The Engineering of Optical Energy Gap with Composition in $(ZnS)_x (CdTe)_{1-x}$ Thin Films

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ABSTRACT.   The optical energy gap (E_g^{opt}) of the as deposited and annealed $(ZnS)_x(CdTe)_{1-x}$ thin films could be designed for the range $0.0<x<1.0$.

The E_g^{opt} showed a decrease in its value as CdTe increased in the films with slight increase in the case of respective annealed films at 473K for one hour. Suitable equations to E_g^{opt} with respect to the composition (x) have been investigated.

The value of the width of tails of localized states in the gap (E_t) was also determined and showed a fluctuation according to the content x. A suggested model of the density of states of these films were obtained.

Introduction

Cadmium telluride (CdTe) and zinc sulphide (ZnS) belong to II-VI compounds and usually have direct optical band gaps of 1.5eV and 3.7eV respectively (Abrikosov, 1969, Brian,1969). The optical energy gap of the system CdS$_x$Te$_{1-x}$ has been determined by Hill and Richardson (Hill,1973a, Hill,1973b). They found that the energy gap of the system varied with the composition (x) according to the form $E_g^{opt} (x) = E_{g1}^{opt}+ (E_{g1}^{opt} - E_{g2}^{opt} - b) x$, where E_{g1}^{opt} and E_{g2}^{opt} are the energy gaps of the pure compounds 1 and 2 and b is the bowing parameter . Makadsi *et al.* (Makadsi *et al.*, 1994) showed that the energy band gap of CdTe$_{1-x}$S$_x$ films having values in the range from about 1.45 eV for CdTe to about 2.45 eV for CdS .

Sanchez et al (Sanchez et al , 1996)studied the temperature dependence of the fundamental band gap (E_g^{opt}) of Cd$_{1-x}$Zn$_x$Te alloys with zinc concentration in the range (x) from 0.0 to 0.3 . They found E_g^{opt} varies from 1.511eV for x = 0 to 1.667±0.008 eV for x= 0.3 at room temperature.

Deshmukh *et al.* (Deshmukh *et al.*, 1997) showed a linear increase in the band gap for x<0.3 whereas a non linear dependence was observed beyond x = 0.3.

In the previous work (Al-Ani, 2001a, Al-Ani, 2001b) the electrical, structure and optical properties of $(ZnS)_x (CdTe)_{1-x}$ thin films were investigated. In this paper we are going to give a new design of the optical energy gap of $(ZnS)_x (CdTe)_{1-x}$ compound which may help to give the best mixing ratio for the solar cell applications .

Experimental Procedure

Thin films of $(ZnS)_x$ $(CdTe)_{1-x}$ compound were $0<x<1.0$, of thickness 300nm were deposited at room temperature (303K) on a cleaned glass substrates by thermal evaporation technique using Balzer unit . The rate of deposition was 2nm/sec . Some of the as deposited films were subsequently subjected to annealing at 473K for one hour . The optical absorbance of the films was measured , using UV 8800 Double Beam Spectrophotometer , in the spectral range of 320-850 nm.

Results and Discussion

The optical absorption coefficient (α) of the as deposited and annealed films were calculated from the absorbance spectra at various incident photons (hv) . The optical energy gap (E_g^{opt})of $(ZnS)_x(CdTe)_{1-x}$ have been obtained using the formula (Tauc,1974 , Mott,1979).

$$\alpha h v = B(h v - E_g^{opt})^r \qquad (1)$$

where B is constant and r is an exponential which can assume values 1,2,3,1/2 and 3/2 depending on the nature of the electronic transitions.

The obtained (E_g^{opt}) showed an increase in their values as the ZnS contents increased in the films .This is because of the high resistivity of the films when the amount of ZnS increased, since the resistivity of CdTe is about $10^5\Omega$ cm whereas that for ZnS is about 10^7 Ω.cm. A similar behavior have been shown for the annealed films but with values somewhat greater than that of the as deposited.

Figures1 and 2 exhibted the variation of (E_g^{opt}) against the composition x for the as deposited and annealed films respectively. The variation of (E_g^{opt}) with content (x) gives non linear dependence according to the obtained equations :
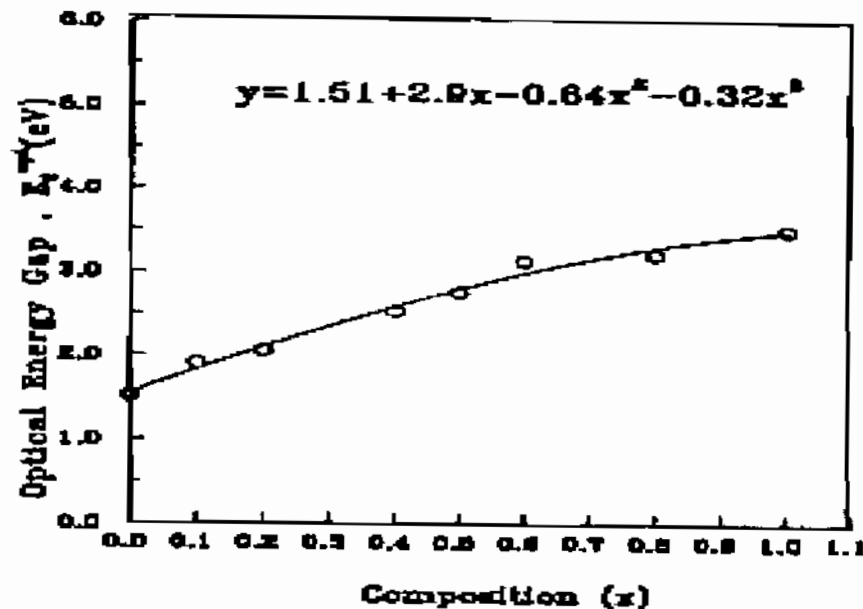

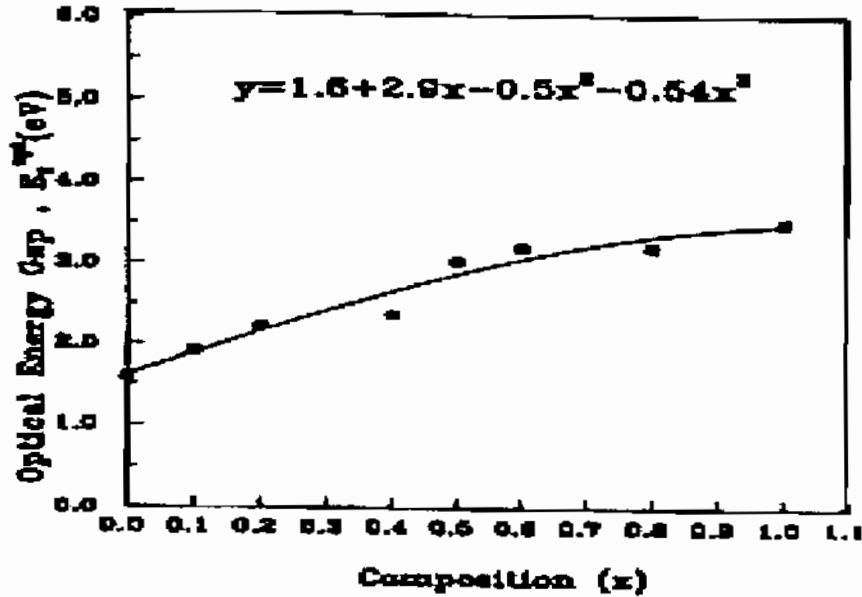Fig. 1. Shows the variation of E_g^{opt} VS. the composition (x). For as deposited (ZnS) (CdTe) films.

Fig. 2. Shows the variation of E_g^{opt} VS. the composition (x). For annealed (ZnS) (CdTe)films.

For as deposited films

$$E_g^{opt}(x) = 1.51 + 2.9x - 0.064x^2 - 0.32x^3 \qquad (2)$$

For annealed films

$$E_g^{opt} = 1.6 + 2.9x - 0.5x^2 - 0.54x^3 \qquad (3)$$

The width of tails of the localized states in the gap (E_t) of the as deposited and annealed films with respect to x was also obtained and as shown in figures 3 and 4 respectively. It is clear from the figures that the E_t was wavering from low value for CdTe and ZnS to maximum value at x = 0.5. This behaviour was in agreement with the structure results (Al-Ani, 2001b).
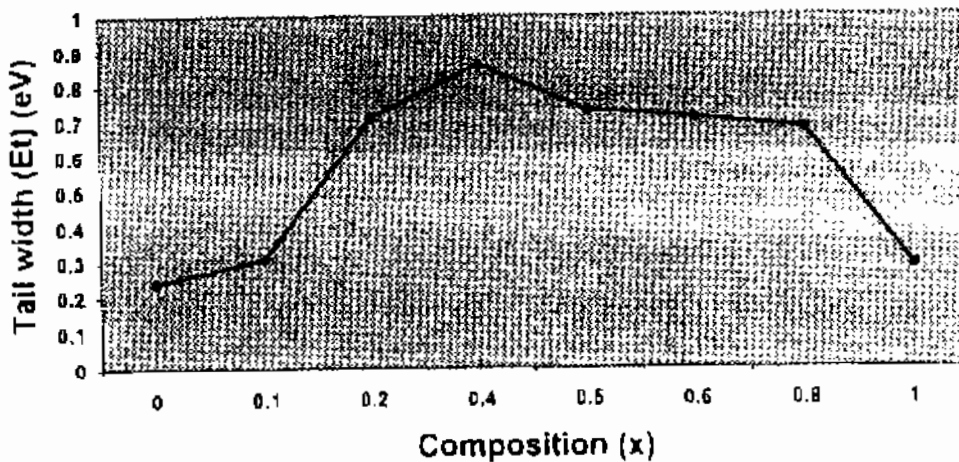

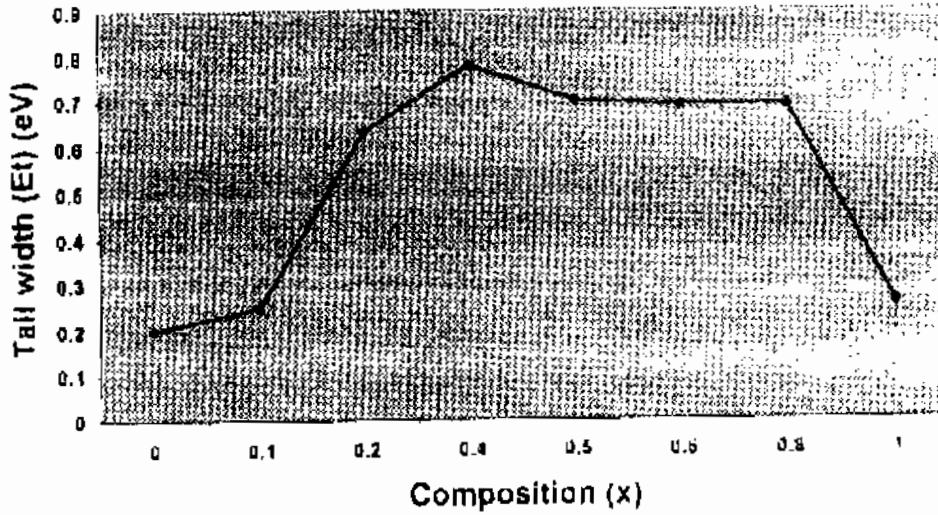Fig. 3. Tail width (E_t) versus the composition (x) for as deposited (ZnS) (CdTe) films.

Fig. 4. Tail width (E_t) versus the composition (x) for annealed (ZnS) (CdTe) films.

This change in E_t as well as the structure refers to the difference in the lattice constants of the compounds ZnS and CdTe (Hand Book ,1978), hence the more difference in the lattice constants the more disorder appears in the films.

A suggested model for the density of states for these films has been investigated as shown in figure 5. This model exhibited the change in E_g^{opt} with respect to x and according to the values of E_t. Figures (5a) and (5b) for the pure ZnS and CdTe films and figure (5c) for the mixture $(ZnS)_x (CdTe)_{1-x}$ films in which the maximum E_t is of about 0.86 eV and this has been reduced depending upon the dominance of CdTe or ZnS ratio in the films.
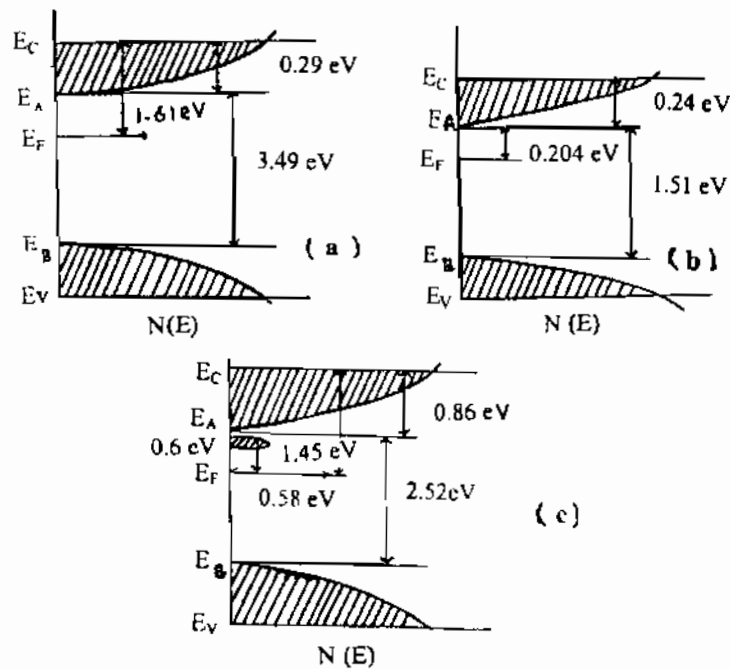

Fig. 5. Shows suggested model of density of states of $(ZnS)x (CdTe)1-x$ thin films.
a) pure ZnS   b) pure CdTe   c) mixture

Conclusions

The engineering of the optical energy gap of the system $(ZnS)_x (CdTe)_{1-x}$ is varied non linearly with the content (x), so we have a new candidate compound for fabricating the solar cell. This gives rise to the usefulness of this compound in optoelectronic devices over a wide spectral range. The variation of the tail width of the films gives different phases and structures of the compound and depends on the ZnS content.

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هندسة فجوة الطاقة البصرية لأغشية المركب (ZnS)$_x$ (CdTe)$_{x-1}$ الرقيقة

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المستخلص .   عيّنت فجوة الطاقة البصرية (E_g^{opt}) لأغشية (ZnS)$_x$ (CdTe)$_{x-1}$ الرقيقة حيث (0<x<l) بعد ترسيبها مباشرة والمعالجة الحرارية .

وقد وجد أن E_g^{opt} تقل قيمتها بزيادة نسبة CdTe في الأغشية. كما وجـد أن هناك زيادة طفيفة لفجوة الطاقة للأغشية بعد عملية التلدين عند درجة حـرارة 473K ولمدة ساعة. وقد وضعت صيغة توضح العلاقة بين E_g^{opt} والنسبة x للأغشية كما تـم ترسيبها والمعالجة حراريًا .

تم حساب عرض ذيول الحالات الموضعية (E_l) في فجوة الطاقة البـصرية . وقد لوحظ أن هناك تذبذبا في قيمتها وفقا للنسبة x . اقترح نموذجا لكثافــة الحــالات للأغشية التي تم دراستها .