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Analysis of Structural and Electrical Properties of Iron Sulfide (FeS_2) Thin Films doped with Aluminum and Strontium impurities.

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Abstract: *Thin films of iron sulfide (FeS_2) prepared by CBD technique were doped with aluminum (Al: 0.02-0.04M) and strontium (Sr: 0.02-0.04M) impurities at room temperature of 26 °C. X-Ray diffraction (XRD) and four-point probe were used to analyze the structural and electrical properties of the thin films. The XRD results show that 0.02M of strontium impurities produced polycrystalline structure of the thin films with diffraction peak values located at Bragg's angles, 2Θ of 14.71°, 25.03° and 34.95°, while the un-doped polycrystalline FeS_2 thin films have diffraction peaks at 2Θ values of 19.81°, 24.43°, 31.45° and 36.73°. Clearly, the contributing in-phase reflections for the different diffraction angles occur from different orientations of lattice planes and/or different crystallite sizes caused by the Sr impurity. On the other hand, 0.02M of aluminum dopant produced mono-crystalline structure of the FeS_2 thin film with 2Θ value of 24.97° and a broadened full width at half maximum (FWHM). It is remarkable that the single peak of the mono-crystal due to Al impurity coincides with the highest intensity and sharper peak of the un-doped FeS_2 thin film. The electrical resistivity of the thin films decreased while the conductivity increased with increase in impurity concentrations with non-uniform changes occurring from 0.02M for both impurities. The film thickness remained between 0.09-0.1µm but showed a more dramatic increase with impurity concentration from 0.02M for both impurities.*
Keywords: *iron sulfide, aluminum and strontium impurities, Bragg's angle, film thickness*

I. Introduction

Iron sulfide thin films have attracted sustained research due to the natural abundance of iron sulfide and its environmental compatibility as well as the potential applications of FeS_2 thin films in photovoltaic, optoelectronic and photochemical systems among others [1-4]. Other merits of FeS_2 thin films include ease of impurity doping, low production cost and high carrier mobility. As with many other thin films, the benefits accruable from FeS_2 thin films can also be enhanced by varying the deposition techniques, deposition time, annealing temperature, pH concentration, complexing agent etc.[5-8] The effects of these lead to different optical, structural and electrical properties of the thin films [9-11] making them amenable to more applications.

In this paper, the effects of aluminum and strontium doping on the structural and electrical properties of iron sulfide thin films are investigated.

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 °C. The reaction kinetics are as in [11] providing different concentrations of FeS_2:Al and FeS_2:Sr in separate beakers.`

III. Results And Discussions.

The structural analysis of the FeS_2 thin films was performed using X'PERT PRO diffractometer with CuK_α radiation of wavelength 1.54068A in the 2θ scanning mode to obtain the XRD data while Vander Pauw Four-Point probe was used to measure the electrical properties. Fig. 1 (a,b,c) show the diffraction patterns of the un-doped and for 0.02M doping with Sr and Al impurities for FeS_2 thin films Fig. 1(a) shows four diffraction peaks of the un-doped FeS_2 thin films at 2θ values of 19.81°, 24.43°, 31.45° and 36.73°, depicting its polycrystalline structure. Fig. 1(b) shows the effect of 0.02M Sr doping on the FeS_2 thin film with only three diffraction peaks also revealing a polycrystalline structure whose diffraction angles, 2θ, occur at 14.71°, 25.03° and 34.95°. The occurrence of these different diffraction peaks with Sr impurity are clearly due to constructive interference from reflections different from those of un-doped FeS_2 thin films.

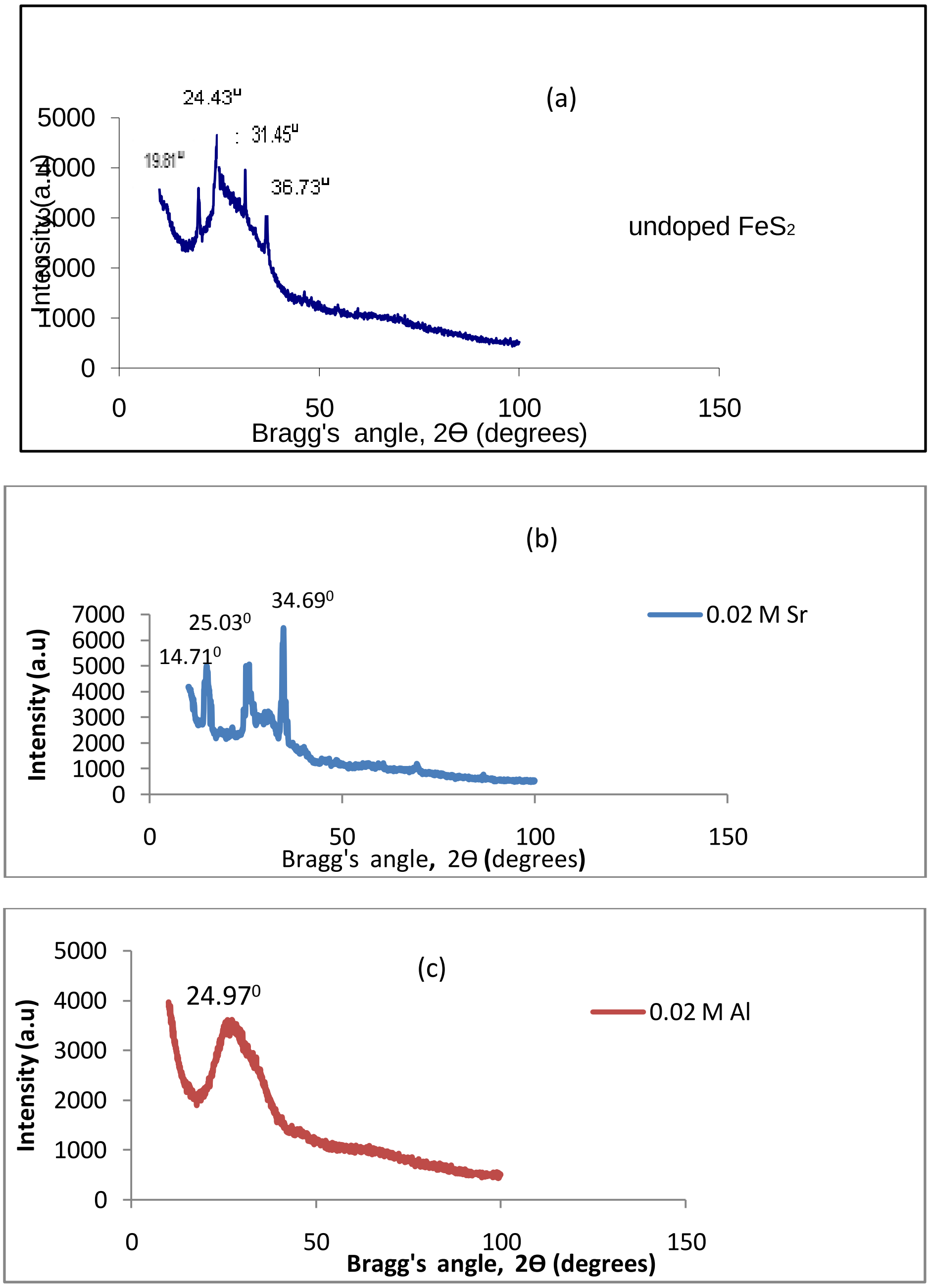

Fig. 1 XRD patterns for Iron Sulfide (FeS_{2z}) thin films for (a) un-doped (b) 0.02M Sr doping and (c) 0.02M Al doping.

Fig. 1(c) on the other hand shows a mono-crystalline structure when the FeS_2 thin film is doped with 0.02M Al impurity. It is also remarkable to note that the broadened single peak of the mono-crystalline due to Al impurity occurs at Bragg's angle, 2θ of 24.97° which practically coincides with the sharp diffraction peak of the highest intensity for the un-doped FeS_2 thin film which occurs at 2θ of 24.43°.

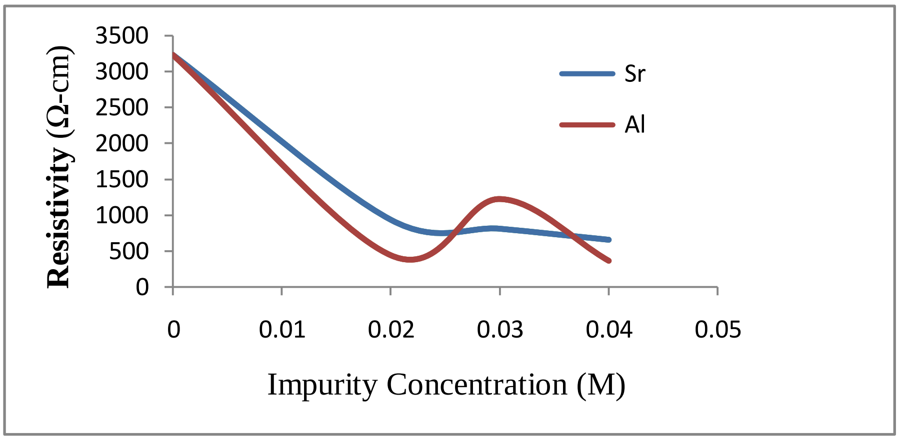

Fig. 2: Graph of resistivity against impurity concentration for FeS_2: Sr and FeS_2: Al

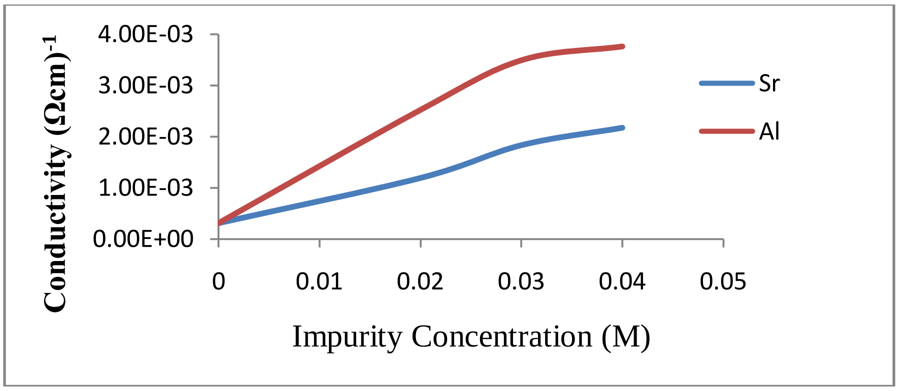

Fig. 3: Graph of Conductivity against impurity concentration for FeS_2: Sr and FeS_2: Al

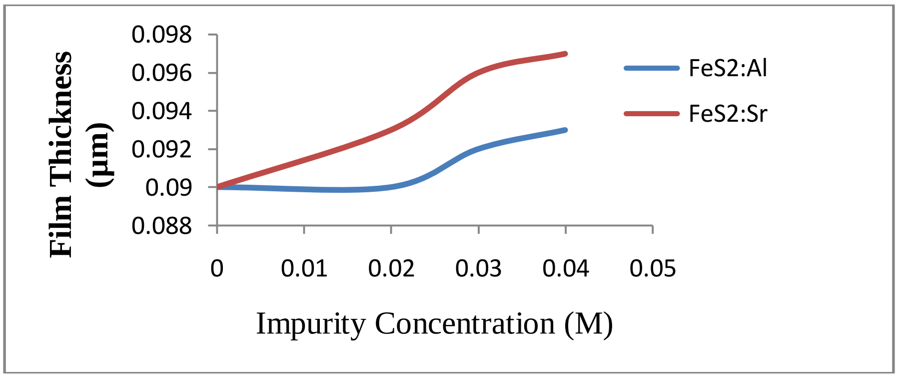

Fig.4: Graph of Thickness against impurity concentration for FeS_2: Sr and FeS_2: Al

Fig. (2, 3 and 4) respectively show the resistivity, conductivity and the variations in film thickness due to impurity concentrations of Sr and Al on the FeS_2 thin films. In all the cases, non-linear changes of decrease or increase occur from 0.02M concentration for both impurities. Fig. 5(a and b) and Fig. 6(a and b) respectively, show the variations in real and imaginary dielectric constants for different doping concentrations of the impurities.

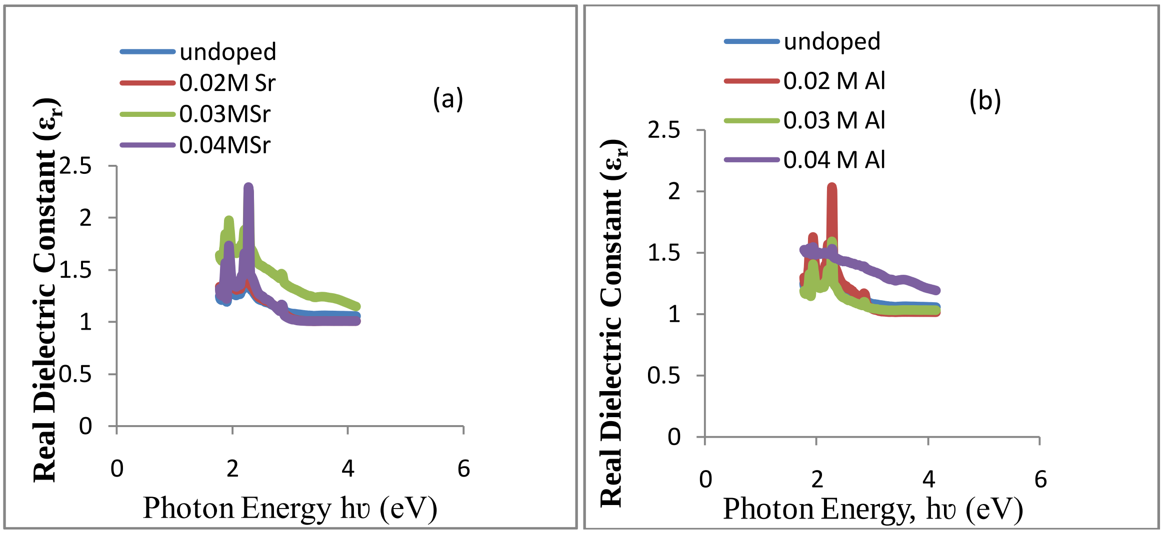

Fig.5: Real Dielectric constant against photon energy of (a) FeS_2:Sr and (b) FeS_2:Al

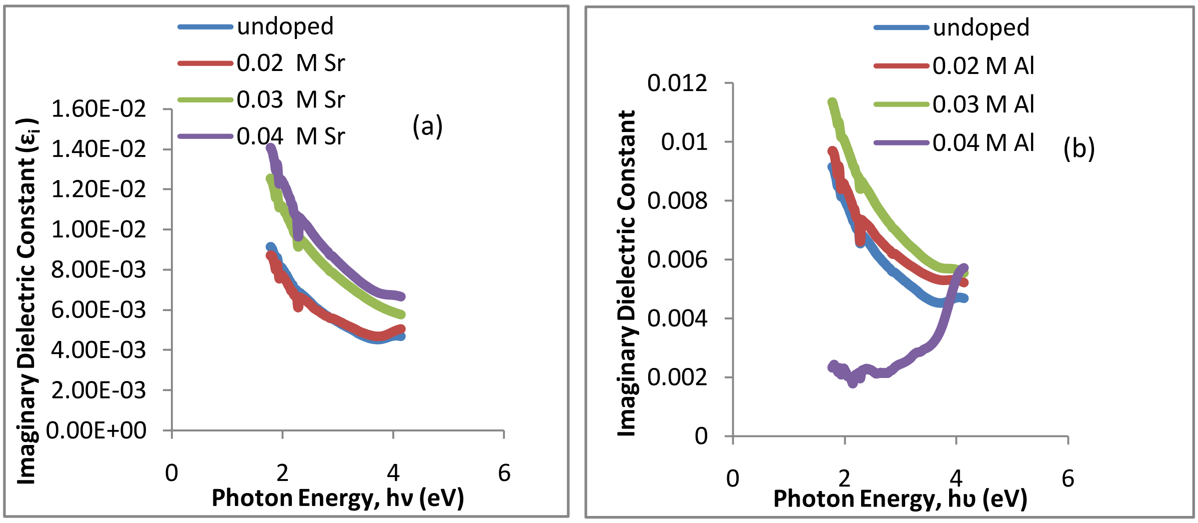

Fig.6: Imaginary Dielectric Constant against Photon energy of (a) FeS_2:Sr and (b) FeS_2:Al

IV. Conclusion

The deposition and analyses of un-doped FeS_2 thin films and those doped with varying concentrations of Sr and Al have been successfully investigated. The results show that Sr doping produced polycrystalline structure of the thin films that are different from the polycrystalline structure of the un-doped FeS_2 films while Al doping changed the polycrystalline to mono-crystalline structure. The impurity concentrations used also lowered the resistivity and increased the conductivity of the thin films. The film thickness also increased with impurity concentrations. Variations in both real and imaginary dielectric constants due to the impurities are as reported in this paper.

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