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STUDY OF OPTICAL PROPERTIES OF ZnS THIN FILM USING SIMULATION SOFTWARE

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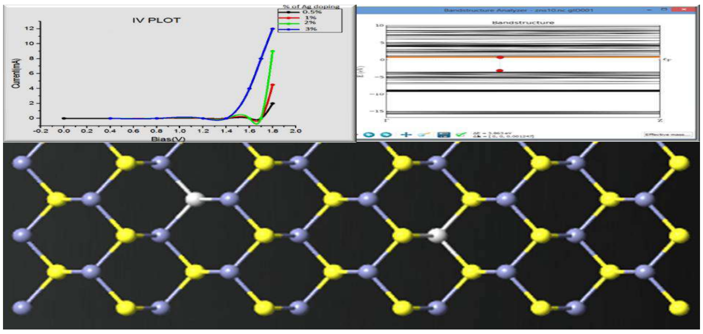
ABSTRACT

Semiconductor nonmaterials have been receiving great attentions. Among these various semiconductors nonmaterial's zinc sulfide is a versatile material because of its physical, chemical and optical properties. ZnS has a wide band gap (3.5-3.9 eV) when in bulk but band gap increases when it is in nano form. It is used in various applications electronic devices, biomedical field, variety of sensors and many more. In the present study, thin layer of ZnS was formed using VNL-ATK software and results were compared with the nano particle synthesized via chemical route. The ZnS was doped with nickel, cobalt and silver and the effect of doping with different materials was studied. Optical properties were studied using UV-VIS spectroscopy, Simulation was done using VNL-ATK software and the experimental results were compared and found to be similar within error limits.

Graphical Abstract



KEYWORDS: Band Gap, Nano Particle, Sol-Gel Method, VNL-ATK Software, Zinc Sulphide

INTRODUCTION

In the recent years, particularly compound semiconductors comprising of group II-VI have gained importance due to their optically active nature and size dependent excitation energy [1]. More over they have relatively high band gap energy, short carrier diffusion and large ionicity, in comparison to III-V compounds [2]. Group II-VI nanomaterials show promising behavior in optoelectronics devices. They are also much used in electronics, photonics, sensors, nano devices etc [3]. ZnS is direct band gap semiconductor which makes it suitable for electronic as well as optoelectronic applications [4]. The band gap ranges from 3.66 eV for cubic and 3.9eV for hexagonal phase of ZnS[5][6]. Zinc sulfide, has high bulk refractive index (n = 2.36 at 620 nm calculated by Abbe method) and due to its lack of absorption in the visible and near IR region (from 400 nm to 2400 nm),it is an attractive material for the use as a suitable inorganic component to improve the properties of nanocomposites [7]. Zinc sulfide is mainly used as an optical material transmitting from visible light to infrared region. It can be used as an optical window or shaped into a lens [8].

MATERIALS AND METHODS

The simulation was done using VNL-ATK [9]. The thin film was simulated using 10 layers using DFT calculator and (3x3x3) K-point sampling and LDA exchange correlation. After obtaining simulation results ,one set of sample was actually synthesized using sol-gel chemical precipitation[10] method at room temperature in which 1M zinc acetate and 1M sodium sulfide were mixed in the magnetic stirrer mixing them drop wise. The precipitate was washed five times with water and two times with ethanol. Thereafter the obtained particles were dried overnight at 90^{o} C. This set of samples was doped with cobalt with 1,2,5,6 and 8% using 1M cobalt acetate. Another set was doped with 1%, 3% and 5% Nickel. The UV-Vis spectra were obtained using Lambda750 (Perkin Elmer) Spectrometer. The optical bandgap was obtained from Tauc plot.

RESULTS AND DISCUSSIONS

The band structure and electronic properties of ZnS thin film was studied using density functional theory and the results were compared with experimental data. Software analysis showed that the effect of doping due to cobalt, nickel and silver influences the band structure. It was found that in case of undoped ZnS thin film the Fermi level is near the conduction band with a band gap of 3.86 eV as shown in **figure1** and the peak amplitude of density of states is found to be near the valence band but when it is doped with cobalt, nickel and silver the Fermi level shifts

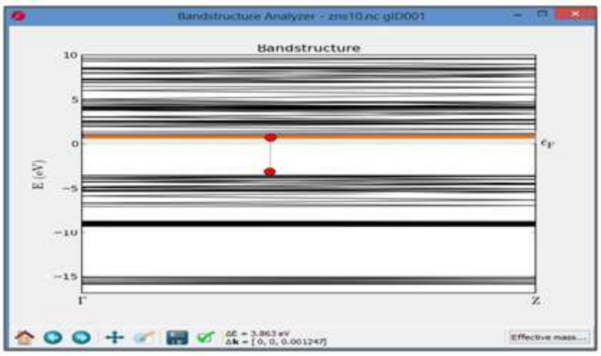


Figure 1: Band Structure Analyser of 2.71 Nm ZnS Thin Film Showing Band Gap of 3.86 eV

Also it was found that the band gap increases in case of doping with cobalt and nickel from the intrinsic semiconductor characteristics but in case of the silver doping the band gap was found to be decreased even at very low concentration of doping atoms of silver. The observed change in band gap for different concentrations of cobalt was 505eV to 5.35eV shown in Table 1. And that for nickel was 5.31eV to 5.87eV Table 2. But in case of silver the band gap decrease was 3.40eV to2.40 eV Table 3. The observed band gaps by observed with simulation are shown in figure 2(a) and 2(b). This suggest that the the band structure of ZnS film can be modified with the help of doping using different doping materials.

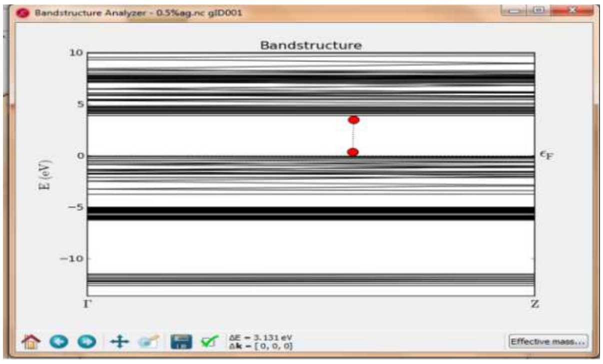


Figure 2(A): Band Structure for 0.5% Ag Doped ZnS

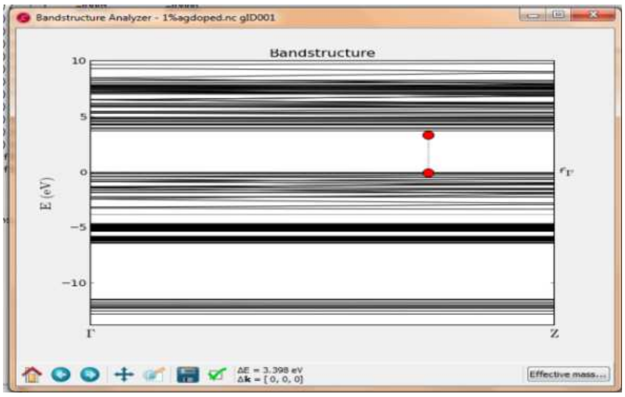


Figure 2(B): Band Structure for 1% Ag Doped ZnS

With tuning of the band gap the electronic properties of ZnS thin film can be tuned. The large band gap produced in case of doping that is the blue shift can be attributed to the confinement effect in nano structure. This shift in wavelength has made the material useful in ultraviolet range.

Table 1: Bandgap of the Co Doped Samples

Sr. No	Sample	Bandgap (eV) (With Simulation)	Optical Band Gap(eV)
1.	ZnS:Co 1%	5.35	5.1
2.	ZnS:Co 2%	5.56	4.8
3.	ZnS:Co 5%	5.70	5.6
4.	ZnS:Co 6%	5.05	5.0
5.	ZnS:Co 8%	5.04	5.0

Table 2: Bandgap of the Ni Doped Samples

Sr. No	Sample	Bandgap(eV) (With Simulation)	Optical Band Gap(eV)
1.	ZnS:Ni 1%	5.64	5.5
2.	ZnS:Ni 3%	5.31	5.13
3.	ZnS:Ni 5%	5.87	5.66

In case of Nickel and Cobalt doping the band gap results obtained from simulation were found to be similar to that obtained with experimental UV-vis spectroscopy data which showed the change of 5.0eV to 5.6 eV for different doping concentrations in case of cobalt and 5.1eV to 5.66 eV in case of Nickel doping.

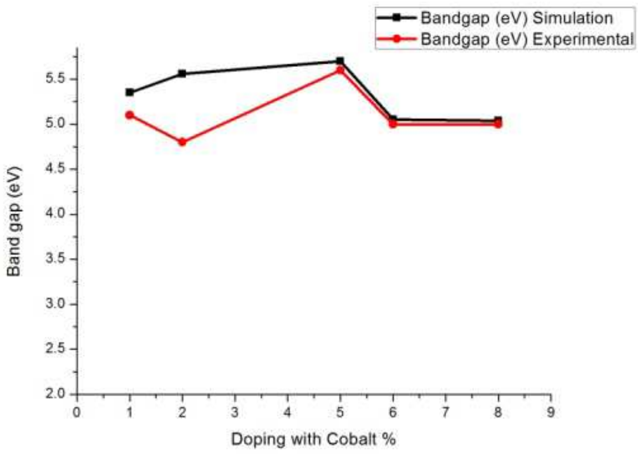


Figure 3: Cobalt Doping vs Band Gap

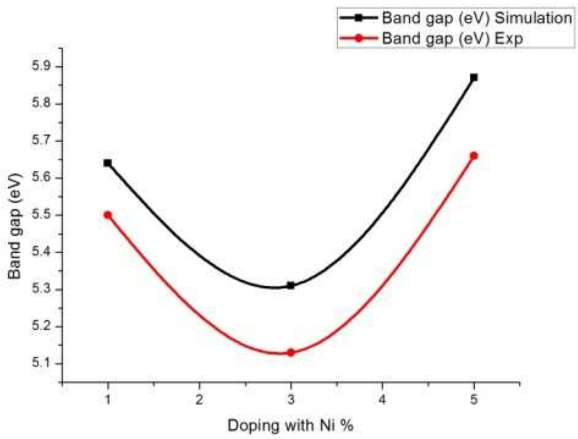


Figure 4: Nickel Doping vs Band Gap

Further one set was simulated using Silver as a do pant and p-n junction was simulated. The IV curve for the silver doped Zinc sulphide diode showed large increase in current for increasing concentrations of silver.

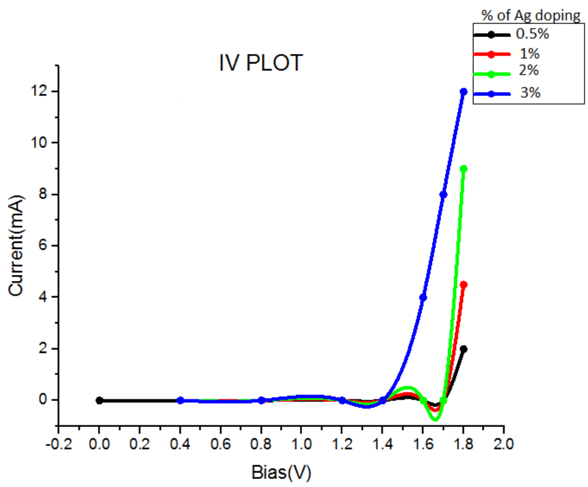


Figure 4: I/V for Different Concentrations of Ag

Table 3: Bandgap of the Ag Doped ZnS with Software Simulation

Sr. No	Sample	Bandgap(eV)
1.	ZnS:Ag 0.5%	3.13
2.	ZnS:Ag 1%	3.40
3.	ZnS:Ag 2%	2.79
4.	ZnS:Ag 3%	2.54

The band gap observed using silver as a dopant showed decrease in band gap and it was observed that band gap decreases with increase in silver concentration,

CONCLUSIONS

The optical band gap values for undoped and doped ZnS nanoparticles were found from software analysis as well as from experimental observations using Tauc plot. It was observed that the band gap of pure ZnS is 4.9 eV when observed experimentally. The band gap of cobalt and nickel doped ZnS changes as the function of doping concentration. The increased doping widens the bandgap which means blue shift of energy. The band gap of silver doped ZnS decreases with increasing concentration of Silver. Which means that band gap of ZnS can be increased or decreased with use of different type of dopants and their concentrations. Therefore, by varying the doping concentration band gap can be modified and can be tuned to obtain suitable material for fabrication of LED from UV range to visible range.

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