Characterization and Processing of CdS/ZnS Thin Layer Films Deposited onto Quartz for Solar Cell Applications

N Dahbi a, D-E Arafah b, a*

a Laboratory of semiconductor devices physics (LPDS), university of Béchar n°417, Béchar (08000), Algeria
b University of Jordan, Physics Department, Amman 11942; Jordan

Abstract

In this work, synthesis and processing of CdS/ZnS multilayer thin film systems are studied; compositional changes within these thin films structures are investigated by the Rutherford backscattering (RBS) technique to determine the depth distributions of the mixed region and stoichiometry according to Rump simulation which is used to estimate layer thickness and compositions even for complex samples; depth profiling using this program is also determined. The RBS data reveal a more homogeneous film could be obtained after annealing in 400°C and stoichiometric film structures with composition Cd_{1-x}Zn_xS, where x=0.6 are synthesized in ZnS/CdS bilayer.

Keywords: Thin film; ZnS/CdS; Chemical treatment; Thermal treatment; RBS; Depth profiles; Vacuum deposition; Solar cell

1. Introduction

Over the years, CdS and ZnS thin films have been intensively investigated mainly for their applications in large-area electronic devices such as thin-film field-effect transistors and solar cells. Among several n-type semiconductor materials, it has been observed that the large band gap n-type window material CdS is the most promising hetero-junction partner for the well-known photovoltaic

* N Dahbi. Tel.: +213-49-81-55-81/91; fax: +213-4-81-52-44.
E-mail address: algirierose@yahoo.com.
materials, e.g. ZnS [1, 2]. This latter thin film has a vast potential for use in short-wavelength optoelectronic such as electroluminescent devices due to his band gap which is of 3.66eV [3, 4]. So by the addition of ZnS, the band gap energy of CdS can be increased, hence combination of the two thins films produce Cd$_{1-x}$Zn$_x$S thin film which has a larger energy gap make it transparent to practically all wavelengths of solar spectrum [5] also by using this higher band gap materials i.e. Cd$_{1-x}$Zn$_x$S as a heterojunction partner to CdTe can improve the window band gap then improve the short wavelength spectral response of CdTe solar cell.

Cd$_{1-x}$Zn$_x$S can be prepared by a variety of techniques, including spray pyrolysis, ion beam deposition, molecular beam epitaxial growth, chemical bath deposition, thermal evaporation, and screen printing methods [7].

The Rutherford Backscattering technique (RBS) is one of the most powerful methods to investigate the composition, stoichiometry and depth profile of solids and consequently any structural changes in their composition as a result of ion beam modifications. This technique has been considered for the measurement of dose accumulation in a semiconductor substrate during an implant. The RBS involves measuring the number and energy of ions in a beam (usually He ions) that backscatter after colliding with atoms at surface and near-surface regions of a sample at which the beam was targeted. With this information and the scattering geometry, it becomes possible to determine quantitatively mass information and elemental concentrations versus depth below the surface [8].

The most extensive use of the RBS technique finds itself in various fields of electronic and optical materials and applications, e.g. special coatings and in the study of various physiochemical processes on solid surfaces [9].

Our goals in this work are to study mixing effects of synthesized CdS/ZnS multilayer thin film systems deposited on quartz substrate by using vacuum deposition method, chemical and thermal treatment will be used to achieve homogeneous Cd$_{1-x}$Zn$_x$S thin films, also compositional changes within the thin films structures will be investigated by the RBS technique to determine the depth distributions of the mixed region and stoichiometry.

2. Experimental methods

In the preparation of CdS/ZnS thin film layer, a ZnS film was first deposited on Quartz substrate with thick of 700Å by vacuum deposition with a typical working pressures of $10^{-4}$ Pa were used during evaporation, this was then dipped in 1% CdCl$_2$ methanol solution for about 30 s, then dried with an infrared lamp, and then rinsed in the Deionized water. This was followed by an additional deposition of CdS thin film with thick of 500Å; finally the samples were annealed in air at 400 °C for 15min.

Rutherford backscattering (RBS) was used to characterize the films, using 2 MeV $\alpha$-particles beam supplied from the Jordan University Van de Graaff accelerator (JOVAC). Detection of backscattered particles was done using normal incidence and a scattering geometry with angle 135° relative to the incident beam and the reflected particles were collected using a silicon surface barrier detector of 12keV resolutions and 50 active area. To assist in the evaluation, Rump simulation was used in order to estimate of the layer thickness, compositions and determine the depth profile of our samples [10].

3. Results and discussion

Typical and theoretical results of Rutherford backscattering (RBS) experiment for our multilayer ZnS/CdS samples are reported in figure 1 for two cases: before and after chemical treatment, the calculated (theoretical) spectrum which is obtained from Rump simulation and is shown as a solid curve appear to be in good agreement with the measured spectrum (experimental) which is represented by open
circles. The simulation reproduces the nominal thickness of the top surface layer namely, 50nm (CdS) layer, the interface layer on the other hand was found to be about 14% thicker. Such a layer was found to contain quite a large percentage, 80%, of oxygen; this may be expected, and this work is indeed consistent with other work [11] in which oxygen is present in large concentration and noted to be active.

Fig. 1 Typical 2 MeV RBS spectrum of ZnS/CdS thin film deposited onto quartz glass: (a) before chemical treatment; (b) after chemical treatment.

However, one source of its presence is air during sample preparation, in addition a small amount of silicon was noted to be present within the layer; this indicate that the matrix is an active ingredient that may mix within the film components at room temperature. However, this observation is noted sooner than expected, and silicon can cross the interface layer by its higher diffusivity which dominates all other matrix elements present in the sample. The process which can justify the transform of silicon is the presence of a high concentration gradient.

Close examination of the signal reveals sloping on the front edges of sulfur, oxygen and silicon as well as the back edge of Zn. After chemical treatment, which involves dipping the samples in a saturated solution of CdCl₂ at room temperature for 30s in air, represent excellent match with the measured spectra. Once again, the input data for calculation are based on the experimental conditions which makes in the results obtained more reliable. Examination of figure 1 reveals wide variations and marked changes and can be summarized in the following points: First, the ratio of Cd after chemical treatment is doubled due to incorporation of Cd from the solution. Second, the Cd is extending over layer that is 12% wider with larger concentration at large depths such that its peak is detected at deeper depth by about 30%. Third, the Zn signal appears to be drastically reduced by about 30% from its original peak value, accompanied by movement towards the surface by an almost the same proportion. The amount of material is extending over a layer that is 13% larger, the motion of Zn towards the surface appears to conserve about 0.3% of Zn to be retained in the sample; perhaps, if larger dipping times were used, then the amount of Zn retained would be smaller. Forth, a similar observation to Zn was noted with the sulfur signal; in particular, sulfur was observed to exhibit movement towards the surface such that its peak concentration has moved by 13% and has increased by an almost 15% with a more defined and narrow region. Fifth, film components are homogeneous being that the signals distributions are not widely varying. Finally,
both oxygen and silicon within the bulk are homogenous but their concentration near the surface region exhibit variation from stoichiometry by an amount not exceeding 50% (see Fig. 3).

Figure 2 shows the measured and simulated spectra of the sample after annealing at 400 °C for 15 min, which indicates a clear and marked change in the signals.

![Figure 2 Typical 2 MeV RBS spectrum of ZnS/CdS thin film deposited onto quartz glass after annealing at 400 °C](image)

The computer simulation of the spectrum shows an excellent agreement with measured one based on the formation of mixed layer $\text{Cd}_{1-x}\text{Zn}_x\text{S}$, Isaiah et al. [12] found that a homogeneous $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ can be fabricated from ZnS/CdS structure.

Thermal annealing activated diffusion appears too and has intimate mixing within the layers, this latter process has resulted in about 40% change in the Cd while that due to Zn is larger and reaches about 60%. Heat and CdCl$_2$ treatments exhibit marked changes; however, annealing in air following chemical treatment acts to drive chlorine to the interior, rather than to the surface. Such that it is trapped at vacancy type defects and complexes [13].

The lattice mismatch between ZnS and CdS proposes the presence of $\text{Cd}_{1-x}\text{Zn}_x\text{S}$ mixed layer at the ZnS/CdS interface region to reduce the structural disconnection. In addition, the interdiffusion between the two layers appears to reduce the interface defect density [14, 15]. The depth profiles of the structure obtained from the simulation by RUMP calculation are also shown in Fig. 3 and it confirm the above results.

Finally, we have demonstrated that using chemical and thermal activated diffusion that $\text{Cd}_{1-x}\text{Zn}_x\text{S}$, with $x=0.6$ thin films can be synthesized from vacuum deposited ZnS/CdS multilayer. Structural study by RBS depth profiles reveals that Cd diffuses within ZnS film more readily than Zn diffuses into CdS film.
Fig. 3 Depth profile of ZnS/CdS layer before and after chemical and thermal treatments.
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References


