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Effects of strontium and aluminum impurities on optical properties of iron sulfide (FeS_2) thin films.

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Abstract: *Chemical bath deposited iron sulfide (FeS_2) thin films were grown at room temperature (26 ^oC) on glass substrates and the effects of impurity concentrations of strontium (Sr, 0.02-0.04M) and aluminum (Al, 0.02-0.04M) on the optical properties of the FeS_2 thin films were investigated using a spectrophotometer in the UV-VIS region. The highest transmittance of 70% occurred for 0.04M Al impurities and 27% for 0.02M of Sr impurities as compared to 18% for un-doped iron sulfide thin films, while the reflectance exhibited varying peak values at 550 nm and 650 nm wavelengths for all concentrations of both impurities. Other optical properties obtained from the spectrophotometer data using appropriate relations showed a corresponding low absorbance of 0.2 for 0.04M Al impurity and fairly high absorbance of 0.6 for 0.02M of Sr impurity. A significant increase in the energy band gap occurred from 1.9 - 2.2eV for Strontium impurity concentrations and 2.0 - 3.8eV for Al impurity concentrations with the highest of 3.8eV at 0.04 Al doping. The effects of Sr and Al dopants on the extinction coefficient and refractive index of the thin films are also reported in this paper.*
Keywords: *iron sulfide, Sr and Al impurities, spectrophotometer, transmittance, reflectance.*

I Introduction

Metal chalcogenides have band gap energy between 1 to 2 eV which attracts the attention of researchers due to their good potentials for photovoltaic, electronic and photo electrochemical applications [1-4].

Iron sulfide, also called pyrite, is of particular interest due to its natural abundance and non toxic nature making its photovoltaic and optoelectronic applications sustainable. Other attractive qualities of iron sulfide thin films include low production cost, excellent environmental compatibility, ease of n/p doping and high carrier mobility. However, only limited progress has been made to explore the potential of this material for solar and other applications [5-8].

In this investigation, iron sulfide thin films are doped with strontium and aluminum impurities to explore their effects on the optical properties of the thin films for consequent expansion of their applications.

II Experimental Details

Analytical grade reagents used for the FeS_2 thin films deposition include iron (iii) chloride [$FeCl_3$] as the precursor for iron ions, sodium thiosulphate [$Na_2S_2O_3.5H_2O$] as the precursor for sulfur ions and tri- ethanol amine (TEA) as a complexing agent. Aluminum Chloride [$AlCl_3$] and Strontium Chloride [$SrCl_2$] were used to obtain Al^{3+} and Sr^{2+} dopants.

The glass substrates were initially degreased in trioxonitrate (V) acid for 24 hours and then washed with distilled water and dried by holding the tips of the glass slide/substrates in synthetic foam and exposed to air. For the deposition of FeS_2 thin films, seven beakers each of 100 ml, were set up and to each beaker 10 ml of 0.1M iron (iii) chloride and 5 ml of tri-ethanolamine were added. This was followed by addition of 10 ml of 0.15M sodium thiosulphate with proper stirring. Addition of two drops of hydrochloric acid, adjusted the pH of the reaction mixture to 2.

Then, into the beakers, in two sets of three, were mixed 2 ml of 0.02, 0.03 and 0.04M of Al^{3+} and Sr^{2+} dopants respectively, leaving one beaker as un-doped. The beakers were then kept in water bath maintained at room temperature of 26 ^oC. The reaction kinetics are as follows:

$$FeCl_3.H_2O + (TEA) \longrightarrow [Fe (TEA)]^{3+} + 3Cl^- + H_2O \quad (1)$$
$$[Fe (TEA)]^{3+} \longrightarrow Fe^{3+} + (TEA) \quad (2)$$
$$Na_2S_2O_3.5H_2O \longrightarrow Na_2O_3 + 5H_2O + S^2 \quad (3)$$
$$Fe^{3+} + 2S^{2-} \longrightarrow 2FeS_2 + e^- \quad \{4)$$

The dopants dissociated in the solution as follows:

$$AlCl_3 \longrightarrow Al^{3+} + 3Cl^- \quad (5)$$
$$SrCl_2 \longrightarrow Sr_2^+ + 2Cl^- \quad (6)$$

The results in separate baths are FeS_2:Al and FeS_2:Sr

III Results and Discussion

The optical data for the doped and as grown FeS_2 thin films were measured with UV-VIS spectrophotometer in the wavelength range of 300 – 700nm. Fig, 1 (a and b) show the reflectance of the FeS_2 thin films doped with Sr and Al impurities. Fig. 1 (b) reveals increase in reflectance with doping concentrations of Sr when compared with the reflectance of the as grown sample, while Fig. 1(a) reveals lower than as grown reflectance for 0.03M Al and a steady increase for 0.04M Al impurity concentrations. Varying peak values of the reflectance occur for both impurities at 550 and 650 nm wavelengths with the highest peak values for 0.02M Al and 0.04M Sr at 550 nm wavelength.

The transmittance of Fig.2(a) shows distinctive differences in the transmittance of FeS_2 thin films doped with Sr with the highest transmittance of 28% occurring for 0.02M Sr and least transmittance of 5% for 0.03M Sr while the un-doped FeS_2 transmittance is about 17%. In Fig.2(b), the transmittance of up to 70% occurs for 0.04M Al and the least is about 10% for 0.03M Al doping Fig. 3(a and b) show a slowly decreasing absorbance with increasing wavelength from 100% at 300 nm to 60% at 700 nm for both strontium and aluminum impurities except for 0.04M Al doping which decreases rapidly to less than 10% in the visible range.

Fig. 4(a and b) show the energy band gap which ranges from 1.9eV – 2.2eV for the Sr doping used and 2.0 – 3.8eV for all the Al impurity concentrations with the highest of 3.8eV occurring for 0.04M Al doping.

Figs. 5 and 6 show the effects of Al and Sr doping on the extinction coefficient and refractive index of the FeS_2 thin films with the greatest change in the extinction coefficient occurring for 0.04M Al doping. The refractive index varied from 1.0 to peak value of 1.5 for 0.02M of both impurities and 1.55 for 0.04M of Sr doping.

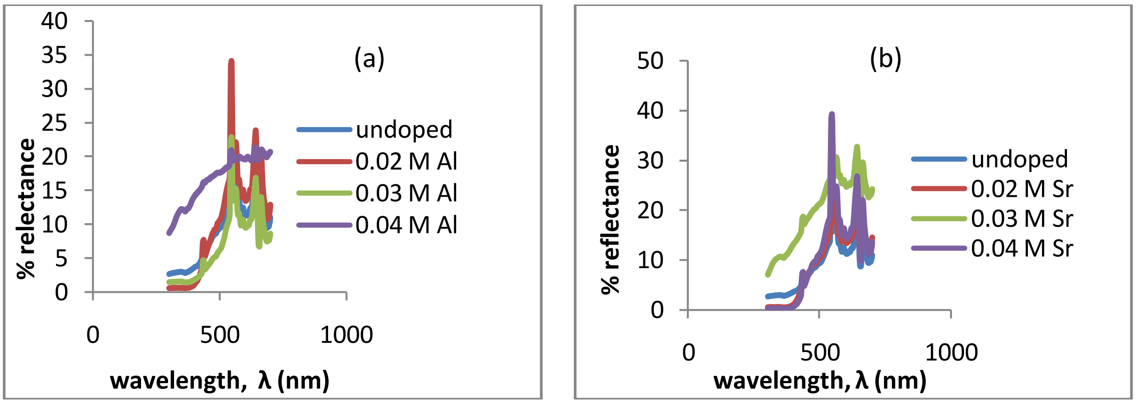


Fig.1: Graph of Reflectance against Wavelength for FeS_2 thin films doped with varying concentrations of (a) Aluminum and (b) Strontium.

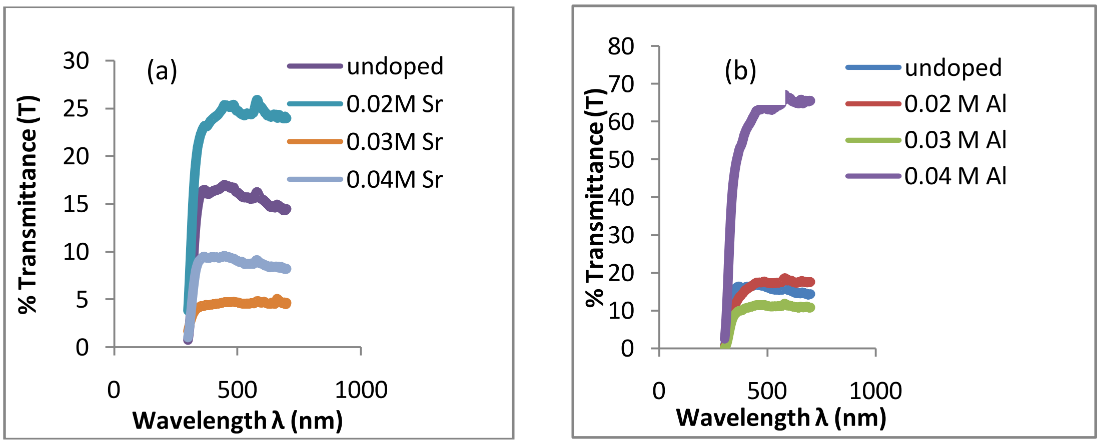


Fig.2: Graph of transmittance against Wavelength for FeS_2 thin films doped with varying concentrations of (a) Strontium and (b) Aluminum

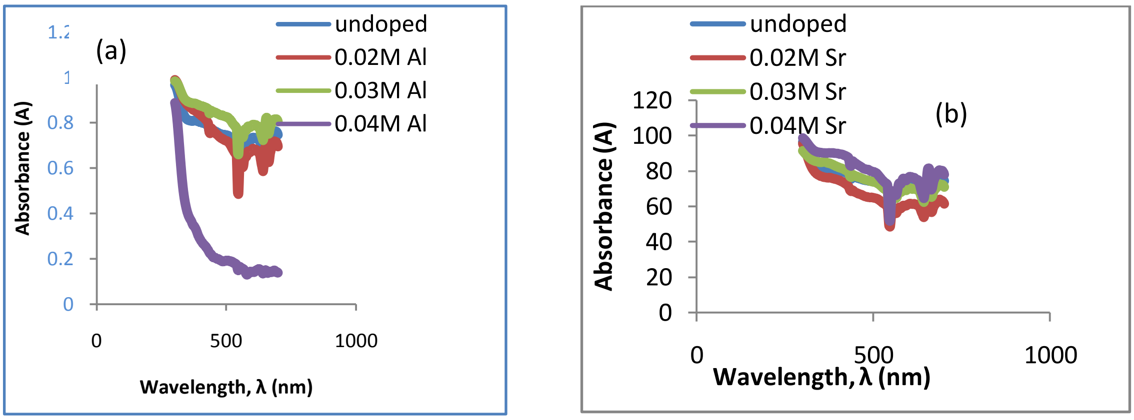


Fig.3: Graph of absorbance against Wavelength for FeS_2 thin films doped with varying concentrations of (a) Aluminum and (b) Strontium.

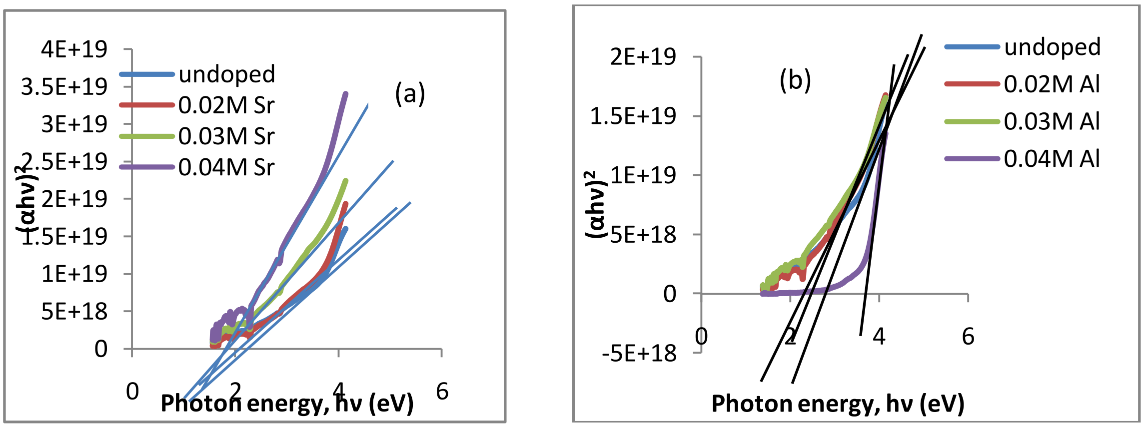


Fig.4: Graph of $(\alpha h\nu)^2$ against Photon Energy for FeS_2 thin films doped with varying concentrations of (a) Strontium (b)Aluminum.

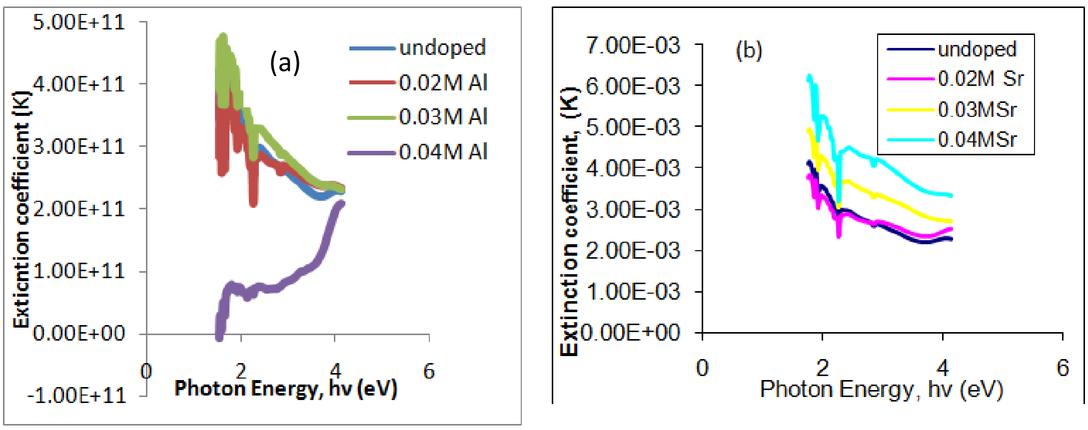
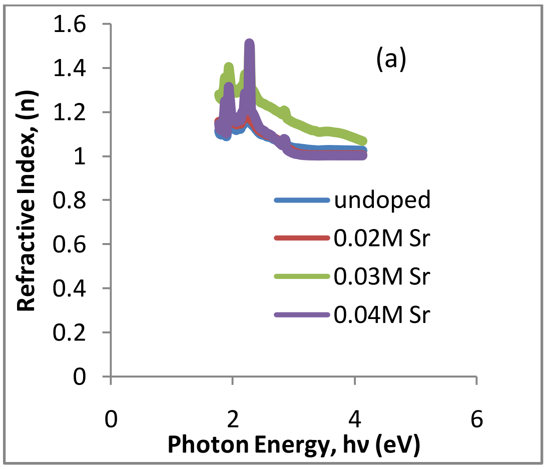


Fig.5: Graph of Extinction coefficient against Photon Energy for FeS_2 thin films doped with varying concentrations of (a) Aluminum and (b) Strontium.



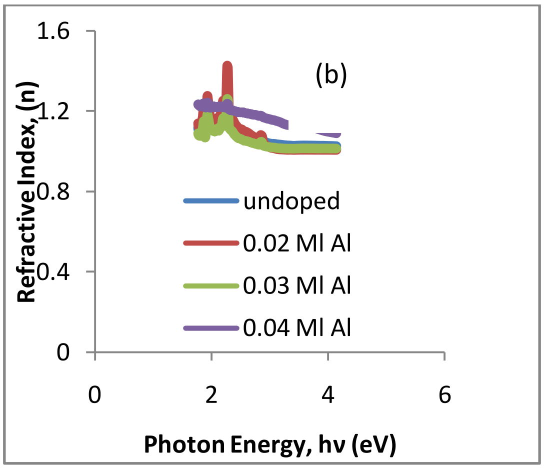


Fig.6: Graph of Refractive Index against Photon Energy for FeS_2 thin films doped with varying concentrations of (a) Strontium and (b) Aluminum.

IV. Conclusion

The effects of aluminum and strontium doping on the optical properties of CBD deposited FeS_2 thin films have been successfully investigated. The results show that different concentrations of the doping materials used, produced different effects on the optical properties of FeS_2 thin films. Pronounced changes in the transmittance, absorbance, extinction coefficient and energy band gap occurred for 0.04M Al doping as reported in this paper. Strontium impurity concentrations also produced distinctive changes in the transmittance, extinction coefficient and refractive index of the FeS_2 thin films. Thus, the doping of FeS_2 with Sr and Al impurities provide expanded values of the optical properties of the thin films for more versatile applications.

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