Effect of The Cu Doping on The Structural and Optical Properties of AlSb Thin Films Deposited by Thermal Evaporation Method

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Abstract. AlSb thin film was prepared on a glass substrate with a thickness of (200 nm) at room temperature using the thermal evaporation technique under high vacuum conditions (10^{-6} mbar). The effect of Cu doping at ratios (1%, 3% and 5%) on the structural and optical properties were investigated. The structural properties of the films were evaluated by X-Ray Diffraction (XRD) and atomic force microscopy (AFM). The optical properties of the films were measured using the (UV-Vis) spectra in the ranges from 400 to 1000 nm. XRD results showed that all the samples have a polycrystalline cubic structure, and the average grain size of AlSb increases with increasing the Cu ratios. According to the AFM analysis, it is noticed that the average surface roughness (RMS) of AlSb nanocubic thin film decreases with increasing Cu doped concentration. From UV–Vis absorption spectra, it is noticed that all the samples have high absorption in the visible region, and the direct energy gap values for the samples were 1.83 eV, 1.81 eV, 1.80 eV, and 1.78 eV for pure, 1% Cu, 3% Cu and 5% Cu respectively.

Keywords: High vacuum, Cu doped, micro strain, roughness, energy gap.

1. Introduction

The III-V semiconductors are stoichiometric compounds obtained by combining group III elements (essentially Al, Ga, In) with group V elements (essentially N, P, As, Sb) (1, 2). This gives us 12 possible combinations and important properties of the surface crystal planes (3). One of these compounds is AlSb. AlSb has a high energy gap, high electronic mobility, long wavelength, and conversion efficiency of more than 27% (4). Therefore, it is used in a wide range of applications such as solar cells, thermoelectric and opto-electronic devices. In addition, Al and Sb are relatively abundant, non-toxic and low-cost making AlSb compound an attractive material for device applications (5, 6). AlSb also has potential applications as a detector of the radiation and as a material in high mobility hetero structures. Several methods have been used for the development of the thin films of AlSb like pulse laser deposition (7), co-evaporation (8), liquid phase epitaxy (9), hot wall epitax(10) co-sputtering (11) and doped AlSb thin films. Thermal evaporation technique is the most cost effective method among all other used techniques. In this work, AlSb thin film was successfully deposited onto glass substrates and doped with...
copper at (1%, 3%, and 5%). The structural properties are evaluated by XRD and AFM techniques, and UV-vis was used to investigate the absorption spectra and calculate the energy gap.

2. Experimental

AlSb alloys have been prepared by mixing the a purity aluminum powder (99.99%) and antimony powder (99.99%) made by the Riedel-de Haen Chemicals Ltd., and putting in a quartz tube under (1x10^{-2} torr), then the tube placed inside an oven at 1100 °C for 5 hours. The sample was cooled down using a slow cooling method. Thermal evaporation method was used to deposite AlSb thin films onto pre-cleaned amorphous glass substrate under high vacuum about (5 × 10^{-6} torr). The glass substrate was placed on the substrate holder above a molybdenum boats that carrying the materials, and the process was performed at a deposition rate of (0.5 ± 0.05 nm sec^{-1}). The films had been doped with Cu at ratios (1, 3 and 5) %.

The XRD machine (6000 SHIMADZU-Japan) was used to study the structural properties. The morphology of the samples (average diameter, roughness, and root mean square) were studied using the atomic force microscopy (AFM). The optical absorption was measured at a range of (400-1000) nm using ( UV-VISIBLE 1800 spectrophotometer )

3. Results and Discussion

Figure (1) shows the XRD pattern of AlSb alloy. The peaks observed at 25.1943, 29.1411, 41.6611, 49.2683 and 66.4085 exhibit the formation of a polycrystalline cubic phase of AlSb which correspond to the (111), (200), (220), (311), and (331) reflection planes of. This result matches with the ASTM card number (00-006-0233). Table (1) shows a matching between the experimentally measured alloy and ASTM card (19).

![Figure 1. X-ray diffraction pattern of AlSb alloy.](image)

| Standard | observed |
|----------|----------|
| 2θ       | intensity | d    | hkl | 2θ     | intensity | d    | hkl |
| 25.1354  | 100       | 3.54 | 111 | 25.1943| 100       | 3.53195 | 111 |
| 29.0913  | 35        | 3.067| 200 | 29.1411| 27        | 3.06195 | 200 |
| 41.6030  | 75        | 2.169| 220 | 41.6611| 66        | 2.16617 | 220 |
the average crystallite size \(D\) can be estimated from the peak width with Scherrer’s formula (12):
\[
D = \frac{K\lambda}{\beta_{\text{FWHM}} \cos \theta} \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (1)
\]
where \(D\) is the average crystal size, \(K\) is the Scherrer coefficient (0.94), \(\lambda\) is the x-ray wavelength = 1.5406 Å, \(\theta\) is Bragg’s angle and \(\beta\) the full width at half-maximum (FWHM) in radians.

The lattice parameter \(a\) of a cubic system is calculated according to the following equation (13):
\[
a = \frac{d_{hkl}}{(h^2 + k^2 + l^2)^{\frac{1}{2}}} \quad \ldots \ldots \ldots (2)
\]
where \(d_{hkl}\) is the inter-planar distance of each plane and \((hkl)\) are Miller indices.

The dislocation density \(\delta\), defined as the length of displacement lines per unit size of the quartz is expected from the formula (14):
\[
\delta = \frac{1}{D^2} \quad \ldots \ldots \ldots (3)
\]

The strain that made peak lengthening resulting from lattice deformation (microstrain) can be stated by Wilsok plan (15):
\[
\mu \varepsilon = \frac{\beta_{\text{FWHM}} \cos \theta}{4} \quad \ldots \ldots \ldots (4)
\]

The crystal layers number \(N_{\circ}\) calculated by using the following relation (16).
\[
N_{\circ} = \frac{t}{D^3} \quad \ldots \ldots \ldots (5)
\]
where \(t\) is the thickness of the samples

Figure (2) (a, b, c and d) shows the XRD patterns for pure and doped AlSb thin films at different Cu ratios (1%, 3% and 5%). From this figures, it is noticed that all samples have polycrystalline cubic structure with preferred orientation along (111) plane, and Cu addition causes slight offset shifting in the diffraction angle with a little decreasing in peak intensity and increasing the grain size for the film doped with 1% Cu. This film also appears less micro strain and dislocation density which attributed to the atomic radius of copper being less than the atomic radius of AlSb (\(r_{\text{Cu}} = 128\) pm, \(r_{\text{Al}} = 143\) pm, \(r_{\text{Sb}} = 140\) pm) (20). In addition, Cu may fill the interstitial spaces and reducing the crystal defects and hence reduce the roughness and the average diameter that seen clearly from the AFM images in figure (3) (a, b, c and d).
Figure 2. X-ray diffraction patterns of AlSb thin films for pure and doped samples.

Table 2. The grain size Micro strain, Dislocation density and Number Layers crystal for pure thin films and at different ratios of Cu (1%, 3%, 5%).

| sample        | G.S       | Micro strain \( \times 10^{-4} \) | Dislocation density \( \times 10^{14} \) | \( N/10^{15} \) \times Number Layers Crystal |
|---------------|-----------|---------------------------------|------------------------------------------|---------------------------------------------|
| Alloy         | 55.3907   | 6.603                           | 3.25                                     | 1.176                                       |
| Pure thin film| 33.5776   | 10.923                          | 8.87                                     | 5.283                                       |
| Cu 1%         | 35.7995   | 10.153                          | 7.802                                    | 4.359                                       |
Cu 3%  35.462  10.226  7.95  4.484
Cu 5%  34.8683  10.417  8.22  4.717

Figure 3. 3D AFM images AlSb / glass thin films pure and different Cu ratios

Table 3. Average Diameter, Roughness and root mean square for AlSb / glass thin films pure and different Cu ratios

| Samples | Avg.Diameter (nm) | Roughness (nm) | r.m.s (nm) |
|---------|------------------|----------------|------------|
| pure    | 74.65            | 33.3           | 38.4       |
| 1% Cu   | 62.64            | 6.23           | 7.19       |
| 3% Cu   | 66.85            | 2.32           | 2.7        |
| 5% Cu   | 58.87            | 1.79           | 2.11       |
Figure 4. Absorption spectra of the AlSb thin films pure and different Cu ratios

Figure (4) shows the absorption spectra of the samples. We can see that all samples have a high absorption in the visible region, and the absorption coefficient ($\alpha$) is given by the following equation (17).

$$\alpha = 2.303 \times \left( \frac{A}{t} \right)$$  \hspace{1cm} (6)

where $A$ is the absorbance of the sample

To calculate the energy gap for the direct allowed transitions using Tauc equation

$$ahv = B_o \left( h \nu - E_{opt} \right)^r$$  \hspace{1cm} (7) (18)

where $r = 1/2$ for allowed transitions and $r = 3/2$ for forbidden transitions; $E_g$ is the direct energy gap and $B$ is a parameter that depends on the transition probability. The energy gap of all samples was calculated from figure (5) by plotting $(ahv)^2$ versus photon energy for pure and doped AlSb thin films. The energy gap for direct allowed transitions decreases with increasing the Cu addition assigned to be 1.83 eV, 1.81 eV, 1.80 eV, and 1.78 eV for pure, 1% Cu, 3% Cu and 5% Cu respectively. These results can be attributed to the uniformity of the surface when adding copper. In addition, the copper added additional localized levels of electrons, hence reducing the energy gap.
4. Conclusions
AlSb thin films were successfully deposited on glass substrates by thermal evaporation method. All the samples have a polycrystalline cubic structure, and adding Cu enhances the uniformity of the samples by decreasing the strain and increasing the grain size. The best structure property is found the film doped with 1% Cu, and the energy gap also decreases with increasing the Cu content.

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