



# STRUCTURAL AND OPTICAL STUDIES OF ELECTRODEPOSITED YTTRIUM CHALCOGENIDE FILMS

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**ABSTRACT:** Electrodeposition of yttrium chalcogenide films on the variety of substrates using non-aqueous bath has been carried out. Sulphur, selenide and telluride are taken as chalcogenide elements. All baths were prepared in formaldehyde solution. Sodium acetate was used as a complexing agent for all non-aqueous baths. Corning glass vessel of volume 12cc was used as a bath container. High purity graphite plate of size  $4 \times 2.5 \times 0.2 \text{ cm}^3$  is used as a counterelectrode. In order to hold substrate and counterelectrode at appropriate distance a bakelite holder was used. Saturated calomel electrode (SCE) was used as a reference electrode in. Substrate, temperature, chemical composition, terminal thickness etc., has been optimized for desired deposition potential for individual bath. For structural properties all films were deposited on to a stainless steel substrate and for optical properties they were deposited on to an ITO coated glass. The structural property of film was studied by X-ray diffraction and optical property was studied by optical absorption technique, which confirms the deposited material and the band gap energy of respective compound.

## Introduction:

Since from 19<sup>th</sup> century, due to vast consumption of non-renewable fossil fuels resulted in a severe anxiety for energy deficiency and the corresponding carbon emissions, creates new environmental issues. There is urgent need of clean, affordable and reliable energy that can substitute fossil fuels and limits the carbon emission issue. Therefore, the interest of researchers focused towards the development of technology to make availability of clean and renewable energy, especially the intermittent energy, energy conversion and storage [1, 2]. Many high-tech applications are found in rare earths due to their unique properties [3]. Currently rare earth several applications in modern technologies ranging from cell phones and televisions to LED light bulbs and wind turbine [4]. Lokhande and et al have been reported electrodepositions of some of the rare earth metals chalcogenides from aqueous as well as non-aqueous media [5,6]. Spray pyrolysis method also used to prepare thin films chalcogenides of various rare earths [7]. Many theoretical models have been proposed with their electrical, magnetic, structural and other properties. Some field compounds have found to be high field technology applications [8-10]. Umbach has shown that, in case of rare earth compounds only  $\text{HoMo}_6\text{S}_8$  exhibits the co-existence of superconducting and ferromagnetic states [11]. Many researchers reported rare earth films and their characterization by various methods [12, 13]. As the rare earth metal exhibits different valance states, yttrium chalcogenide system may consists some apparent compounds.

In this paper we report on the structural and optical study of yttrium chalcogenides thin films from non-aqueous bath. Sulphur, selenide and telluride are taken as chalcogenide elements. By dissolving yttrium nitrate in formaldehyde, a non-aqueous bath of yttrium nitrate was prepared. Sodium acetate was used as a complexing agent.  $\text{CH}_3\text{CSNH}_2$  was used as a sulphur ion source,  $\text{SeO}_2$  as a selenium ion source and non-aqueous  $\text{T}_2\text{O}_3$  solution as a telluride ion source.

## Experimental Details:

The bath 0.05M  $\text{Y}(\text{NO}_3)_3$  containing 0.05M  $\text{CH}_3\text{CSNH}_2$  and 0.05M  $\text{CH}_3\text{COONa}$  composition was suitable for electrodeposition of Y-S at room temperature (above  $25^\circ\text{C}$ ). About 0.5 micron thickness film was electrodeposited onto a stainless steel substrate and its structural property was studied by X-ray diffraction. Using same composition film was deposited onto a FTO coated glass and used for the optical study. The X-ray diffraction studies showed the films are polycrystalline and deposited material is to be  $\text{YS}_{1.71-1.76}$ . From optical absorption studies, the band gap energy was calculated to be 1.85eV.

The Y-Se films were electrodeposited from bath containing 0.05M Y (NO<sub>3</sub>)<sub>3</sub>, 0.05M S<sub>e</sub>O<sub>2</sub> and 0.05M CH<sub>3</sub>COONa at room temperature on variety of substrates. The XRD pattern was obtained from film deposited onto a stainless steel substrate. The X-ray diffraction studies showed the peaks of YSe<sub>2</sub>, having crystalline nature of the film. For optical absorption study, the film was deposited onto a FTO coated glass with same composition and band gap energy was calculated to be 1.96eV.

TeO<sub>2</sub> solution forms precipitate when mixed with non-aqueous solution of Y (NO<sub>3</sub>)<sub>3</sub>. Therefore, it is difficult to obtain electrodeposition by co-deposition method. Therefore Y-T<sub>e</sub> films were deposited by using layer-by-layer process. Initially yttrium was electrodeposited from the complexed bath 0.05M Y (NO<sub>3</sub>)<sub>3</sub> onto a stainless steel substrate at room temperature. Then layer of tellurium was electrodeposited over it, from the bath consisting of saturated solution of TeO<sub>2</sub> - 0.05M CH<sub>3</sub>COONa at same condition and same substrate. The film was characterized by X-ray diffraction. The possible compounds of yttrium-telluride are YT<sub>e3</sub>, Y<sub>2</sub>T<sub>e3</sub>, YT<sub>e2</sub> and Y-T<sub>e</sub> was observed. Optical absorption of Y-T<sub>e</sub> films deposited on FTO coated glass in proper wavelength range shows the band gap energy equal to 1.74eV.

### Results and Discussion:

Fig.1 shows the polarization curves for the reduction of yttrium chalcogenide (Y-S, Y-Se, Y-T<sub>e</sub>) from desired baths onto a stainless steel substrate. The sharp nature of curves indicates single outset potential. The deposition potentials for the reduction of Y-S and Y-Se onto a stainless steel substrate were -0.75 and -0.27 respectively, while for reduction of tellurium onto a yttrium deposited stainless steel was -1.90. Fig 2 shows the polarization curves for the reduction of 1) Y-S, 2) Y-Se onto a FTO coated glass and 3) Te on yttrium deposited FTO coated glass.

Table 1 shows the estimated deposition potentials for the reduction of Y-S, Y-Se and Y-T<sub>e</sub> onto a stainless steel and FTO coated glass substrate.

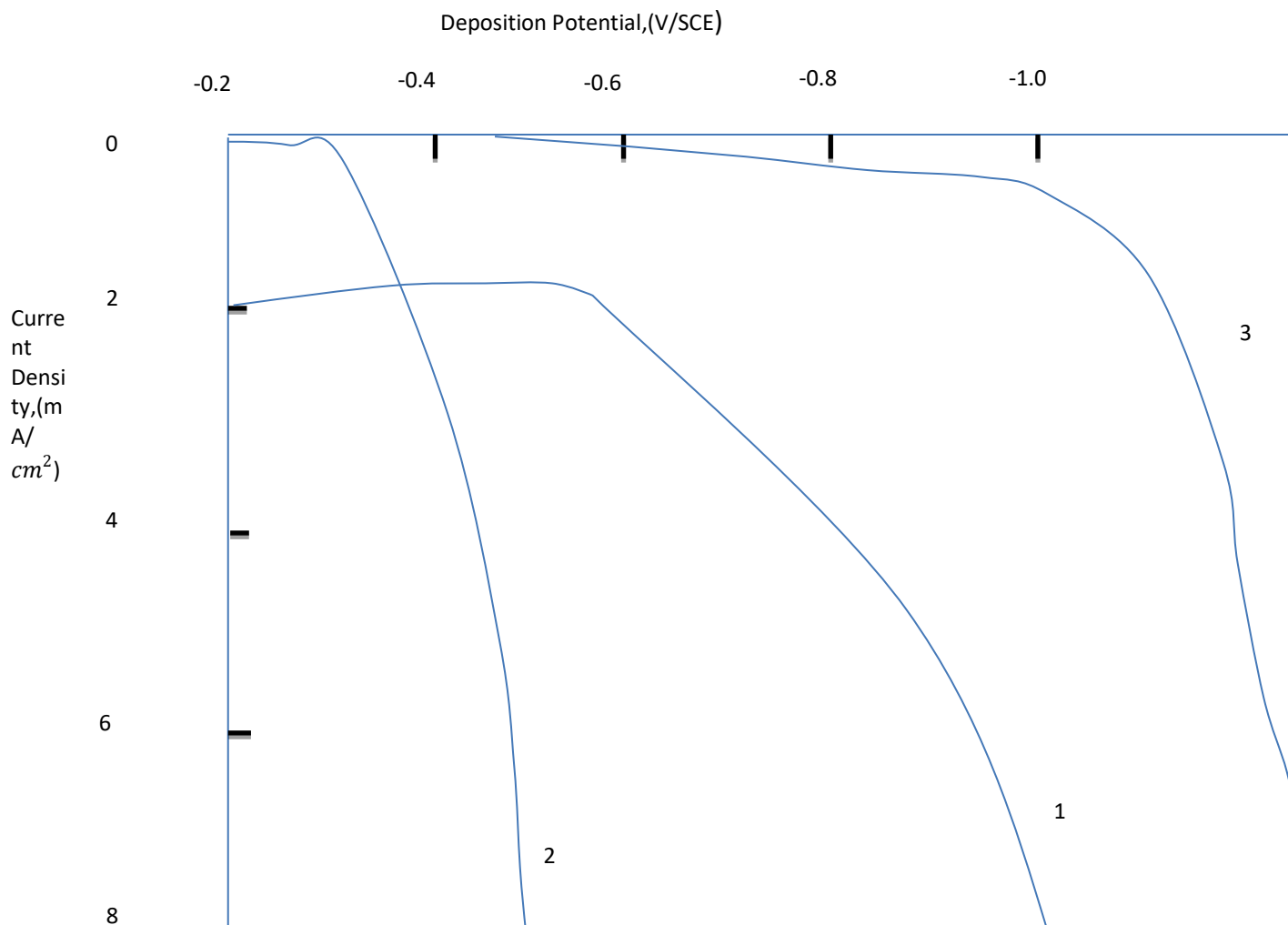


Fig.1: polarization curves for the reduction of 1) Y-S, 2) Y-Se onto stainless steel substrate and 3) Te on yttrium deposited stainless steel substrate.

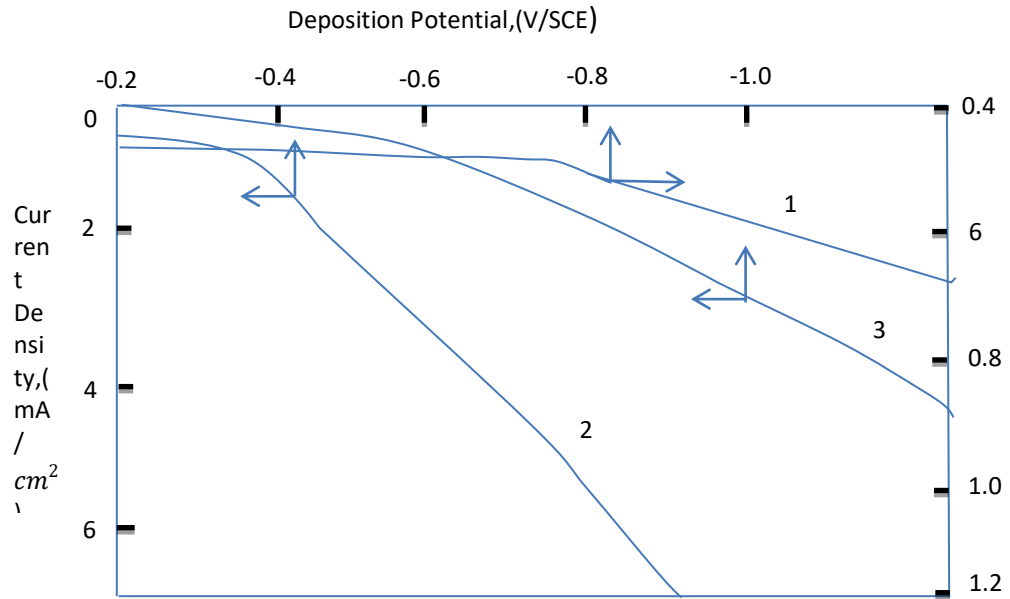


Fig.2: polarization curves for the reduction of Y-S, Y-Se and Y-Te on FTO coated glass.

Table 1: Estimated deposition potentials for the reduction of Y-S, Y-Se and Y-Te onto a stainless steel and FTO coated glass substrate.

Film Deposited	Bath composition	Deposition potentials (V/SCE)	
		St.Steel	FTO coated glass
Y-S	0.05M $Y(NO_3)_3$ - 0.05M $CH_3CSNH_2$ - 0.05M $CH_3COONa$ .	-0.72	-0.79
Y-Se	0.05M $Y(NO_3)_3$ - 0.05M $SeO_2$ - 0.05M $CH_3COONa$ .	-0.27	-0.36
Y-Te	Sat. $TeO_2$ - 0.05M $CH_3COONa$	-1.9	-1.95

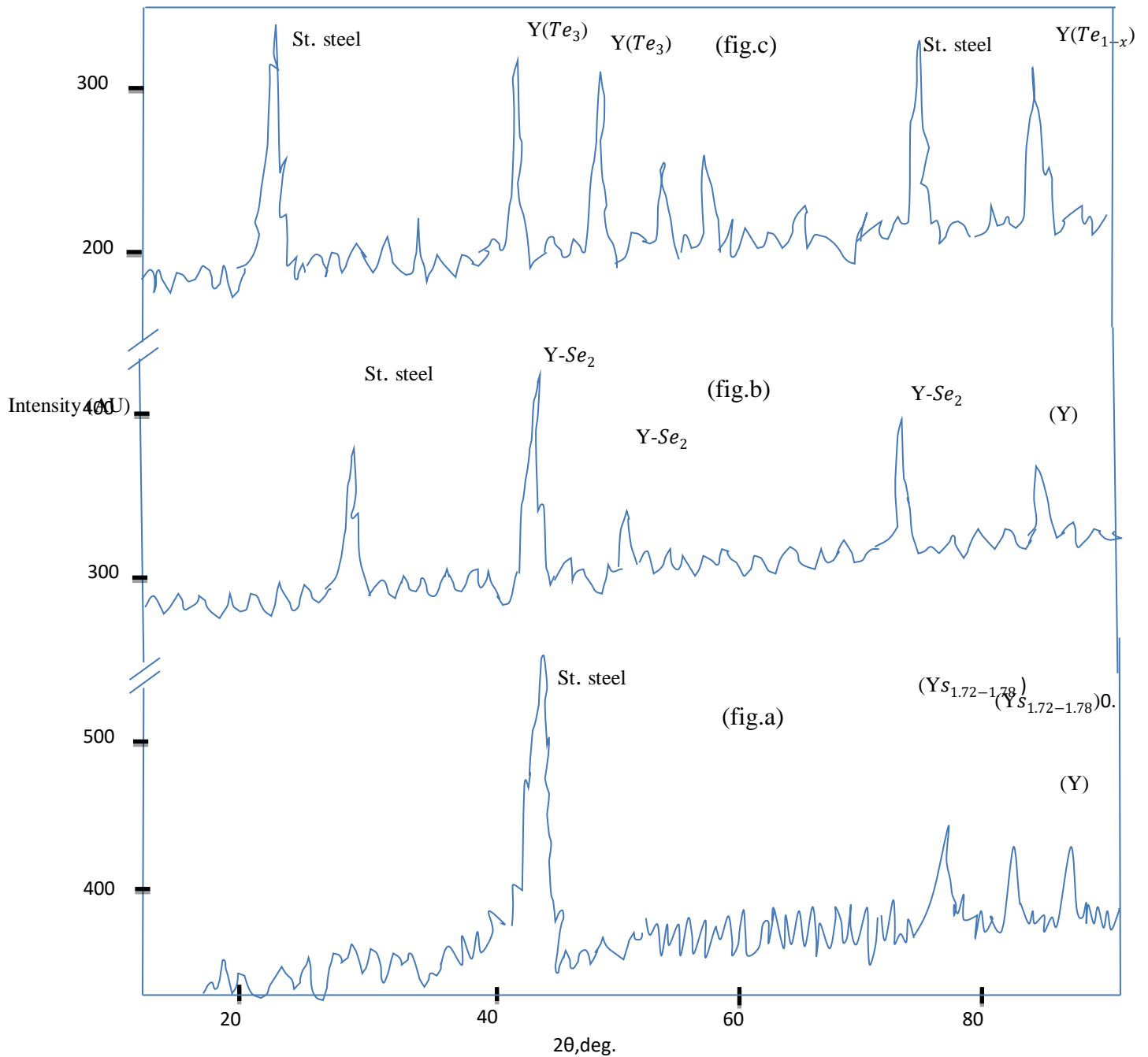


Fig. 3: XRD pattern of Y-S, Y-Se and Y-Te film deposited onto stainless steel

The structural properties of yttrium chalcogenide films are studied by X-ray diffraction technique. The study has been carried out with the films deposited onto stainless steel substrate. A different concentration of chalcogenide ions was tested, however, 0.05M concentration is found to be suitable for them, in which there is no yttrium hydroxide presence. Fig.3 shows the XRD pattern of Y-S, Y-Se and Y-Te films deposited onto a stainless steel substrate.

Table 2: Comparison of interplaner distances ‘d’ for Y-S, Y-Se and Y-Te films

Deposited film	Bath Composition	Observed ‘d’ values	Standard ‘d’ values	Compound formed	references
Y-S	0.05M $Y(NO_3)_3$ -0.05M $CH_3CSNH_2$ - 0.05M $CH_3COONa$ .	1.27 1.09	1.26 1.07	$(Ys_{1.72-1.78})$ $(Ys_{1.72-1.78})$	14
Y-Se	0.05M $Y(NO_3)_3$ -0.05M $S_eO_2$ - 0.05M $CH_3COONa$ .	1.26 2.72 1.80	1.26 1.74 1.80	$Y-Se_2$ $Y-Se_2$ $Y-Se_2$	15
Te on yttrium (Y-Te)	Sat. $TeO_2$ - 0.05M $CH_3COONa$	2.06 1.91 1.79	2.07 1.93 1.79	$Y(Te_3)$ $Y(Te_3)$ $Y(Te_{1-x})$	16,17

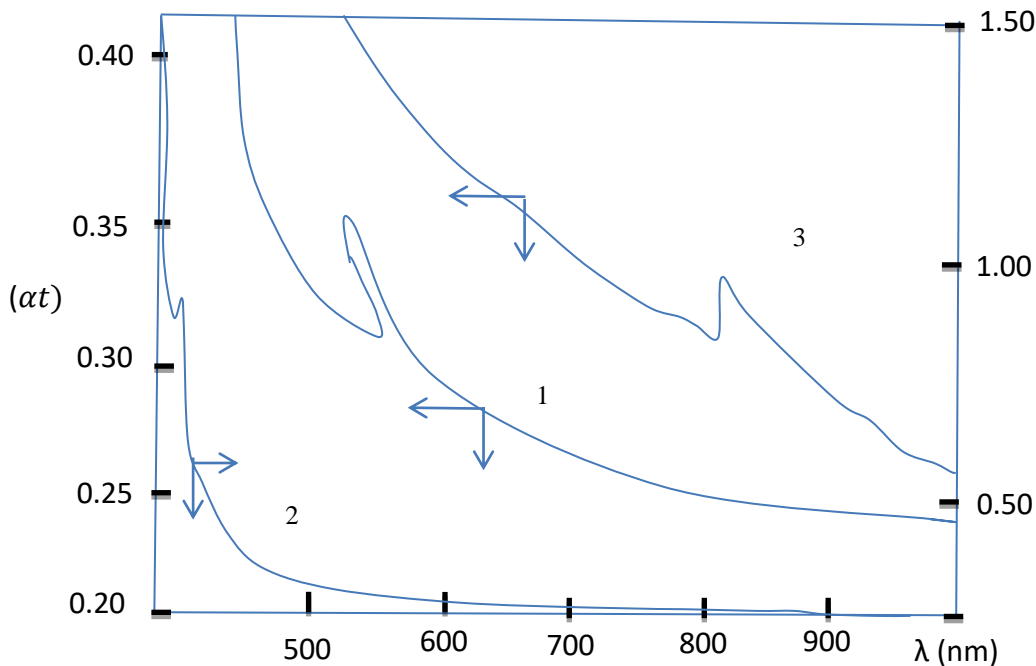


Fig 4: Optical density ( $\alpha t$ ) versus wavelength ( $\lambda$ ) spectra of of 1) Y-S, Y-Se and Y-Te film.

Table 2 shows the Comparison of observed ‘d’ values with ‘d’ values from standard ASTM data [14-17], which shows that material deposited corresponding to Y-S, Y-Se and Y-Te.

We have carried out optical absorption of yttrium chalcogenides films deposited on conducting (FTO coated) glass substrates at room temperature ( $27^{\circ}C$ ) in the wavelength range 400 to 1,000 nm.

Fig.4 shows that optical density ‘ $\alpha t$ ’ starts decreasing up to 700nm, which is large towards the shorter wavelength side. The absorption coefficient ‘ $\alpha$ ’ is if the order of  $10^2-10^3 cm^{-1}$ .

In order to estimate bandgap ‘ $E_g$ ’ of the Y-S, Y-Se and Y-Te, a plot of  $(\alpha h\nu)^2$  versus  $(h\nu)$  is plotted as shown in fig.5. The ‘ $E_g$ ’ were estimated to be 1.85, 1.96 and 1.86 respectively.

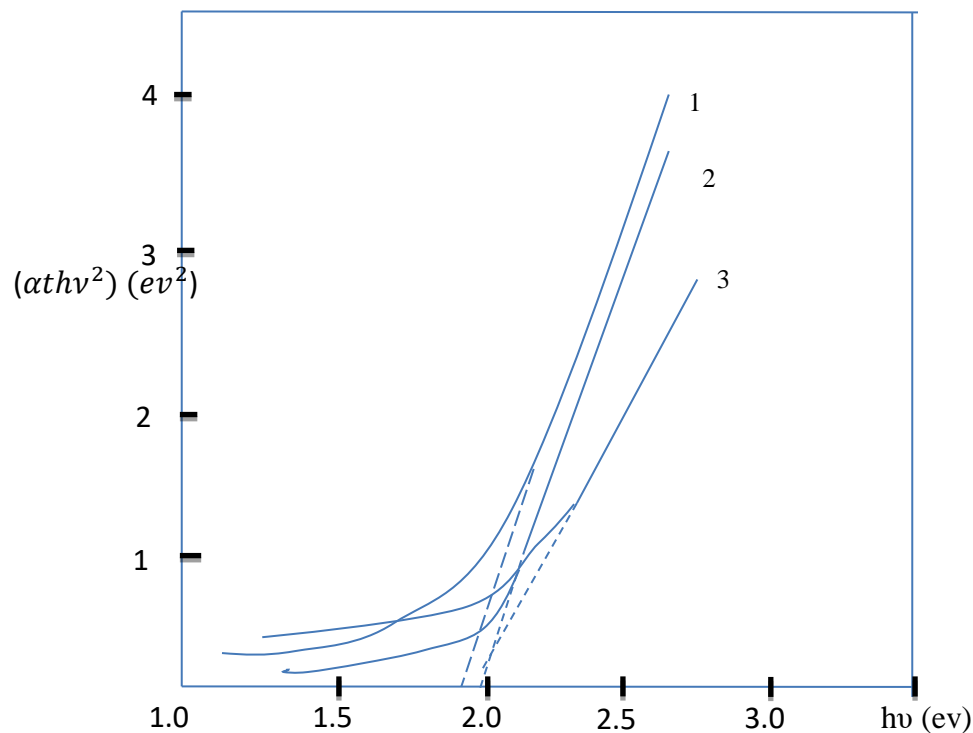


Fig. 5 : Graph of  $(\alpha thv^2)$  versus  $(h\nu)$  for 1) Y-S, 2) Y-Se and 3) Y-Te Films

### Conclusions:

Our study shows that yttrium chalcogenide (Y-S, Y-Se and Y-Te) films can be deposited at room temperature onto a stainless steel substrate and ITO coated glass using suitable complexing agent. The deposited yttrium chalcogenide films had the composition  $YS_{1.72-1.78}$ ,  $Y-Se_2$ ,  $Y(Te_3)$  and  $Y(Te_{1-x})$  with the band gap energies 1.85, 1.96 and 1.86 eV respectively.

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