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GRAIN SIZE DEPENDENCE OF THE ELECTRICAL AND OPTICAL PROPERTIES OF THE SPRAYED Cd0.5Zn0.5S:B FILMS DEVELOPED IN SCIENCE PARKS

By selçuk mert

GRAIN SIZE DEPENDENCE OF THE ELECTRICAL AND OPTICAL PROPERTIES OF THE SPRAYED $Cd_{0.5}Zn_{0.5}S$:B FILMS DEVELOPED IN SCIENCE PARKS

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Energy Systems Engineering Department ,Yalova University, Yalova, Turkey

Science park has been widely recognized for its importance to the development of high-tech industries. Boron doped $Cd_{0.5}Zn_{0.5}S$ films which were developed in Science parks were prepared by spray pyrolysis technique at 400 °C substrate temperature, which is a low cost and large area technique to be well-suited for the manufacture of solar cells, using boric acid (H_3BO_3) as dopant source and their properties were investigated as a function of doping concentration. $Cd_{0.5}Zn_{0.5}S$ films were obtained with incorporation of Cd element into ZnS by spray pyrolysis technique using aqueous solutions of $CdCl_2$, $ZnCl_2$ and $(CS(NH)_2)_2$, which were atomized with compressed air as carrier gas. Effects of the grain size of the films on optical and electrical properties of sprayed cadmium zinc sulfide (CdZnS) films were investigated.

(Received January 12, 2016; Accepted March 1, 2016)

Keywords: Thin film structure, Semiconductor, Optical properties, Grain, Microstructural properties

1.Introduction

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$Cd_{0.5}Zn_{0.5}S$ films were obtained using spray pyrolysis method on the glass substrates at a temperature of 400°C. Spray pyrolysis is basically a chemical process, which consists of a solution that is sprayed into a substrate held at high temperature, where the solution reacts forming the

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desired thin film. In this technique, the $Cd_{0.5}Zn_{0.5}S$ films were deposited on heated microscope glass (Objekttrager, 1 cm × 1 cm) substrates by spraying an aqueous solution in air atmosphere. The spray solutions are comprised of zinc chloride and cadmium chloride (0.5 M, Merck, ≥ 99%) and boric acid (H_3BO_3) as dopant source in the deionized water. The substrate temperatures 400°C was used and the temperature was controlled within ± 5°C through a chromel–alumel thermocouple as a sensor for the temperature controller. Before deposition, the glass substrates were ultrasonically cleaned in acetone solution, and then rinsed in deionized water. The atomic percentage of dopants in (B/(Zn-Cd)) solution were 1.0, 1.5, and 3.0 at.% in spray solution. In this procedure, compressed air was used to atomize the solution containing the precursor compounds through a spray nozzle over the heated substrate; air is compressed from the atmosphere. The precursor is pyrolyzed on the heated substrate. The solution was pumped into the air stream in the spray nozzle by means of a syringe pump. The analyses of these films are investigated in Science park. The optical band gap energy Eg was determined by extrapolating the high absorption region of the curve to the energy axis [13]. The resistivity of $Cd_xZn_{1-x}S$ films were determined by four probe measurements at room temperature. The carrier density was determined by Hall effect measurements.

3. Results and Discussions

The dependence of grain size and strain of the $Cd_{0.5}Zn_{0.5}S$ films with the boron concentration is shown in Fig.1. The grain size was found to decrease from 250 to 125 nm as the boron concentration was increased from 0% to 3%. Thus, increasing the boron concentration increases the density of nucleation center and, under these circumstances, a larger number of centers start to decrease, resulting in smaller grains. The smaller grain size is undesirable for most semiconductor applications because of the barrier effect of grain boundary on the mobility in planar direction [14]. Also, the decrease in grain size with the boron concentrations could be attributed to the enhanced reaction kinetics among the sprayed droplets as well as improvement in the ad-atom mobility on the substrate surface. It can be explained that the decreasing trend of grain size with the increase of strain due to the retarded crystal growth as the stretched lattice increases the lattice energy and diminishes the driving force for the grain shrinkage. The lattice strain provide a driving force for the grain shrinkage during the increasing boron concentration. The lattice strain arises from a high atomic packing density and frozen-in crystallographic defects in the grains and grain boundaries [15]. Since the intragranular defects and grain boundaries contain more free energy than crystalline phase, the decrease of the grain sizes in the films higher free energy with increasing boron concentration. Moreover, the particle size and strain are manifestations of dislocation network in the films the increase in strain with an decrease in the grain size indicates the formation of the non-good quality films.

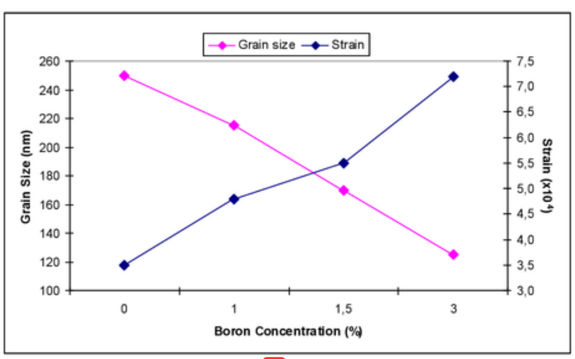
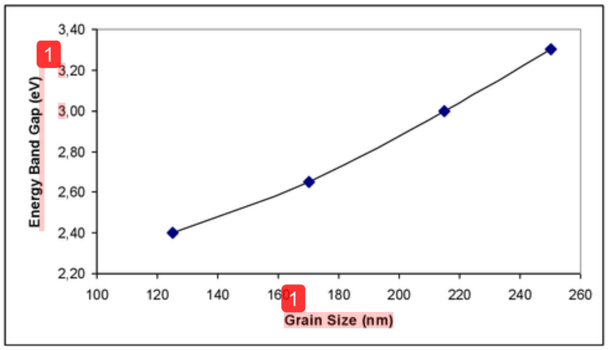


Fig. 1: Variation of boron concentration in the polycrystalline films with grain size and lattice strain of $Cd_{0.5}Zn_{0.5}S$:B films deposited by spray pyrolysis method.

The dependence of the band gap of $Cd_{0.5}Zn_{0.5}S$ films with the boron concentration is shown in Fig.2. It can be seen that the band gap increases from 2.40 to 3.30 eV as the grain size decreases from 250 to 125 nm. This increase in the band gap can be due to the influence of various factors such as grain size, structural parameters, carrier concentration, presence of impurities, deviation from stiochiometry of the film and lattice strain [16–18]. A detailed analysis is needed to bring out the effect of each of these parameters on the value of grain size. Hence, we consider that the observed increase in Eg with decreasing grain size is due to the increase in lattice strain. From these results, it is clear that energy band gap increases with increase in boron concentration. Earlier studies show that strain changes the inter atomic spacing of semiconductors which affects the energy gap [19]. It is concluded that the effect of grain size on the bandgap, as the result of electron confinement in grains [20] and also the effect of lattice strain.



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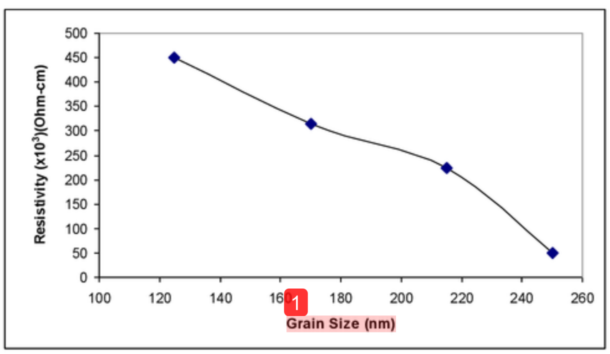

Fig. 3: Variation of grain size in the polycrystalline films with resistivity of $Cd_{0.5}Zn_{0.5}S:B$ films deposited by spray pyrolysis method.

Figure 3 shows the variation of film's resistivity with grain size. This behaviour can be explained as follows: when the grain size decreases, the grain boundaries increases and hence resistivity is rises. The increase of the resistivity of the films as a function of the grain size is also due to re-crystallization of the crystallites in the films, which induces the increase of the number of faults at the grain boundary. As a consequence, the quality factor of the film decreases with decreasing grain size. It can be explained that the decrease of the grain size to increase the number of grain boundaries; the increase of the barrier height at the grain boundaries. Thus, it can be show that the increase of resistivity with the decreasing grain size of the films probably is due to the distortion of the crystallinity of the films. This observation is attributed to the size effect observed in semiconductor films.

4. Conclusions

Boron doped $Cd_{0.5}Zn_{0.5}S$ films have been prepared by the spray pyrolysis method on glass substrates heated at 400 ∘C using different boron concentration. It is seen that the optical and electrical properties of $Cd_{0.5}Zn_{0.5}S$:B films are found to be grain size dependent. The resistivity measurement shows that films are semiconducting in nature. With the increase of boron concentration, coalescence of the small grains took place, leading to the formation of lower crystallites in the film along with an distortion of the crystallinity. Therefore, it is observed that the electrical and optical properties of the films have a direct dependence on the grain size. As a result, the observed increase in E_g and strain with decreasing grain size are due to the increase of resistivity and the increase of boron concentration of the films. The results of these analyses provide some policy implications and government of the local university for Yalova. Thus, a science park is learning site, combining in a pre-established territorial area productive, scientific, technical, educational and institutional agents, based on the assumption that the co-location of these agents is expected to enhance the technological and innovation capability of the host region.

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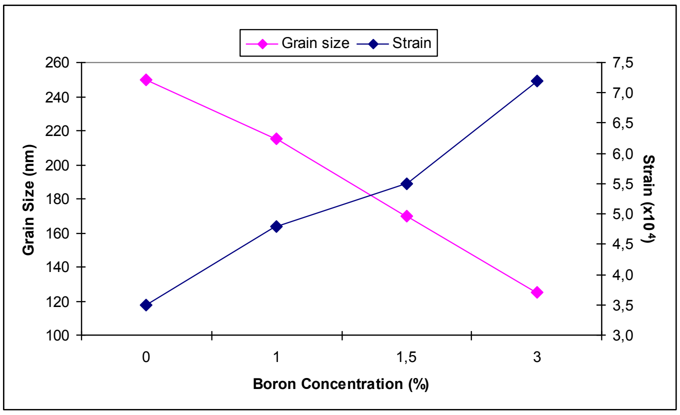

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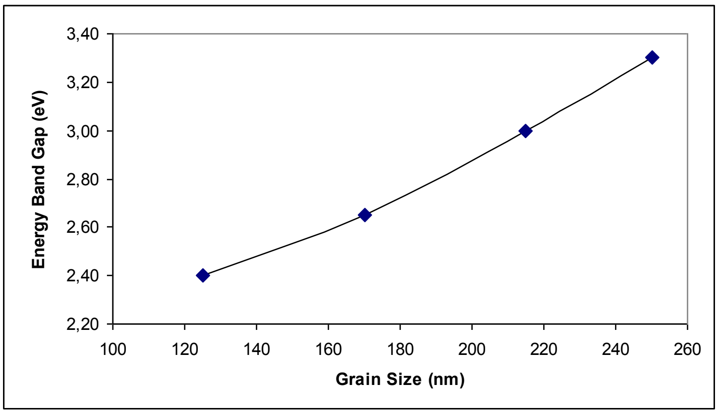

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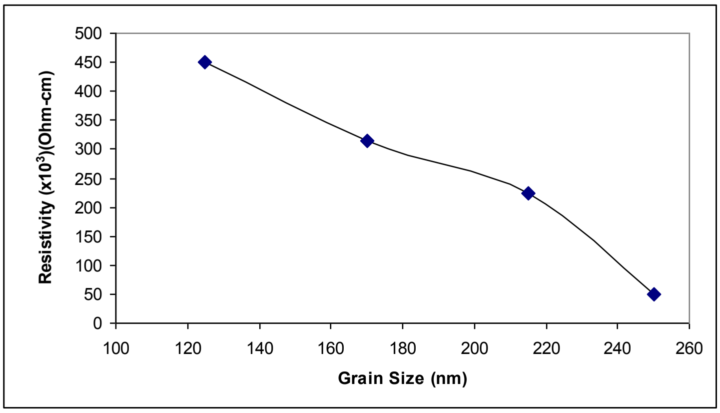

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