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PROSPECTS OF INDIUM SULPHIDE AS AN ALTERNATIVE TO CADMIUM SULPHIDE BUFFER LAYER IN CIS BASED SOLAR CELLS FROM NUMERICAL ANALYSIS

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Indium sulphide (In_xS_y) is a prominent candidate to be an alternative buffer layer to so-called toxic cadmium sulphide (CdS) in CIS based solar cells. In this study, buffer layer parameters layer thickness and buffer layer bandgap have been investigated by Solar Cell Capacitance Simulator (SCAPS) to find out the higher conversion efficiency. A promising result has been achieved with an efficiency of 16.76% (with V_{oc} = 0.610 V, J_{sc} = 34.63 mA/cm^2 and fill factor = 79.37) by using In_XS_y as a buffer layer. It is also found that the high efficiency of CIGS absorber layer thickness is between 1.5µm and 3µm. The bandgap of In_xS_y buffer layer was taken 2-2.9 eV to simulate which is related to the feasible value and In_xS_y bandgap is relatively higher compared to CdS buffer layer bandgap. Moreover, it is found that J_{sc} is very high for the buffer layer thickness of 30-50nm and quantum efficiency is almost 80% in 350-500 nm region attributed to less absorption of light in the buffer layer. In addition, it is revealed that the highest efficiency cell can be achieved with the buffer layer bandgap of 2.74-2.90 eV. This result can be explained in the practical work as non-stoichoimetric composition of indium sulphide may result in different bandgaps. Hence, a specific non-stoichoimetry composition which results in the highest bandgap is desirable to achieve high efficiency In_xS_y-CIGS solar cells. From the simulation results, numerous influences of buffer layer are investigated in CIGS solar cell which can lead to the fabrication of high efficiency devices.

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Keywords: CIGS solar cells; Buffer layer; Indium Sulphide; SCAPS.

1. Introduction

Buffer layer is an intermediate layer film between the absorber and window layers with two main objectives, to provide structural stability to the device and to fix the electrostatic conditions inside the absorber layer [1]. Meanwhile, it will have to make good p-n junction with the p-type absorber layer for the electrical conduction and to allow the transmission of photons into the absorber layer to generate electron-hole pair. Indium sulphide, In_2S_3 is a n-type promising buffer layer in CIGS thin film solar cells because of its stability, bandgap energy (2-2.3 eV) and (2.8 eV), transparency and photoconductor behavior [2]. In_2S_3 can be a good replacement of conventional toxic CdS films with high bandgap as buffer layers in solar cells. Efficiency of 16.4% can be achieved with indium sulphide buffer layer [2]. Another optimistic characteristic is, the bandgap of indium sulphide can increase upto 3.0 eV with the doping of sodium (5%), which can be found on the surface of CIGS layers on soda lime glass substrates [3]. In addition, the interface analysis of In_2S_3/CIGS shows good result in increasing the bandgap because of materials diffusion from absorber layer to buffer layer [4]. However, Cu diffusion from absorber layer into buffer layer can degrade the electrical performance of the total device. On the other hand, for a thinner In_2S_3 layer the absorption edge is in the 400-500 nm while for CdS it is in 500-550 nm [5]. In this work, In_2S_3 bandgap is simulated from 2eV t o 2.9 eV to show the effect of each bandgap towards the

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properties of the solar cell. Apart from that, it is also found that the thickness of In_2S_3 buffer layer is laid within 40 nm to 50 nm. The solar cells with indium sulphide shows light soaking effect, due to this effect fill factor goes down slightly but V_{oc} increases greatly and which results in the solar cell's efficiency increasing by approximately 16%. Additionally, the high buffer sensitivity to light soaking can be explained by enhancement in In_xS_y/CIGS interface quality [5]. The resistivity of In_XS_y can vary from $1x10^2$ Ωcm to $1x10^6$ Ωcm. We need to keep high resistivity of buffer layer to prevent the diffusion from window layer. Due to comparatively high bandgap, less light will be absorbed in the n-In_2S_3 buffer layer. In this paper, other buffer layer CdS with a bandgap of 2.4 eV has also been studied for a comparative analysis with the In_2S_3 layer. In the present work the main focus is to find out the best electrical performances of the thin film solar cells with CIGS/ In_2S_3 structure. Moreover, the effects of various operating temperatures have been investigated for the CIGS/ In_2S_3/ZnO structured solar cells.

2. Methodology

The AC and DC electrical characteristics of thin film heterojunction solar cells can be investigated with SCAPS 2802. The best electrical performance for CdTe and CIGS solar cells can also be simulated. SCAPS is used to imitate and investigate all the available research-level CIGS/CdTe solar cells with various buffer layers. For solar cell and detector structures, collection efficiencies as a function of voltage, light bias, and temperature can also be obtained. Additionally, important information such as electric field distributions, free and trapped carrier populations, recombination profiles, and individual carrier current densities as a function of position can be evaluated from SCAPS. In addition, output such as current voltage characteristics in the dark and under illumination can be achieved by using the different layer parameters. Temperature can be varied to find the impacts on current voltage characteristics of the proposed structure. The schematic view of the structure used in this study is shown in figure 1. In the simulation, n-type ZnO, In_2S_3, CdS, CIGS layer parameters are emphasized to investigate the benefits of using In_2S_3 as buffer layer in CIGS solar cells and comparative study with CIGS/CdS structure. By incorporating the various material parameters into SCAPS for all of the analysis aspects, changes in the values for efficiency, open circuit voltage, short circuit current and fill factor as well as the effect of operating temperature are observed. In case of CIS/CIGS solar cells CIGS, is polycrystalline material and some physical parameters depend on doping conditions [6]. For the indium sulphide buffer layer, the bandgap is used from 2.3 to 2.84 eV to find out the best efficiencies and for the higher bandgap the device has given the best efficiency of 16.63 %. In addition, the thickness of the buffer layer is also varied between 30 nm and 1 μm to find out the effects in the cell performance. The description and the baseline values of the physical parameters those are used in the In_2S_3/CIGS solar cells simulation are shown in tables 1 and 2, respectively.

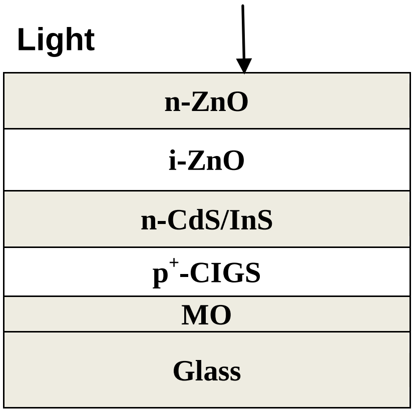

Figure 1: Schematic structure of CIGS solar cell with InS or CdS buffer layer used in numerical analysis

Table (1) Electronic properties.

EPS	Dielectric permittivity (relative) □
MUN	Electron band mobility μ_n (cm^2/Vs)
MUP	Hole band mobility μ_p (cm^2/Vs)
NA	Acceptor concentration ($1/cm^3$)
ND	Donor concentration ($1/cm^3$)
EG	Electrical bandgap (eV)
NC	Effective density of states in conduction Band ($1/cm^3$)
NV	Effective density of states in valance band ($1/cm^3$)
CHI	Electron affinity χ_e (eV)

Table (2) Physical parameters used in simulation (either CdS or InS is used).

	n-ZnO	i-ZnO	n-In_2S_3	n-CdS	p-CIGS
Layer thickness (µm)	0.20	0.080	0.050	0.050	3.00
EPS	9	9	13.5	9	13.60
MUN (cm^2/Vs)	100	100	4.00E+2	3.50E+2	1.00E+2
MUP (cm^2/Vs)	25	25	2.10E+2	5.00E+1	2.50E+1
NA ($1/cm^3$)	0	0	1.00E+1	0	2.00E+16
ND ($1/cm^3$)	1.0E+18	1.0E+18	1.00E+18	1.00E+17	1.00E+1
EG (eV)	3.3	3.3	2.800	2.410	1.010
NC ($1/cm^3$)	2.20E+18	2.20E+18	1.80E+19	1.80E+19	2.20E+18
NV($1/cm^3$)	1.80E+19	1.80E+19	4.00E+13	2.40E+18	1.80E+19
CHI (eV)	4.6	4.6	4.70	4.50	4.50

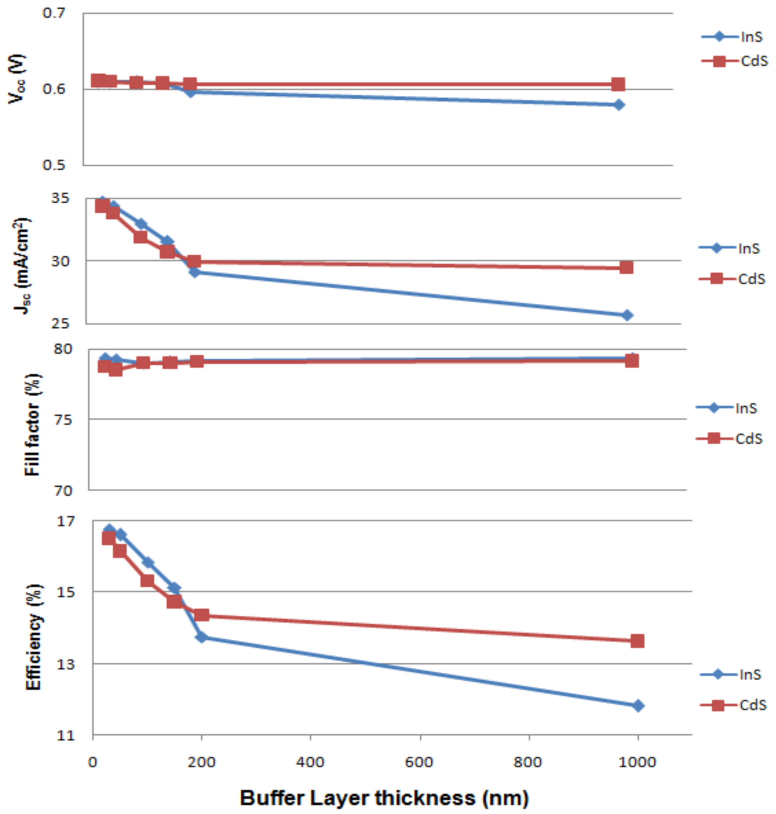

Figure 2: Effect of In_xS_y buffer layer thickness in CIGS performance

3. Results and discussions

3.1 Effects of various layer thicknesses of In_2S_3

To rationalize the simulation, the novel p-CIGS heterojunction solar cells with In_2S_3 buffer layer has been verified in terms of buffer layer thicknesses and bandgaps. At the beginning of the simulation, the buffer layer thickness has been varied from 30 nm to 1 μm to carry out the optimum electrical performance of these heterojunction solar cells. In addition, 3.0 μm of CIGS layer thickness is used during the simulation. It has been investigated that the efficiency of the solar cell is decreasing with the thickness of In_2S_3 buffer layer. The highest efficiency 16.76% is measured, when the buffer layer thickness is 30 nm. The best possible buffer layer thickness of In_2S_3 is between 30 nm and 50 nm. The observed efficiency is 16.76% and 16.61% at the thickness of 30 nm and 50 nm. It can be attributed to thinner layer thickness where less photon energy will be absorbed. Moreover, the bandgap of CIGS layer is 1.100 eV. Therefore, due to low bandgap lower photons energy will be captured in the absorber layer, which will influence to produce higher J_{sc} and V_{oc}.

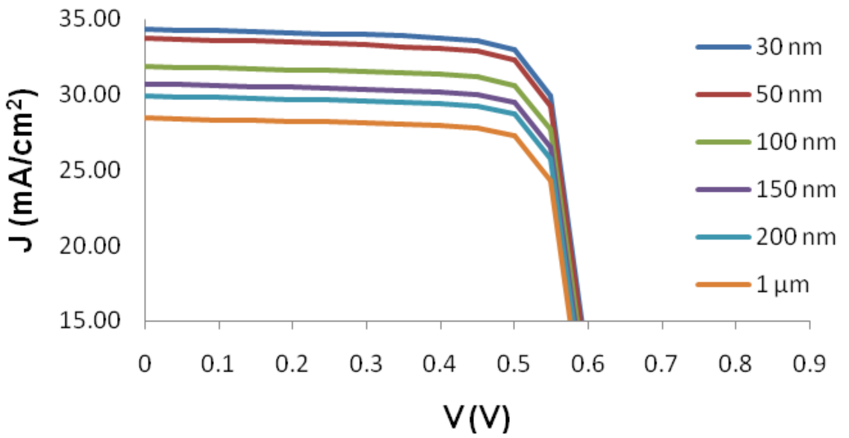

Figure 3: J-V characteristics for CIGS cells with different In_xS_y buffer layer thicknesses

Overall performances of the CIGS solar cells are also shown in Figure 2. Both open-circuit-voltage (V_{oc}) and short-circuit-current-density (J_{sc}) are decreasing with the increasing thickness of the buffer layer, which is the n-type region in solar cell. Electron-hole pair (EHP) generation is the major factor, which happens for the collection of longer wavelength of lights in the absorber layer. It is also found that for In_2S_3 phase S> 60% and less than that it will be InS or In_6S_7. And, for $In_2S_{(3+x)}$ best electrical performances can be achieved [6]. In addition, fill factor (FF) increases with the thinner In_2S_3 layer, which can be related to the no band discontinuity or spikes at the valance band interfaces.

However, low V_{oc} and J_{sc} can be found for the recombination at the CIGS absorber layer due to an electron (or hole) is trapped by an energy state in the forbidden region which is introduced through defects. Therefore, fewer electrons will contribute to the quantum efficiency of the solar cell and the value for Voc and Jsc will be low. The J-V characteristics and spectral response of the solar cells are shown in figures 3 and 4, respectively. It has been found that the quantum efficiency of the solar cell is very high, which is almost 80% in 350-500 nm region. On the other hand, for CIGS/CdS it is around 78% for the above mentioned region (Figure 7). It can be described as more photons will be captured in the absorber layer. Thus a greater percentage of electron-hole pairs would be produced from the absorbed photons. A decrease in the numbers of photons at the absorber layer would decrease the quantum efficiency of the solar cell.

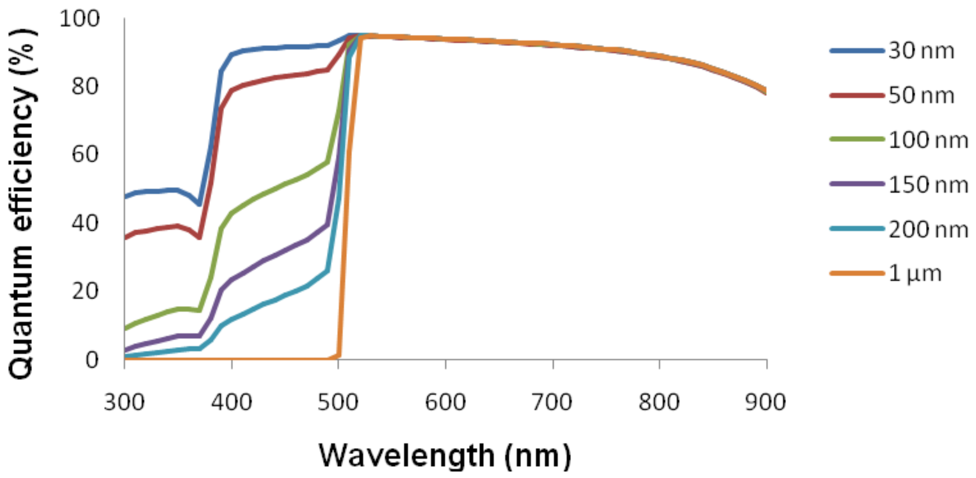

Figure 4: Spectral response for CIGS cells with different In_xS_y buffer layer thicknesses

3.2 Effects of In_2S_3 layer bandgaps

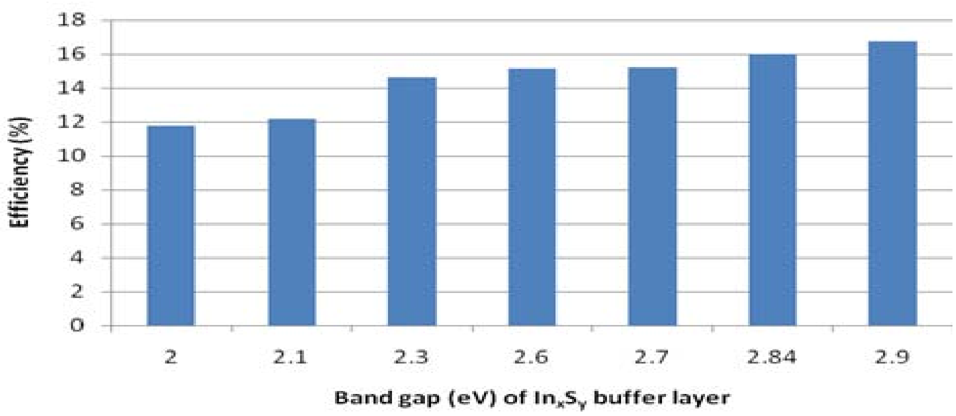

Figure 5: Efficiency of CIGS solar cells for 50 nm thick In_xS_y buffer layer with various bandgaps

In this work, the In_2S_3 layer bandgap has been varied from 2.0 to 2.9 eV to see the effects on electrical performance, where 1.100 eV CIGS layer bandgap has been used. It has been found that while the bandgap increases upto 2.9 eV with the layer thickness of 50 nm, an efficiency of 16.76% can be achieved. In addition, for the bandgap of 2.0 eV the efficiency goes down to 11.18%. It happens due to higher bandgap of n-type region which will allow more photons to be absorbed in the absorber layer. Moreover, conduction band offset and valance band offset play an important role to achieve the higher efficiency. The optimum band offset is $\Delta E = 0.25$ eV at 2.84 eV. So, this will affect the J-V characteristics of the solar cell. From Figure 5, it can be seen that the efficiency decrease with the decrease of In_2S_3 bandgaps for 50 nm of thickness. Therefore, insufficient absorption of photon is occurred in case of higher bandgap of buffer layers. It is also found that if sulphur ratio increases, the bandgap will be higher for the In_2S_3 buffer layer. However, too much sulphur will make the film amorphous [7]. The efficiency of indium sulphide/CIGS solar cells with various bandgaps have been shown in Table 3.

Table (3) Effects of different buffer layer thickness and bandgap in CIGS solar cells

Buffer layer	Thickness (nm)	Bandgap (eV)	Voc (V)	Jsc (mA/cm^2)	FF (%)	Efficiency η (%)
In_xS_y	30	2.90	0.6100	34.626	79.37	16.76
In_xS_y	50	2.84	0.6098	34.353	79.27	16.61
In_xS_y	100	2.60	0.6088	32.938	79.02	15.84
In_xS_y	150	2.70	0.6078	31.487	79.04	15.13
In_xS_y	200	2.50	0.6070	29.094	65.82	13.75
In_xS_y	1000	2.30	0.5795	26.9524	79.33	11.81

3.3 Comparative study of various layer thicknesses and bandgaps of CdS

CdS buffer layer has the bandgap energy of 2.4 eV. In this simulation, the thickness of the CdS buffer layer has been varied between 30 nm and 1 µm. V_{oc} and J_{sc} decrease with increasing CdS buffer layer thickness as shown in figure 6. Due to the thicker buffer layer, more photon will be absorbed in this region. Fill factor increases slightly as the buffer layer thickness approaches 1 µm. It can be due to less discontinuity at the absorber and buffer layer interface. Solar cell with 30 nm of CdS buffer layer recorded the highest efficiency for the whole CdS/CIGS cases. This is because, a thin buffer layer means majority of photons can pass through the buffer layer without being absorbed. As the buffer layer is increased to 1 µm, the efficiency of the solar cell drops rapidly. This is due to the photon loss that occurs inside the buffer layer. When less photon makes it through the buffer layer, less electron-hole pair is produced hence less electricity is produced. However, bandgap of CdS (2.4 eV) is comparatively lower than the bandgap of In_2S_3 (2.84 eV). For this reason, the absorption of photons at lower wavelength region will be less for InS/CIGS cases which is shown in figure 8. Therefore, the spectral response of InS is higher than CdS for 30 nm of thickness in 350-450 nm region.

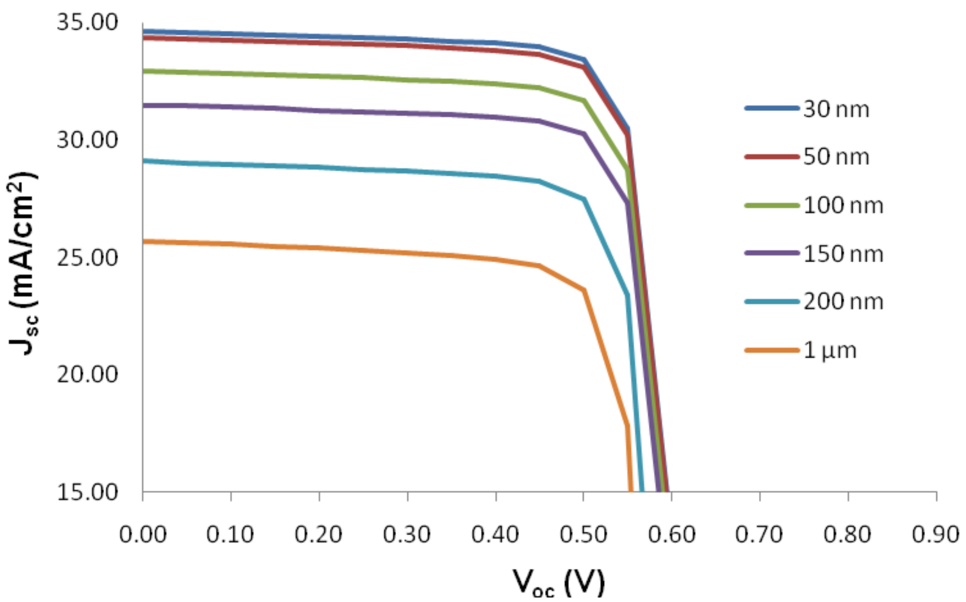

Figure 6: J-V characteristics for CIGS cells with different CdS buffer layer thicknesses

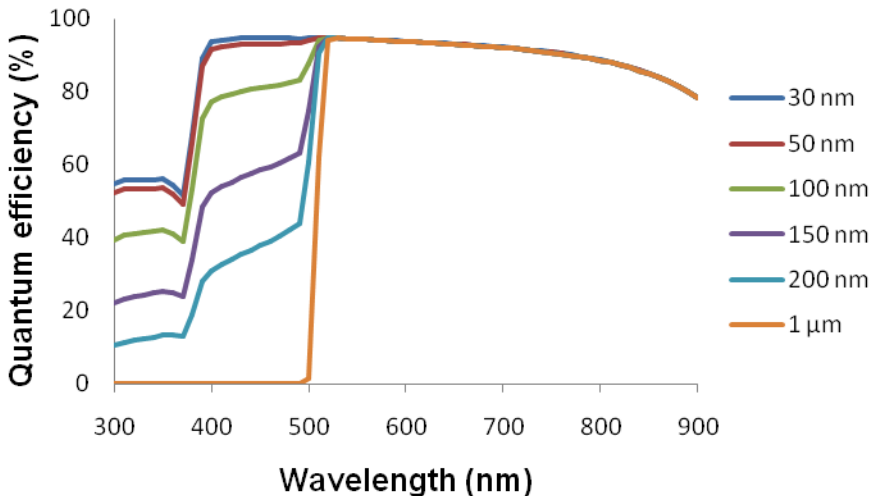

Figure 7: Spectral response for different CdS buffer layer thicknesses

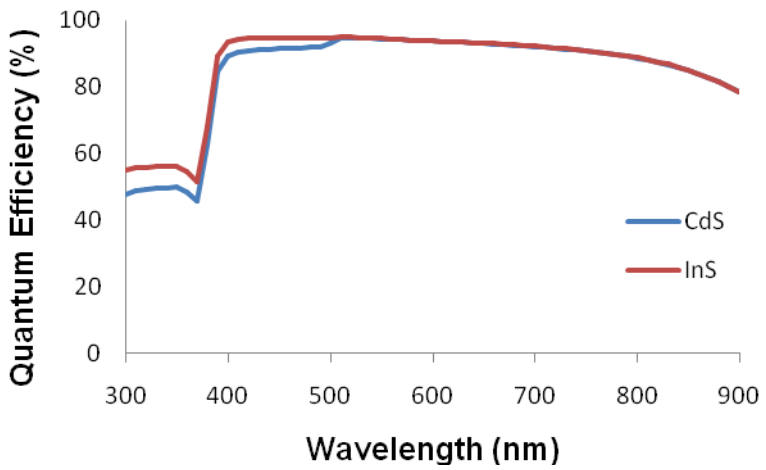

Figure 8: Spectral response for 30 nm InS and CdS buffer layer thicknesses

3.4 Effects of various operating temperatures

The effects of operating temperature on the performance of CIGS/In_2S_3 and CIGS/CdS structure have been investigated. At the room temperature, the highest recorded efficiency is 16.76% for CIGS/In_2S_3 solar cells and the efficiency becomes 16.50% for CIGS/CdS solar cells. All the performance parameters such as efficiency, fill factor, V_{oc} and J_{sc} are decreasing with the increase in operating temperature. When the operating temperature increases, the electrons in the solar cell gains an extensive energy. But instead of contributing to electricity generation, these electrons become unstable and recombine with the holes before the carriers could reach the depletion region and collected [8]. This explains the decreasing V_{oc} and J_{sc} as temperature increases. But, CIGS/In_2S_3 gives a bit better performance in terms of short circuit current and efficiency compare to CIGS/CdS solar cells. The optimum temperature for solar cell operation is at 300 K, which is room temperature. Conventionally, solar cell panels are installed outside in the open environment. Sunlight causes heating of the solar panels hence the operating temperature increases. Therefore, the solar cell usually operates at a temperature higher than 300 K. The changing of V_{oc}, J_{sc}, fill factor and efficiency are shown in Figure 9. From Figure 10, the normalized efficiency of CIGS/In_2S_3 and CIGS/CdS structures with different operating temperatures has been shown and the temperature coefficient is calculated from the slope which is found to be -0.2%/^oC.

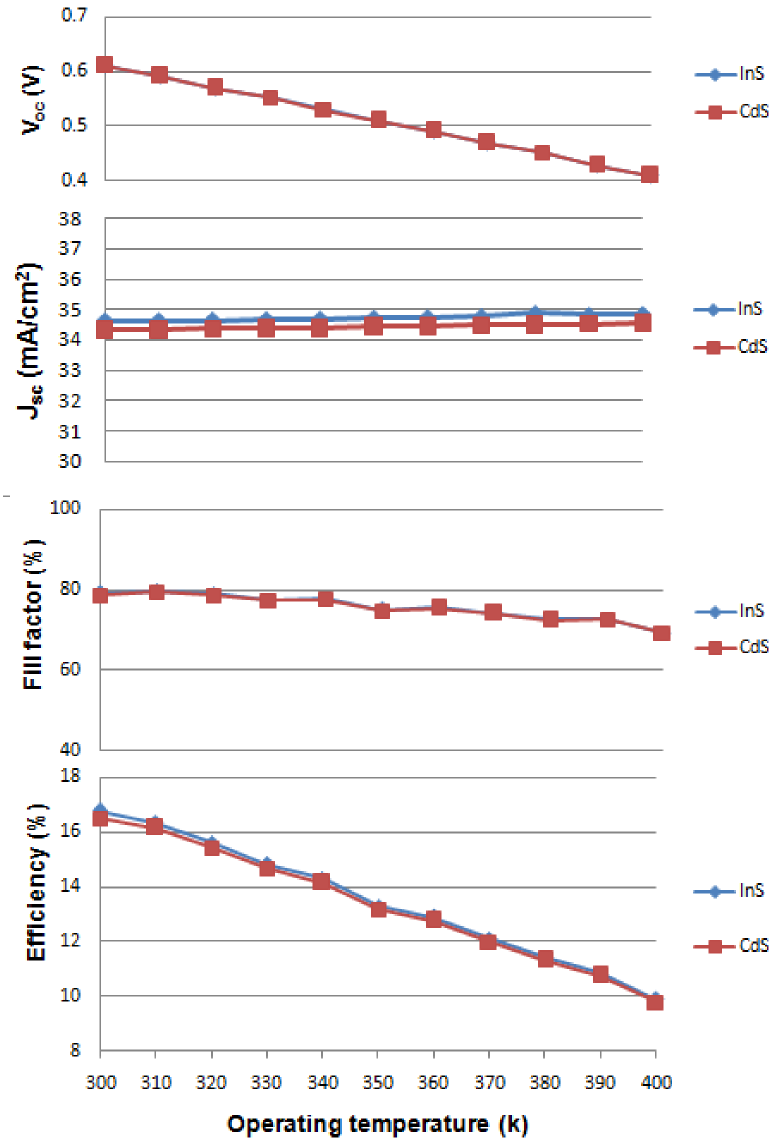

Figure 9: Effects of various operating temperature on CIGS/InS or CdS solar cells

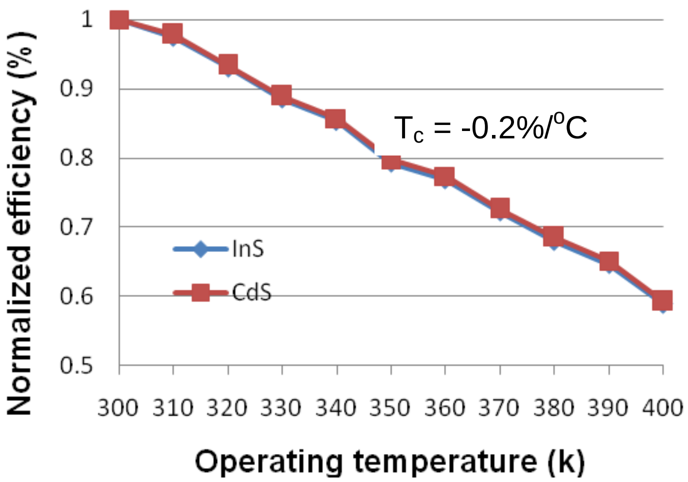

Figure 10: Normalized efficiency of solar cells for different operating temperatures

4. Conclusions

From this numerical analysis of hetero-structure solar cells with In_2S_3 and CdS buffer layers, electrical performances for the CIGS solar cells have been investigated in terms of buffer layer bandgap and thickness. Firstly, decreasing the In_2S_3 absorber layer thickness results in higher J_{sc} and V_{oc}. Secondly changing the buffer layer bandgap also yields better performance. Thirdly, for different operating temperatures CIGS/In_2S_3 solar cells show stability as high as the conventional CIGS/CdS solar cells. In_2S_3 shows very promising result to be an alternative choice of toxic CdS buffer layer in CIGS solar cells. A new challenge to fabricate large-area p-CIGS/ n-In_2S_3 thin film photovoltaic has been opened up by transferring the new device structure case developed in SCAPS.

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