Structural and optical properties of nano-granular In_2S_3 films

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There has been increasing interest in III–VI materials that find application in opto-electronic, photovoltaic and photo-electrochemical solar cell devices [1]. Among these materials, In_2S_3 appear to be a promising candidate for many techno-logical applications due to their stability and energy band gap, optical transmittance and photoconducting behavior [2-3].

Indium sulphide thin films were thermally deposited on glass substrates at low temperature to be applied as buffer layers for thin film solar cells. The various deposition parameters were varied, and the optimum conditions for the deposition of In_2S_3 thin films were identified. The optimum condition for the uniform deposition of In_2S_3 thin film was identified as: substrate temperature Ts = 220–240 °C, average velocity of deposition 0.5 nm/s. The thickness of the films was defined by the time of their deposition in the region 1–30 min.

XRD spectra of the films of different thickness exhibited a broad hump in the 2θ range of around 20°–40°, and this indicated that the all films deposited at low-temperatures are amorphous in nature. Moreover, all investigated films of different *h* are characterized by high transmittance spectra (*T* ~ 85%) in the long wavelength region (500–3000 nm) and a clear absorption edge position

The compositions of the investigated films were analyzed by the AES technique. The AES analysis showed that the film becomes slightly rich in indium starting from half of thickness of the film. Although near substrate regions of the sample exhibited a S/In ratio of about 1, which is sulfur deficient, it is also certain that standard In_2S_3 composition ratio of S/In=1.5 are detected near the film surface. This could be due to the presence of various phases in the films.

The energy band gap of the films was determined by calculating absorption co-efficient α from the optical transmission spectra. In the present study, the films of different thickness exhibited a band gap varied of about 1.96 up to 3.3 eV.

By use the AFM data for the sample morphology it is possible to resolve phase composition of nano-granular In_2S_3 amorphous films of various thicknesses. One phase is related granules with average size d_1 >300 nm, another phase is presented by granules with d_2 ~ 10–60 nm. Both former granules are formed during the deposition process in matrix-like film component composed of very small particles with d_3 = 1–2 nm.

The concentration of granules with different size is changed with variation of the thickness of films deposited at the same conditions. High concentration of granules of bigger size d_1 are characteristic for films with thickness h > 450 nm. The position of band edge of the films is effected mainly by the phase related bigger granules and estimated to be $E_g(1)$ = 1.96 eV (623 nm).

The decrease of the film thickness up to d = 400–250 nm results in a significant reduction of bigger granules content and in an increase of middle-size granules concentration. The value of E_g for In_2S_3 thin films with thickness h ~ 300 nm was determined to be about 2.3–2.35 eV.

In our case, films with d = 200–120 nm have higher concentration of 30–60-nm granules and so we can discard the quantum size effects. It is possible that our films contain some amount of oxygen, however in our case, the bigger In_2S_3 granules exhibited long-wave shifted E_g, while the middle-sized In_2S_3 granules showed E_g ~ 2.3–2.35 eV. These results can indicate that the deposited 300–350-nm granules have more structural defects while the 10–60-nm granules have very few structural defects.

In_2S_3 films are characterized to be mainly composed of small amorphous particles (d_3 = 1–2 nm). The related band edge position is found to be $E_g(3)$ =3.4 eV. This result can be explained by both the oxygen [3] and the quantum size effects [4, 5] took place in the former of In_2S_3 thin films.

This work has been supported by the GPNI "Physical materials, new materials and technologies".

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