CHEMICAL BATH DEPOSITED BARIUM SELENIDE FILMS – STRUCTURAL AND OPTICAL PROPERTIES

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The structural and optical properties of barium selenide films prepared by chemical bath deposition have been studied. X-ray diffraction study indicates that the grown barium selenide films have cubic structure. Optical measurements indicated a direct band gap of 1.70eV.

(Received January 4, 2011; accepted January 23, 2011)

Keywords: Thin film, Barium selenide, Chemical bath deposition, Structural and optical properties

1. Introduction

Barium Selenide (BaSe) is a technological important opto-electronic semi-conducting material with a direct band transition. A number of techniques (Huanyoug et al, 2003, Sankar et al 2003 and Guziewicz et al 2004) are employed in the formation of high quality thin films such as chemical vapour deposition, molecular beam epitaxy, pulsed laser, evaporation and sputtering.

However, the deposition from aqueous solution is attractive due to the low cost which is suitable for the commercial solar cell devices (Natarajan et al, 1994). There are several reports available in the aqueous solution deposition technique such as chemical bath deposition technique (Singh et al, 1987) of BaSe. Chemical bath depositions (Cesar et al, 1994 and Wang et al, 1999) belong to the technique that could also produce high quality films of chalcognide materials. The attractive features of the method are the convenience for producing large area devices and possibility to control the film thickness and morphology of the films by adjusting the deposition parameters. In this paper, we report the chemical bath deposition of BaSe from an aqueous solution bath containing $BaCl_2$ and $SeSO_3$ .The influence of growth conditions such as deposition time on crystallinity and composition of the film was studied. XRD and optical transmission techniques were employed for characterizing the deposited films.

2. Experimental

Thin films of BaSe were deposited by chemical bath techniques on pre-cleaned glass substrates at room temperature. The precursors used were 10ml of 0.5M $BaCL_2$ and 5mL of 0.1M K_2Se04. $Na_2S_20_3$ was used as the complexing agent to slow down the reaction in order to eliminate spontaneous precipitation which is not healthy for the growth. NH_3 was used to provide an alkaline medium for the growth of the films. The equation governing the reaction and deposition of BaSe films are as follow:

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$$BaCL_2+Na_2S_20_3 \rightleftharpoons [Ba\ (Na_2S_20_3)]^{2+} + 2CL^-$$
$$[Ba\ (Na_2S_20_3)]^{2+} \rightleftharpoons Ba^{2+} + Na_2\ S_20_3$$
$$K_2Se0_4 + OH^- \rightleftharpoons k_20_5+HSe^-$$
$$HSe^- + OH^- \rightleftharpoons Se^{2-} + H_2O$$
$$Ba^{2+} + Se^{2-} \rightleftharpoons BaSe \downarrow$$

Once the Ba^{2+} and Se^{2-} are present in the solution. They can combine to form BaSe molecules. The slides were observed to have been coated with depositions. The deposited films were analyzed using Janway 6405 UV – VIS model of spectrophotometer to measure the optical properties of the grown film. This was done in the wavelength range of 0.36µm – 1.10µm. The thickness of the film was determined by optical method.

3. Results and discussion

XRD pattern of the films deposited at different deposition time is shown in Fig. 1. It is observed that the films exhibit cubic structure with peaks corresponding to the (111), (021) and (221) reflections. The inter-planar distances (d) as were indicated in the XRD results are found to be 3.72Å, 3.59Å and 2.00Å. The results of these and all other peaks are presented in Table 1.

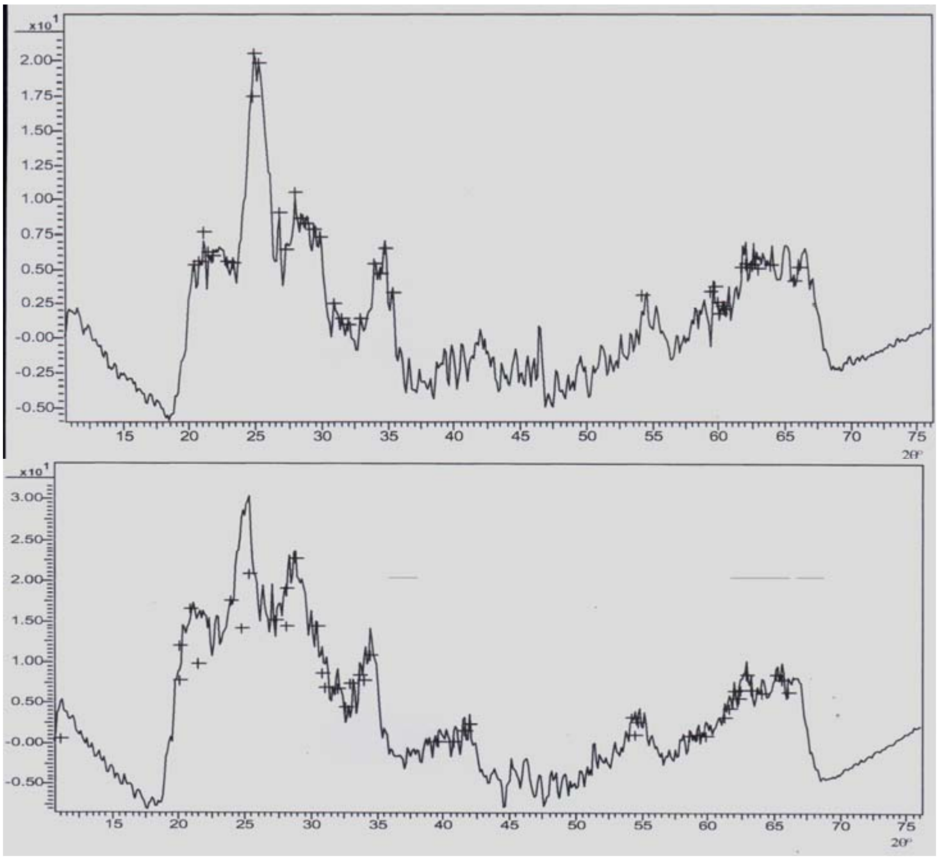

Fig. 1 X-ray diffraction patterns of BaSe.

Table 1 structural parameters of BaSe thin films for Q_{10} and Q_{11}

Reaction Bath	Thickness (µm)	hkl	20 (deg)	(rad)	d (Å) Measured	d (Å) Standard	FWHM	Grain size, D
Q_{10}	0.865	021	26.81	0.468	3.33	3.30	0.380	3.75
		002	35.41	0.618	2.53	2.45	0.385	3.80
		402	54.28	0.947	1.69	1.84	0.383	4.07
Q_{11}	0.967	111	23.90	0.417	3.72	3.53	0.362	3.92
		021	24.78	0.433	3.59	3.60	0.362	3.92
		221	54.24	0.947	2.00	2.00	0.365	4.27

The structural parameters of BaSe film show that the film has average grain size of 3.95Å for film Q_{10} and 4.03Å for film Q_{11}. Table 1 show that the grain size increases with increase in film thickness. This may be attributed to the decrease in imperfections of the films with increasing film thickness.

The above results compare well with the report presented in www. webelements. com which presented BaSe as having cubic structure, and also having the same structure with $NaCl_2$ with each atom having six neighbors.

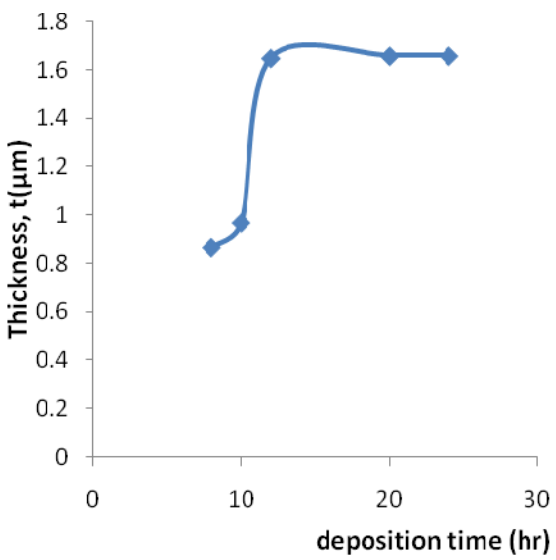

Fig. 2. Variation of thickness vs. deposition time

Fig. 2 reveals that film thickness depends on the growth parameters. It shows that the film thickness increases with the deposition time.

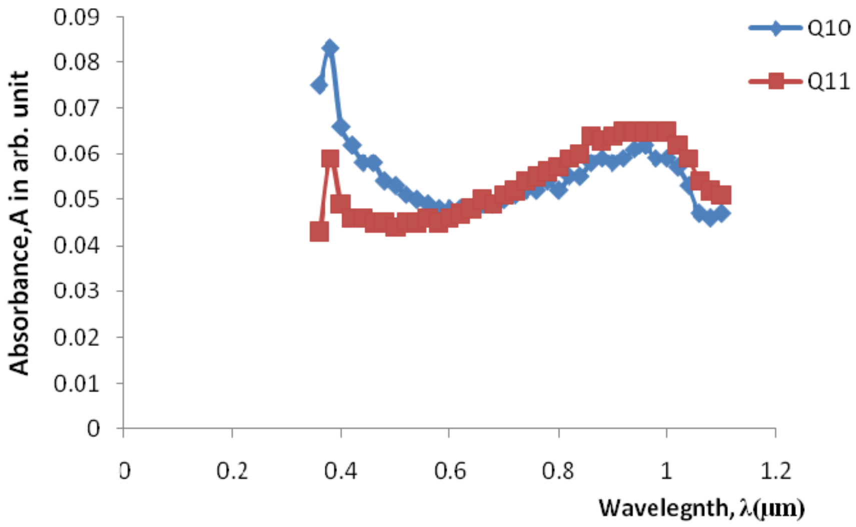

Fig. 3. Spectral absorbance of BaSe for Q_{10}&Q_{11}

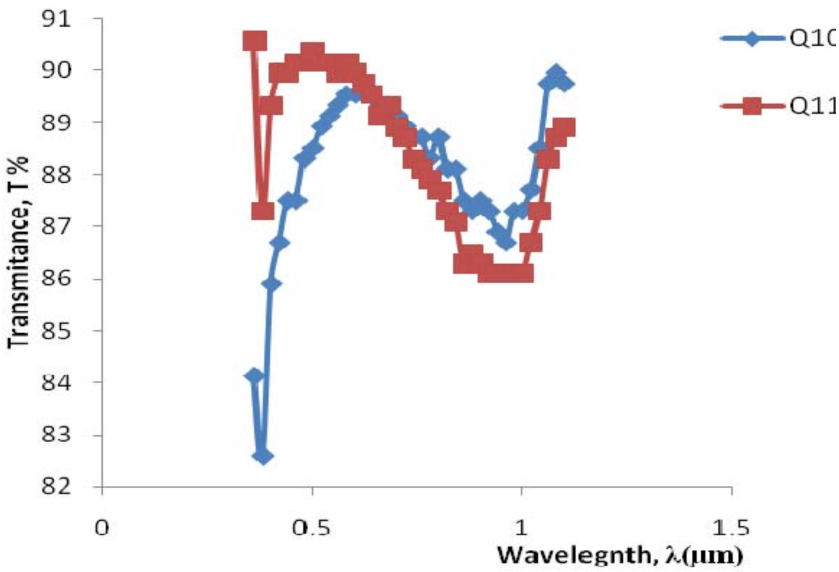

Fig. 4. Spectral transmitance of BaSe for Q_{10} &Q_{11}.

Figure 3 and 4 show the plots of absorbance and transmittance versus wavelength of BaSe thin films deposited in this work. The optical transmission spectra in figure 3 showed uniform value of absorbance (A). All the films have low absorbance. The figure 4 shows that the BaSe transmits heavily about 85% in UV-VIS regions of the spectrum. The very high transmittance in visible region makes the BaSe film useful aesthetic window glaze material. Film thickness has significant effect on the transmittance of the film. Figure 4 reveals that the greater the thickness the higher the transmittance of the film.

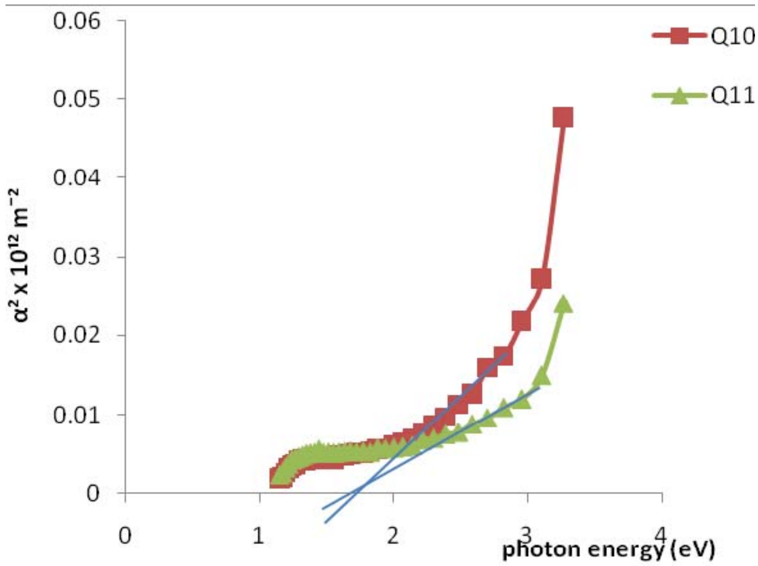

Fig. 5. Plot of α^2 versus hv of BaSe Q10 & Q_{11}

A plot of α^2 versus photon energy (hv) of BaSe film is shown in figure 5.The energy gaps are obtained by extrapolating the linear portion of the curve to the energy axis. The band gap was found to be 1.70eV. The wide band gap possessed by BaSe film makes it likely candidate to replace material like GaN in light emitting laser diodes (Gutowski, et al 2002).

4. Conclusions

The depositions of BaSe thin films have been successfully carried out in alkaline medium using chemical bath deposition technique. The deductions from the XRD and the spectrophotometer revealed a band gap of 1.70eV and the average grain size of 3.95Å. BaSe films were found to have low absorbance in all the regions. They have very high transmitting in UV-VIS region and possess cubic structure.

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