of the layers and give rise to superlattice conduction and valence mini-bands or sub-bands, leading to a band structure which are actually different from those of the host material involves and can be tailored by changing the parameters like thickness of the layers or barrier material, for example.

Because of their completely new properties which are not present in homogenous semiconductors, hetero-structures and superlattices have opened up a new dimension in the field of microelectronics (Capasso, 1990). Devices based on this new concept are being realized both in the area of very fast circuits and in optoelectronics. This whole domain, however, is still in its infancy and promises a great deal for the future [Esaki, 1970].

Calculation of the vibrational features of disordered superlattices is likely to originate interesting development, both for the application such as the spectroscopic characterization of interface disorder and for the fundamental aspects, such as a deeper understanding of the relations between confinement and localization in superperiodic systems.

The combination of double hetero-structure lasers with glass fibers forms the basis of the new light wave communication technology that is gradually replacing transmission of signals over copper wire.

Heterostructures offer extra degrees of freedom in design of semiconductor junction devices, because both the impurity doping and conduction and valence band offsets at the junction can be controlled. This freedom is the basis of the prediction that most devices that utilize compound semiconductors will in the future incorporate heterostructures [Smith, 2002]. They have attracted growing attention over the past twenty years. The technological interest is due to their unique transport properties along the growth direction. Valence Band and Conduction Band Offset (VBO and CBO) are fundamental parameters which control such transport properties in microelectronic devices.

The first attempt to grow superlattices used the chemical vapor deposition technique in $GaAs/GaAs_{1-x}P_x$ ($0.1 \leq x \geq 0.5$) material system [Blakeslee and Aliotta, 1970]. Other methods such as molecular beam epitaxy, metal organic vapor deposition, glow discharge process, etc., have also been used to grow superlattices. Here we report the synthesis of CdS/PbS superlattice using a simple, reproducible, and cost effective technique called chemical bath deposition [Ortega, 1993].

Materials and Methods

We synthesized all the films for this experiment using chemical bath deposition (CBD). Single films of CdS and PbS were first fabricated before the superlattices were made.

The deposition of CdS thin film was based on the reaction between cadmium bromide ($CdBr_2$), thiourea ($CS(NH_2)_2$, using TEA ($N(CH_2CH_2OH)_3$ as a complexing agent, and ammonia solution as a pH adjuster.

The reaction mechanism is of the form:

$$CdBr_2 . 4H_2O + TEA \rightleftarrows Cd(TEA)^{2+} + 2HOBr + 2H_3O$$

$$Cd(TEA)^{2+} \rightleftarrows Cd^{2+} + TEA$$

$$(NH_2)_2CS + OH^- \rightleftarrows CH_2N_2 + H_2O + HS^-$$

$$HS^- + OH^- \rightleftarrows H_2O + S^{2-}$$

$$Cd^{2+} + S^{2-} \longrightarrow CdS$$

The deposition of PbS thin film by CBD was based on the reaction between lead nitrate ($Pb(NO_3)_2$ and thiourea ($SC(NH_2)_2$), using EDTA disodium salt as a complexing agent and ammonia solution as a pH adjuster at 300K.

The reaction mechanism is of the form:

$$Pb(NO_3)_2 + EDTA \rightleftarrows (Pb(EDTA)^{2+} + 2NO_3^{2-}$$

$$(Pb(EDTA]^{2+} \rightleftarrows Pb^{2+} + EDTA$$

$$(SC(NH_2)_2 + OH^- \rightleftarrows CH_2 N_2 + H_20 + HS^-$$

$$HS^- + OH^- \rightleftarrows H_20 + S^{2-}$$

$$Pb^{2+} + S^{2-} \longrightarrow PbS$$

After the deposition of the single layer films were achieved, CdS/PbS superlattice was fabricated by dipping a glass substrate already coated with CdS thin film into a bath containing lead nitrate, thiourea, ammonia solution, and EDTA disodium salt and left to stand for 1hour at a pH value of ~11.

Structural, surface morphology and optical characterization of the films were carried out using an x-ray diffractometer with Cukα radiation, an Olumpus optical microscope, and a Janway 6405 UV/visible spectrophotometer, respectively.

From the spectrophotometer, the absorbance in arbitrary units was measured. Parameters such as band offset, transmittance, reflectance, refractive index, extinction coefficient, dielectric constant, and optical conductivity were then calculated.

RESULTS AND DISCUSSION

Figures 1, 2, and 3 are plots of absorption coefficient squared (α^2) versus photon energy for CdS, PbS, PbS/CdS, and CdS/PbS. From these graphs, the optical bandgap energies for CdS and PbS semiconductor and PbS/CdS and CdS/PbS superlattices were obtained. The values were found to be 2.49eV for CdS, 1.90 for PbS, 2.30eV for CdS/PbS and 2.50eV for PbS/CdS.

Our value is in close agreement with a range of 2.25eV – 3.10eV reported by Liu et al. for PbS - coated with CdS thin film.

A valence band offset (V_{BO}) of 0.2eV was then calculated for the superlattice. The band alignment in this system is normal, making CdS/PbS a type 1 superlattice as shown in the diagram below:

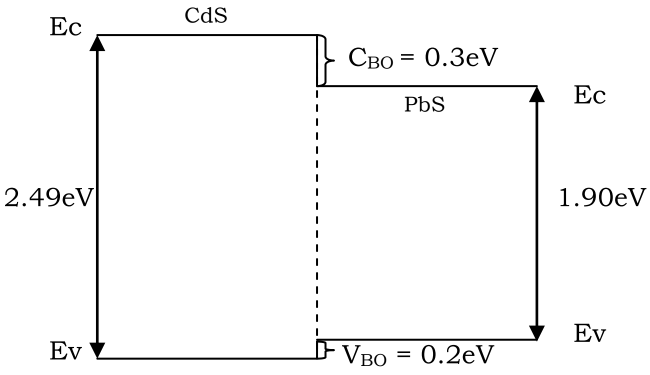


Figure 4 is a plot of transmittance versus wavelength for CdS/PbS and PbS/CdS superlattice. CdS/PbS has a low transmittance throughout the vis-region with 29% at 680nm and 3% at 400nm. PbS/CdS also shows the same trend, with 2% at 400nm and 49% at 680nm. PbS/CdS has a high transmittance in the near infrared region (NIR).

This makes this material useful in the construction of poultry houses to allow enough infrared radiation to warm the very young chicks during the day. This will invariably reduce the cost of energy consumption through the use of stoves, heaters, electric bulbs etc. and the hazards associated with them.

Figure 5 is a plot of absorbance against wavelength in the vis-region for CdS/PbS and PbS/CdS superlattices. Both superlattices show high absorbance at the beginning of the vis-region which decreases as wavelength increases with a range of 1.694-0.310 and 1.587-0.545 for PbS/CdS and CdS/PbS at wavelength range of 400-680nm.

Figures 6, 7 and 8 are plots of refractive index (n), extinction coefficient (K) and optical conductivity (σ_0) for CdS/PbS and PbS/CdS superlattices. A refractive index value of 2.62 and 2.40 at 1.83eV is obtained for PbS/CdS and CdS/PbS.

This high refractive index value makes this material useful in solar cells and anti-dazzling coating. The extinction coefficient for CdS/PbS has a peak value of 12.6x10^{-2} at 3.11eV and a minimum value of 4.3x10^{-2} at 1.83eV. PbS/CdS has a peak value of 13.5 x10^{-2} at 3.11eV and a minimum value of 2.5x10^{-2} at 1.83eV. CdS/PbS superlattice has an optical conductivity (σ_0) value of 4.596x10^{13}S^{-1} at 1.83eV, while PbS/CdS has 2.851x10^{13}S^{-1} at 1.83eV.

Figures 9 and 10 are plots of reflectance and dielectric constant against wavelength and photon energy respectively. For both superlattices, the reflectance shift to lower values as wavelength increases with a relatively low value throughout the region.

This low value of reflectance, have useful application in antireflection coating. For the two superlattices, an almost uniform imaginary dielectric constant is obtained, with values of 0.208 and 0.129 at 1.83eV for CdS/PbS and PbS/CdS. The real part of dielectric constant shows a value of 5.770 at 1.83eV for CdS/PbS and 6.862 at 1.83eV for PbS/CdS.

Figures 11, 12, and 13 show the x-ray diffraction spectra of CdS, PbS and CdS/PbS while Figures 14, 15, and 16 show the optical micrographs at magnification of 100x.

From the micrographs, grain size of 0.3μm was found for both superlattices. The surface of the films was found to be smooth and covers the glass substrate well.

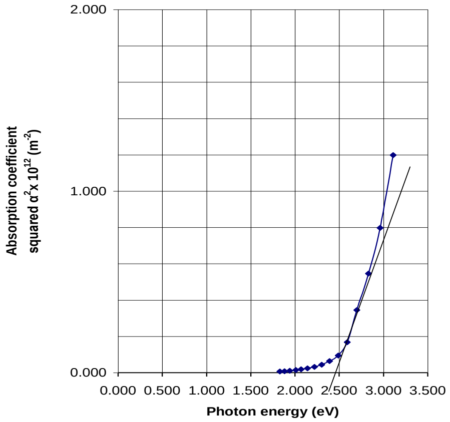


Figure 1: Plot of Absorption Coefficient Squared (α^2) against Photon Energy for CdS Thin Film.

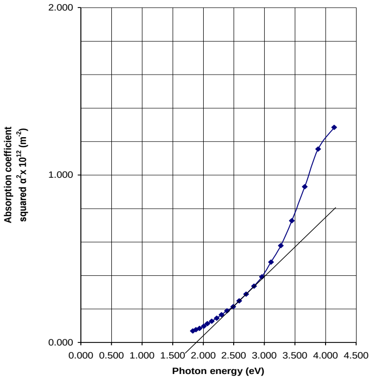


Figure 2: Plot of Absorption Coefficient Squared (α^2) against Photon Energy for PbS Thin Film.

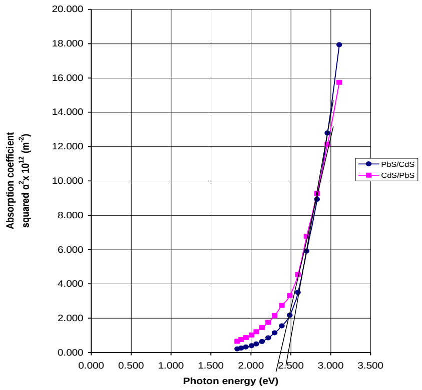


Figure 3: Plot of Absorption Coefficient Squared (α^2) against Photon Energy for PbS/CdS and CdS/PbS Superlattices.

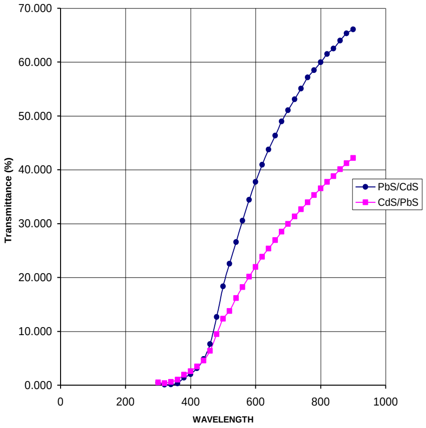


Figure 4: Plot of Transmittance versus Wavelength for PbS/CdS and CdS/PbS Superlattices .

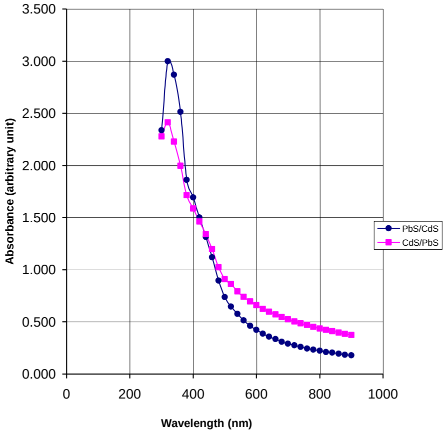


Figure 5: Plot of Absorbance versus Wavelength for PbS/CdS and CdS/PbS Superlattices.

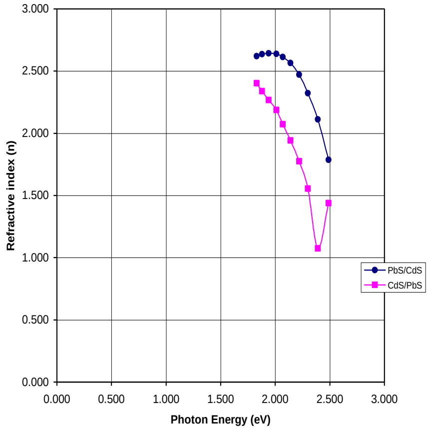


Figure 6: Plot of Refractive Index versus Photon Energy for PbS/CdS and CdS/PbS Superlattices.

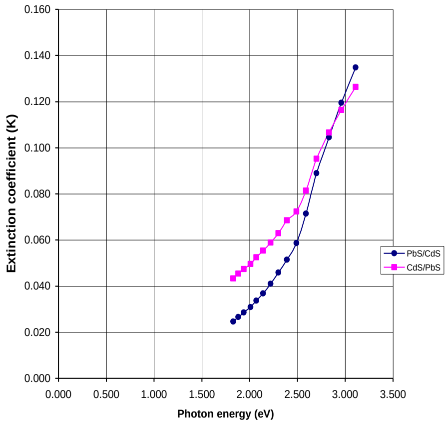


Figure 7: Plot of Extinction Eoefficient versus Photon Energy for PbS/CdS and CdS/PbS Superlattices.

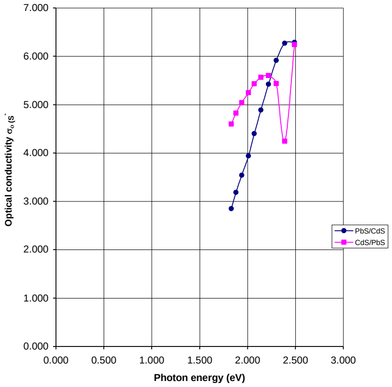


Figure 8: Plot of Optical Conductivity versus Photon Energy for CdS/ZnS Superlattice.

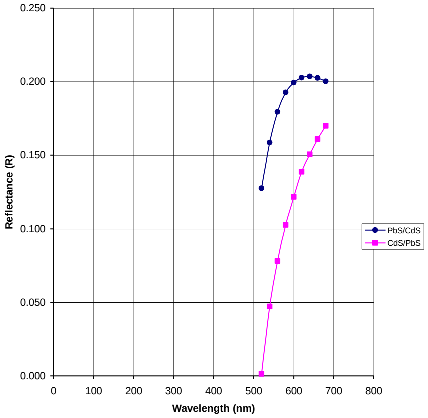


Figure 9: Plot of Reflectance versus Photon Energy for CdS/ZnS Superlattice.

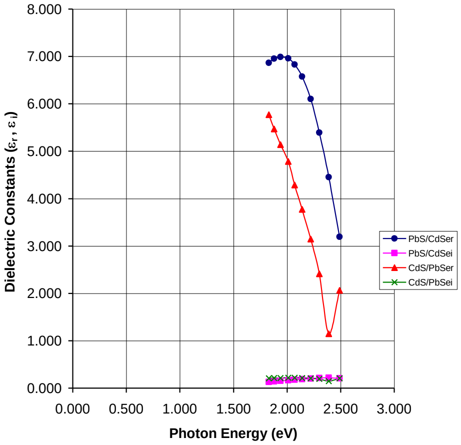


Figure 10: Plot of Dielectric Constants (ε_r, ε_i) versus Photon Energy for CdS/ZnS Superlattice.

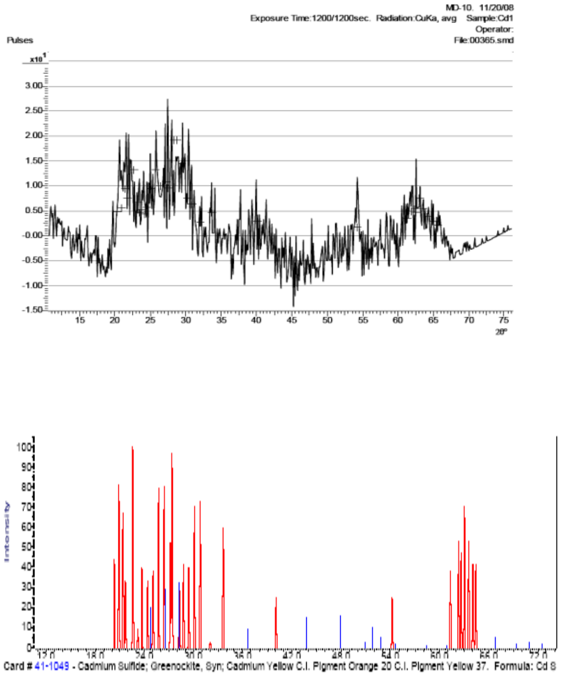


Figure 11: X-ray Diffraction Spectra for CdS Thin Film.

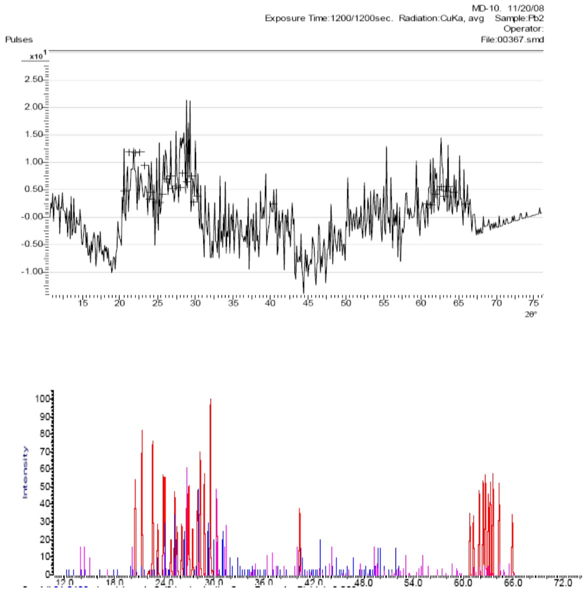


Figure 12: X-ray Diffraction Spectra for PbS Thin Film.

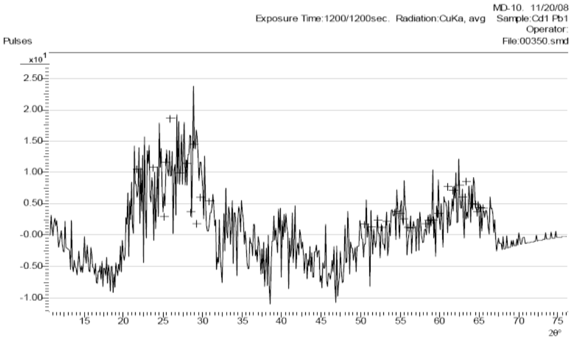


Figure 13: X-ray Diffraction Spectra for CdS/PbS.

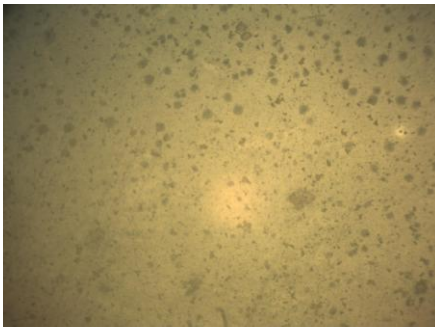


Figure 14: Micrographs of CdS Thin Film.

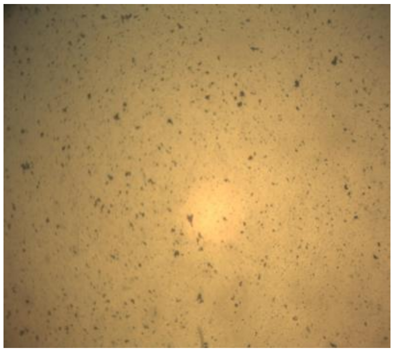
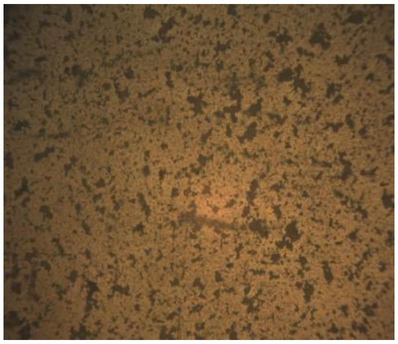


Figure 15: Micrographs of PbS Thin Film.



(b) x 100

Figure 16: Micrographs of CdS/PbS.

CONCLUSION

We have demonstrated using chemical bath deposition technique, the synthesis of CdS/PbS superlattice. A band offset, refractive index and dielectric constant of 0.02eV, 2.40 and (5.77 and 0.208) respectively were obtained for this superlattice. Our results show the band alignment to be a type 1 superlattice.

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