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Effects of Concentration and Annealing Temperature on the Transmittance and Energy Bandgap of Aluminum Doped Palladium Sulphide for Device Applications.

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Abstract
Palladium Sulphide thin films were successfully deposited on a glass substrate using the chemical bath deposition method. The effect of varying concentration of aluminum dopant on the PdS thin film was also investigated by varying the concentration of aluminum in the form Al_x where x = 0.3 and 0.5. Post deposition annealing was also done on the aluminum doped PdS film at temperatures of 50 ^oC, 100 ^oC and 150 ^oC. The optical properties were investigated using UV- spectrophotometer. The result of the analysis showed that while concentration tends to increase the Band gap energy of the films, it decreases with increase in annealing temperature. High value of transmittance in the range of 60- 90 % were observed in the UV region. The band gap of the deposited films lies between 1.20 eV to 1.80 eV. The values obtained for the parameters of the deposited films revealed that the PdS doped with aluminum thin film was a good material for device applications in solar energy collections and photonics etc.

Keywords*: Transmittance, Absorbance, Band gap, Dopant, Palladium Sulphide, Aluminum ,chemical bath, dye, UV– Spectrophotometer, Temperature and annealing.*

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I. Introduction

Palladium is known for its high demand for uses in electrical equipment, dental_materials, implanted medical devices (to add radiopacity), and automobile catalysts. Recently palladium sulphide has attracted much attention within the scientific community as a future material. The renewed interest in this material has arisen out of the development of growth in technologies for the fabrication of high quality simple crystals and epitaxal layers, allowing for the realization of Palladium sulphide based electronic and optoeltectronic devices [4, 7]. Over the last decades, there has been tremendous research on palladium sulphide materials because of their wide range of applications such as smart windows, displays, rearview mirrors, and so forth. Over all, the glazing in building is the most discussed issue due to the fact that it is strongly related to energy saving [6, 12]

A choice of substrates (flexible or rigid, metal or insulator) can be made for deposition of different layers (contact, buffer, absorber, reflector, etc.) using diverse techniques such as; chemical bath deposition techniques (CBD). Successive ionic layer adsorption reaction (SILAR), physical vapour deposition (PVD), chemical vapour deposition (CVD), electrochemical deposition (ECD), plasma-based, hybrid, etc. Such versatility allows scientist and engineers to improve different layers of thin films of which in turn improve device performance [3, 5]. As a result, materials like palladium have been the focus of many studies because of their ability to separate hydrogen from other gases [4]. Palladium is known to have high selectivity and permeance towards hydrogen. Composite palladium membranes are prepared by depositing palladium on the suitable porous supports. Palladium plated on a porous support has higher mechanical strength and lower amount of palladium loading as compared to stand alone palladium films [22].

Dense palladium composite membranes are suitable for separating hydrogen from the products of the steam reforming of methane, which can then be used for energy generation by fuel cells [4, 11, 22] and also for the purpose of our study we propose that chemically deposition of palladium sulphide have potential for solar energy application. The enormous potential of thin films solar cell (TFSC) technology to contribute to the overall photovoltaic (PV) portfolio has been the motivation for this present study.

II. Theory

2.1 Transmittance (T)

It is the Absorbance/Transmittance of thin films that are usually obtained directly using spectrophotometer during optical characterization while other properties are gotten from calculations based on these. Whenever an electromagnetic wave such as light crosses the interface between two different materials such as thin film and glass, a fraction of light is reflected by the inner surface while some amount of electromagnetic wave is refracted through the inner surface and finally transmitted. The reflectance is the amount of reflection in terms of energy while transmittance is the amount of transmission in terms of energy. Mathematically, Transmittance of the specimens is defined as the ratio of the transmitted intensity (flux) (I) to the incident (flux) intensity (I_O).

$$T = {}^{I}/_{I_O} \qquad 1$$

The absorbance A is the logarithm of the reciprocal of the transmittance. Hence, from equation (6) we can deduce transmittance from absorbance in the form,

$$T = 10^{-A} \qquad 2$$

Thus, when one is known, the other can be found. It is the absorbance/transmittance of thin films that are usually obtained directly using spectrophotometer during optical characterization while other properties are gotten from calculations based on these.

2.2 Band gap (E_g)

Band gap is a solid state property and is one of the important parameters in the characterization of a material. The knowledge of optical absorption is necessary in the study of band gap. Photon-induced electronic transitions can occur between different bands which led to the determination of the energy band-gap or within a single band such as free-carrier absorption. The band gap is a difference in energy between the lowest point of conduction band and the highest point of valence band. In other words it is the energy required for an electron to move from the valence band to the conduction band.

The shape of absorption spectrum and dispersion near the fundamental absorption edge are caused by the electron transition from upper part of the valence band to the lower part of the conduction band [2, 3]. This electron transition can be direct or indirect. It is direct when there is no photon participation and without change in crystal momentum of an electron. In other words it is indirect when the interaction with a photon produces a considerable change in the crystal momentum. The various types of transition give rise to different frequency dependencies of the absorption coefficient near the absorption edge.

According to [1, 10], the absorption coefficient for direct transition is given by,

$$ahv \propto \left(hv - E_g\right)^{\gamma} \qquad 3$$

Where γ = ½ if the transition between the upper part of the valence band to the lower part of conduction band are allowed by the selection rules and γ = 3/2, the transitions are forbidden. Hence,

$$ahv = A\left(hv - E_g\right)^{1/2} \qquad 4$$

For allowed transitions, that is

$$(ahv)^2 = B\left(hv - E_g\right) \qquad 5$$

In most cases, indirect transitions [4] are weaker than direct ones by 3 or 2 orders of magnitude. This is because they result only by second order – perturbation and can only be observed in energy regions which are free of direct transition. The dependence of the absorption coefficient on the energy of light quanta near the fundamental edge is given by equations 4 and 5.

A graph of α^2 versus hv gives a straight-line graph with negative band gap as the intercept. However, in the region of absorption edge, the absorption falls to such low values that it becomes difficult to measure the part which is due to band-to-band transition. This is due to the fact that it is now liable to be masked by other incidental absorption or losses in specimens or experimental equipment. Due to this, a plot of α^2 versus hv is not usually straight at the absorption edge region. Hence, the intercept that gives the band gap is extrapolated from the straight portion of the graph to the point.

$$a^2 = 0 \qquad 6$$

[8] Discovered that in some compounds, the density of impurities affected the position of the absorption edge in such a way as to shift it to a shorter wavelength and this causes a large increase in the band gap of such material. In joules, the photo energy for a given wavelength in meters is given by,

$$E = hv = {}^{hc}/_{\lambda} \qquad 7$$

Where, h = plank's constant, c = velocity of light,

λ = wavelength in meter (m), *and* v = frequency of the radiation .

If λ is in nm,

$$hv\,(ev) = \frac{1241}{\lambda} \qquad 8$$

Equation (8) is used in this study in calculating the photon energies in eV for various wavelengths, λ in nm.

III. Experimental Detail

In the experiment, 1.0 M molar concentration of palladium chloride was used. The molar concentrations of aluminum chloride were 0.3M and 0.5M and were used as dopant for the study. The formula for calculating the mass is:

$$g_{ch} = \frac{M.m_{ch} \times Vol \times M.C}{1000} \qquad 9$$

Where, M = the mass of chemical to be weighed, m_{ch} =molar mass of chemical, vol = Volume of water to be used, and M.C = molar concentration used. The chemical bath solution constituted of palladium chloride ($PdCl_2$) as the Pd^{2+} ion source, thiourea $(NH_2)_2CS$) as the source of S^{2-} ion, and disodium thiosulphate ($Na_2S_2O_3$) as the complexing agent. 40 ml of palladium chloride ($PdCl_2$) solution was complexed with 10ml of sodium thiosulphate ($Na_2S_2O_3$) solution in a 100 ml capacity beaker; this was followed by adding 30ml of thiourea (CH_4N_2S) solution in the beaker. For the doped Palladium sulphide, palladium 20 ml aluminum chloride (AlC_3) solution was added to 20 ml of palladium chloride ($PdCl_2$) solution. The glass substrate was immersed vertically suspended into the beaker containing the solution. The deposition was allowed to take place for 60 minutes at temperature of 300 K. After which the substrates were removed from the chemical bath, rinsed thoroughly in distilled water and dried at room temperature.

IV. Results And Discussion

4.1 Optical Characterization

The Transmission spectra of the Aluminum doped palladium sulphide thin film samples are taken in the ultra violet (UV), and visible regions by using UV-VIS-NIR Perker Elmer spectrophotometer lambda 950 with UV Win lab software. The machine measures directly the transmission of the sample. By using the %T data, all other optical parameters were calculated.

The transmittance plot against wavelength for PdS and Al doped PdS thin films are shown in Figure 1 (A-D).

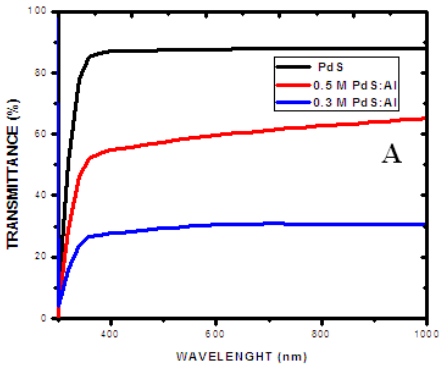

Fig: 1A Plot of transmittance against wavelength for as-deposited PdS.

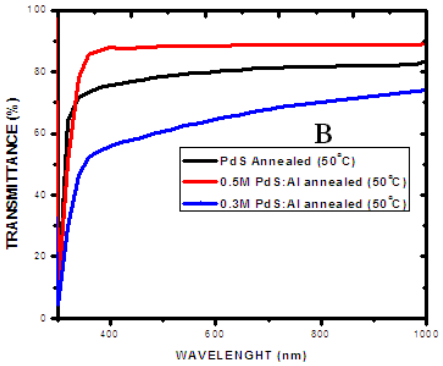

Fig: 1B Plot of transmittance against wavelength for PdS annealed at 50 °C.

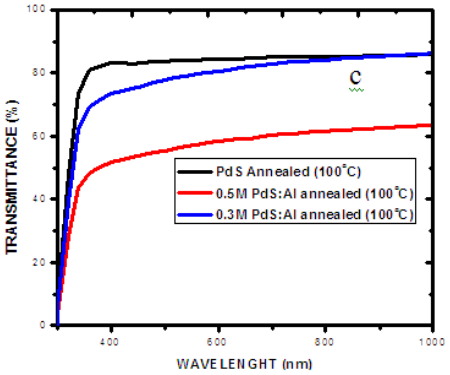

Fig: 1C Plot of transmittance against wavelength for PdS annealed at 100 °C.

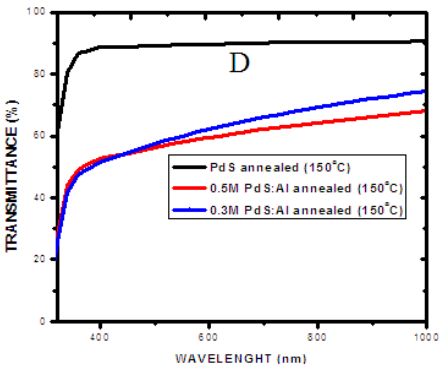

Fig: 1D Plot of transmittance against wavelength for PdS annealed at 150 °C.

The plot of $(\alpha hv)^2$ against hv for PdS and Al doped PdS thin films are shown in Figure 2 (A-D).

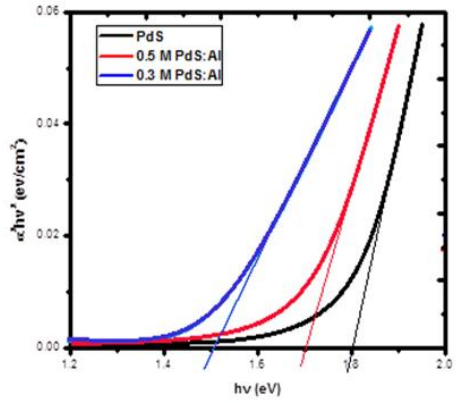

Fig:.2A plot of $(\alpha hv)^2$ against hv for PdS thin film as-deposited.

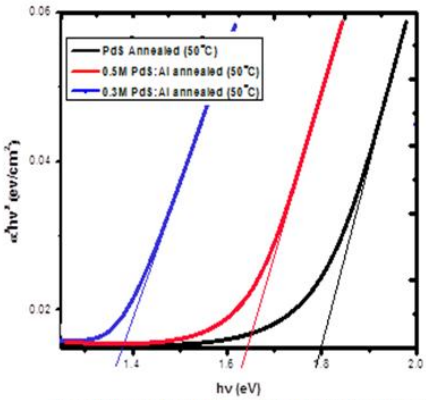

Fig: 2B plot of $(\alpha hv)^2$ against hv for PdS thin film annealed at 50 °C.

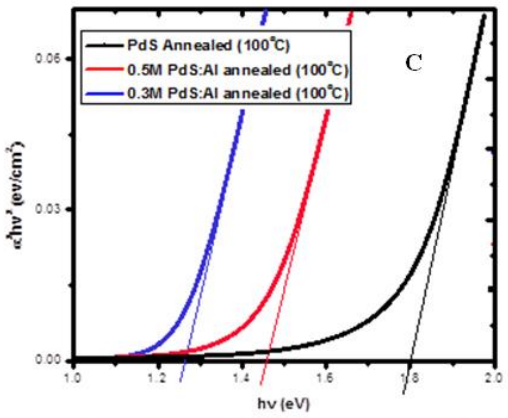

Fig:.2C. plot of $(\alpha hv)^2$ against hv for PdS annealed at 100 °C.

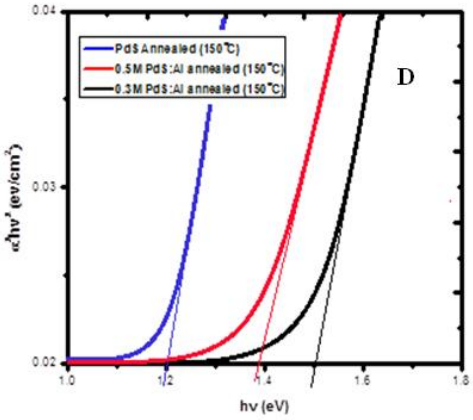

Fig: 2D plot of $(\alpha hv)^2$ against hv for PdS annealed at 150 °C.

The transmittance versus wavelength measurement is shown in figure 1A-D. The transmittance value for all deposited PdS thin films increases with increasing wavelength from 300 to 1000nm. As-deposited PdS thin film in figure 4A showed a transmittance value of >80% while 0.3M PdS:Al showed a transmittance value of 23% and 0.5M PdS:Al showed a transmittance value of 56%.

After annealing the PdS samples at difference temperatures, the transmittance value tends to vary slightly. PdS thin films annealed at 50°C in figure 4B showed for PdS transmittance value of 73% while 0.3M PdS:Al showed a transmittance value of 60% and 0.5M PdS:Al showed a transmittance value of >80%. For the PdS thin films annealed at 100°C in figure 4C showed for PdS transmittance value of >80%, while 0.3M PdS:Al showed a transmittance value of 77% and 0.5M PdS:Al showed a transmittance value of 60%. For the PdS thin films annealed at 150°C in figure 4D showed for PdS transmittance value of >80%, while 0.3M PdS:Al showed a transmittance value of 62% and 0.5M PdS:Al showed a transmittance value of 58%. In general, the transmittance value for PdS thin films shows a high value (60 – 90%) in the spectral region corresponding to maximum sensitivity for photonic vision. This means that the transmittance values in the visible region provides a high lighting sensation than metallic solar control glazing [15]

Band gap energy (E_g), was determined by extrapolating the straight line portion to the hv axis. It is observed that annealing on the PdS thin films reduces the band gap of the films as shown on Figure 2A-D above. Below is the table showing the band gap energy value for all deposited PdS thin films.

Deposited PdS thin films (Annealed and Unannealed)	Band Gap (eV)
As prepared PdS	1.80eV
As prepared 0.3M PdS:Al	1.50eV
As prepared 0.5M PdS:Al	1.70eV
PdS annealed at 50°C	1.80eV
0.3M PdS:Al annealed at 50°C	1.38eV
0.5M PdS:Al annealed at 50°C	1.65eV
PdS annealed at 100°C	1.8eV
0.3M PdS:Al annealed at 100°C	1.25eV
0.5M PdS:Al annealed at 100°C	1.45eV
PdS annealed at 150°C	1.50eV
0.3M PdS:Al annealed at 150°C	1.20eV
0.5M PdS:Al annealed at 150°C	1.38eV

Table 1: Table showing the band gap energy value for all deposited PdS thin films.

These reveals that the band gaps ranges between 1.20eV to 1.80eV which is in close agreement with[4]. The low band gaps make PdS films good materials for Photovoltaic solar cells.

V. Conclusions

In this study, Aluminum doped Palladium Sulphide (PDS) thin films deposited on glass substrate using solution growth technique at different concentrations and annealing temperature have been analysed. The analysis revealed that while concentration tends to increase the Band gap energy of the films, it decreases with increase in annealing temperature. The transmittance value for PdS thin films shows a high value (60 – 90%) in the spectral region corresponding to maximum sensitivity for photonic vision. This means that the transmittance values in the visible region provides a high lighting sensation than metallic solar control glazing. The energy bandgap was observed to be in the range 1.20 eV to 1.80 eV which is within the range reported by other authors in the literature and also confirms the suitability of the films in thermoelectronics.

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