

EXCESS DEFECTS AT THE CdS/CIGS INTERFACE SOLAR CELLS

N. TOUAFEK*, R. MAHAMDI^a

Department of Electronics University Constantine-1 Algeria

^aLea Department of Electronics Hadj Lakhdar University Batna Algeria

The excess defects concentration in the heterojunction solar cells interface CdS/CIGS are investigated by Solar Cell Capacitance Simulator in 1 Dimension SCAPS-1D. The obtained results, for models studied: doping model and pinning model, show that the excess defects concentration at both CdS/SDL and SDL/CIGS interfaces can deteriorate the photovoltaic power conversion efficiency of the solar cells by about 3-5 %, depending on the model and capture cross-sections. The doping model provides a markedly higher tolerance to internal interface recombination when compared to the pinning ones. The excess defects at the interface CdS/SDL is not as critical as the impact of the excess defect at the SDL/CIGS on the performance of the CIGS solar cells. However, the capture cross-sections σ_{np} in both interfaces varying from 10^{-15} to 10^{-13} cm² affect dramatically the performance of the solar cells. The loss in the performance caused by the excess defects concentrations can be recovered by the augmentation of the band gap of SLD layer. The results predict that passed from 1.2 to 1.5 eV increase the efficiency by about 3 %.

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1. Introduction

Thin film solar cells are comprised of several layers of different semiconductors and metals, and thus the device has a large number of interfaces where inter-diffusion of atoms between the different materials is possible [1, 2]. In general the solar cell consists of substrate, TCO, window layer (n-type), absorber layer (p-type) and metal contact layer. Each of the component materials has different physical and chemical properties and each affects the overall performance of the device in some form or the other. The interfaces occur between the different layers, generally play an important role in this film solar cells devices, can cause stresses, defects, interface states, and surface recombination centers. Since each layer has different crystal structure, microstructure, lattice constant, electron affinity, diffusion coefficient, mobility, etc. Also, the interface properties get modified during device processing as a result of growth process involving the sequential deposition of multi-layers at different deposition conditions. In addition, annealing conditions [3], post-deposition treatments involving high-temperature annealing can alter the interface and inter-grain properties, which may result in interface defects, which cause undesirable recombination of carriers. As a result, the device parameters such as open-circuit voltage, current, Fill Factor and efficiency can be modified significantly. Generally, it is not clarified under which conditions defect formation occurs and how it affects the device behavior. In the CIGS solar cells, that have the best performing thin film technologies [4], the Studies show that the electrical properties are strongly affected by the CIGS/CdS interface properties. XPS studies show the presence of an In-rich n-type material at the surface of the p-type CIGS and causes large band bending that contributes to the device performance [5]. This layer identified as a surface defect layer (SDL), structurally similar to the bulk CIGS but have different compositional distributions [5, 6]. However, So far, this layer is not so well known. It is not even clear if it exists in finished CIGS devices. Some research exhibit that this layer is not present in the CIGS high band-gap.

* Corresponding author: ntouafek@yahoo.fr

Recently, it has been proposed that an In-excess n-type conductivity layer is present at the interface region of the CIGS film and the p-n junction is formed between p-CIGS and n-SDL [7] and therefore, the p-n junction in CIGS solar cells is a homojunction located in the CIGS film [8]. So, at the junction CdS/CIGS there are two important interfaces: SDL/CIGS and CdS/SDL.

The purpose of this work is to examine using SCAPS-1D [9] simulation package, the influence of the excess defects at both SDL/CIGS and CdS/SDL interfaces, as well as the effect of the band-gap widening at the surface absorber layer on the electrical parameters of CIGS solar cell.

2. Device simulation Details

2.1 Cell structure

CIGS solar cells with the ZnO/CdS/SDL/CIGS/Mo structure schematically sketched in Fig.1. The CIGS thin -film solar cell consists of the following layers: substrate soda lime glass (SLG); a Molybdenum (Mo), to realize an ohmic back contact; a p-CIGS absorber layer; thin layer of which is usually intentionally made Cu-poor named the Surface Defect Layer (SDL), expected to play an important role in the performance of the high efficiency $\text{CuIn}_{1-x}\text{G}_x\text{Se}_2$ based solar cells [10-11]; an n-type buffer layer; typically CdS [12]; an undoped ZnO layer namely a transparent conduction oxide (TCO), and an n+-ZnO transparent front contact . Metallic Ni/Al contact grids complete the cell.

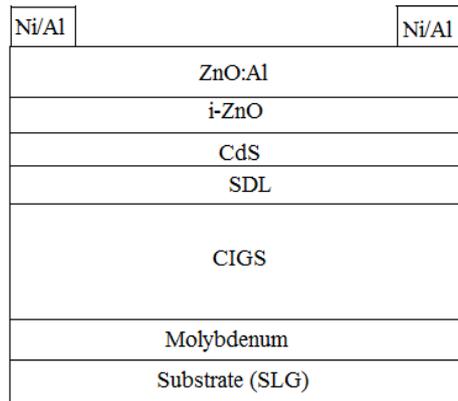


Fig.1. Schematic structure of CIGS based thin-film solar cells (layer thicknesses not to scale)

2.2 Numerical modeling

The merit of the numerical methods is to test and predict the results and the influence of the process parameters on the device without fabrication. In this work, The CIGS solar cells are modeled using the latest version (3.0.0.2) of SCAPS [9,13,14] to predict the changes to CIGS based solar cell performance that are introduced by the excess defects at the interface between CdS and CIGS layers. This software tool is a one dimensional solar cell device simulator, developed at the university of Gent [15], allows the definition of thin-film solar cell devices stacks of layers with a large set of parameters and solves the fundamental solar-cell equations (the Poisson equation and continuity equations for electrons and holes) for each point. Definable parameters include the thickness, doping, defect and interface-state densities and cross-sections, the optical absorption coefficient, the band-gap and the electron affinity. Furthermore, many of the properties can be specified as gradients of various forms. Recombination in deep bulk levels and their occupation is described by the Shockley-Read-Hall (SRH) formalism. Recombination at the interface states is described by an extension of the SRH formalism, allowing the exchange of electrons between the interface state and the two adjacent conduction bands, and of holes between the state and the two adjacent valence bands [16,17] .We consider, in this study, two models: the

doping model, in which the surface layer is an n-type doped material and the pinning model, which views the surface layer as a material that is type inverted due to Fermi-level pinning by donor-like defects at the interface with CdS. The Fermi level pinning was modeled by a high density, 3.10^{13}cm^{-2} , of donor defects close to the CIGS conduction band ($E_F=0.2\text{ eV}$). Here small capture cross sections of 10^{-18} cm^2 were chosen to separate pinning defects from recombination defects. All the bulk defects are at mid gap of the layers [18]. The CIGS cell is simulated under AM1.5 spectrum irradiance with a power density of 100mW/cm^2 and at temperature of 300 K. All electrical properties of SDL were chosen similar to the bulk except the band-gap, doping, and the carrier mobilities. Lower mobilities were chosen since this layer could be more disordered than the bulk material.

3. Results and discussion

The current-voltage (J-V) results from simulation using the parameters given in table 1 are compared with measurement data from [19] in the Fig.2. The results show that the measured JV curve is very well reproduced by the parameters model which validates our set of parameters as a baseline for simulating the effect of the excess defects at the both CdS/SDL and SDL/CIGS interfaces on solar cell performance. The JV parameters from simulations and measurements are displayed in table 2.

3.1. Influence of excess defects at the CdS/SDL interface

The primary function of CdS layer in the structure is to form the heterojunction with CIGS layer and protect the surface defect layer. So, the deposition method should be chosen that the minimum quantity of interface defects is introduced. In the ideal case without interface states, positive charges in the ZnO/CdS part of the junction are balanced by negative charges in the SCR of width W_a in the CIGS absorber:

$$Q_n + qd_wN_w + qd_bN_b = qN_aW_a \quad (1)$$

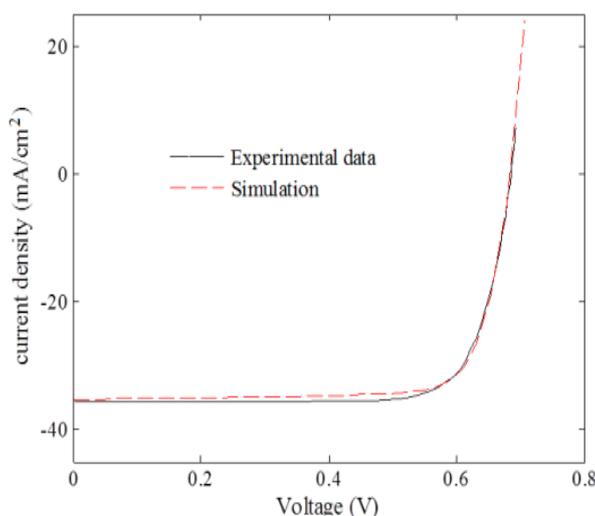


Fig.2. comparison between the (J-V) curves for the simulated and the reported experimental data [19]

Here Q_n are the charges per unit area in a depletion layer of the doped ZnO window layer, q is the elementary charge; N_w , N_b and N_a are the doping concentrations in the i-ZnO, CdS and

CIGS layers with the thickness d_w , and d_b , respectively ; W_a is the width of the SCR in the CIGS layer. From the equation (1), it can be seen that an introduction of negatively charged states at the interface between CdS/CIGS (the left side of the Eq 1) reduces the width W_a of the space charge region in the absorber layer. Therefore, the barrier for holes at the interface decreases which leads to a higher recombination velocity at the CdS/CIGS interface. This explains the importance of the study of the influence of the excess defects at this interface on the solar cell parameters.

The models studied, in Fig.3 the pinning model (black lines) gives the best performance compared to the doping model (red lines). This plot shows the dependence of the photovoltaic output parameters efficiency η , short circuit current density J_{sc} , open circuit voltage V_{oc} , and the fill factor FF on the concentration of the defects at the CdS/SDL interface and captures the cross sections σ_n and σ_p for electrons and holes, respectively, $\sigma_n = \sigma_p = 10^{-15}$, 10^{-14} and 10^{-13} cm². Beyond 10^{10} cm⁻² the performance except the V_{oc} , drops with increasing the defect from 10^{10} to 10^{12} cm⁻² especially for the pinning model. Increasing the capture cross-sections from 10^{-15} to 10^{-13} we note a drop of efficiency about 1.2 %, contrary to the doping model where the drop doesn't exceed 0.2 %. However, for the pinning model, the efficiency of solar cell is strongly influenced by the capture cross-sections. This effect of $\sigma_{n/p}$ is best seen at the highest defect concentration, where the efficiency suffers a reduction of 0.8 to 1.1%, depending on $\sigma_{n/p}$.

3.2. Influence of excess defects at the SDL/CIGS interface

Excess defects located at the SDL/CIGS interface are also important as possible recombination traps at this interface. Fig.4 shows the role of both defect concentration and the capture cross-sections in determining the electrical parameters of cell for doping model (red lines) and pinning model (bleu lines). We can see that the excess defects at the SDL/CIGS interface influence strongly the all electrical parameters (J_{sc} , V_{oc} , FF, and efficiency) that decrease with increasing the defect concentration for both models. It is clear from the plot that beyond 10^{10} cm⁻² of defect concentration, the effect of capture cross-sections appears and becomes significant for high defect concentration. The pinning model is more sensitive to the variation of the capture cross-sections which leads to a drop of efficiency by about 4-5% , For example , for defect concentration equal 10^{12} cm⁻², the efficiency decreased from 18.9 to 14 % for $\sigma_{n/p} = 10^{-15}$ and $\sigma_{n/p} = 10^{-13}$ cm², compared to the doping model which shows a decrease between 3 and 3.5%.

Table2. Measured and simulated solar cell JV-parameters

	V_{oc} (mV)	J_{sc} (mA/cm ²)	FF (%)	Efficiency (%)
simulation	684	-35.239	0.789	19.04
Experimental	688	-35.7	0.781	19.20

Table 1 Input parameter values for the simulation of CIGS solar cells with SCAPS-1D

	Layer properties				
	CIGS	SDL	CdS	i: ZnO	ZnO:Al
W (μm)	2	0.030	0.05	0.2	0.4
E _g (eV)	1.15	variable	2.4	3.3	3.3
χ (eV)	4.5	4.5	4.45	4.55	4.55
ϵ/ϵ_0	13.6	13.6	10	9	9
N _c (cm ⁻³)	2*10 ¹⁸	2*10 ¹⁸	1.3*10 ¹⁸	3.1*10 ¹⁸	3.1*10 ¹⁸
N _v (cm ⁻³)	1.5*10 ¹⁹	1.5*10 ¹⁹	9.1*10 ¹⁸	1.8*10 ¹⁹	1.8*10 ¹⁹
v _n (cm/s)	3.9*10 ⁷	3.9*10 ⁷	3.1*10 ⁷	2.4*10 ⁷	2.4*10 ⁷
v _p (cm/s)	1.4*10 ⁷	1.4*10 ⁷	1.6*10 ⁷	1.3*10 ⁷	1.3*10 ⁷
μ_n (c)	100	10	72	100	100
μ_p (cm ² /Vs)	12.5	1.25	20	31	31
doping (d)	1*10 ¹⁶ (a)	variable	5*10 ¹⁷ (d)	1*10 ¹⁷ (d)	1*10 ²⁰
Bulk defects properties					
N (cm ⁻³)	1.1*10 ¹⁴ (d)	1.1*10 ¹⁴ (d)	5*10 ¹⁶ (a)	1*10 ¹⁶ (a)	1*10 ¹⁶ (a)
σ_n (cm ²)	10 ⁻¹³	10 ⁻¹³	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵
σ_p (cm ²)	10 ⁻¹⁵	10 ⁻¹⁵	5*10 ⁻¹³	5*10 ⁻¹³	5*10 ⁻¹³
Interface properties					
	CIGS/SDL	SDL/CdS	CdS/i-ZnO		
N (cm ⁻³)	variable	variable	10 ⁹ (a)		
σ_n (cm ²)	variable	variable	10 ⁻¹⁵		
σ_p (cm ²)	variable	variable	10 ⁻¹³		

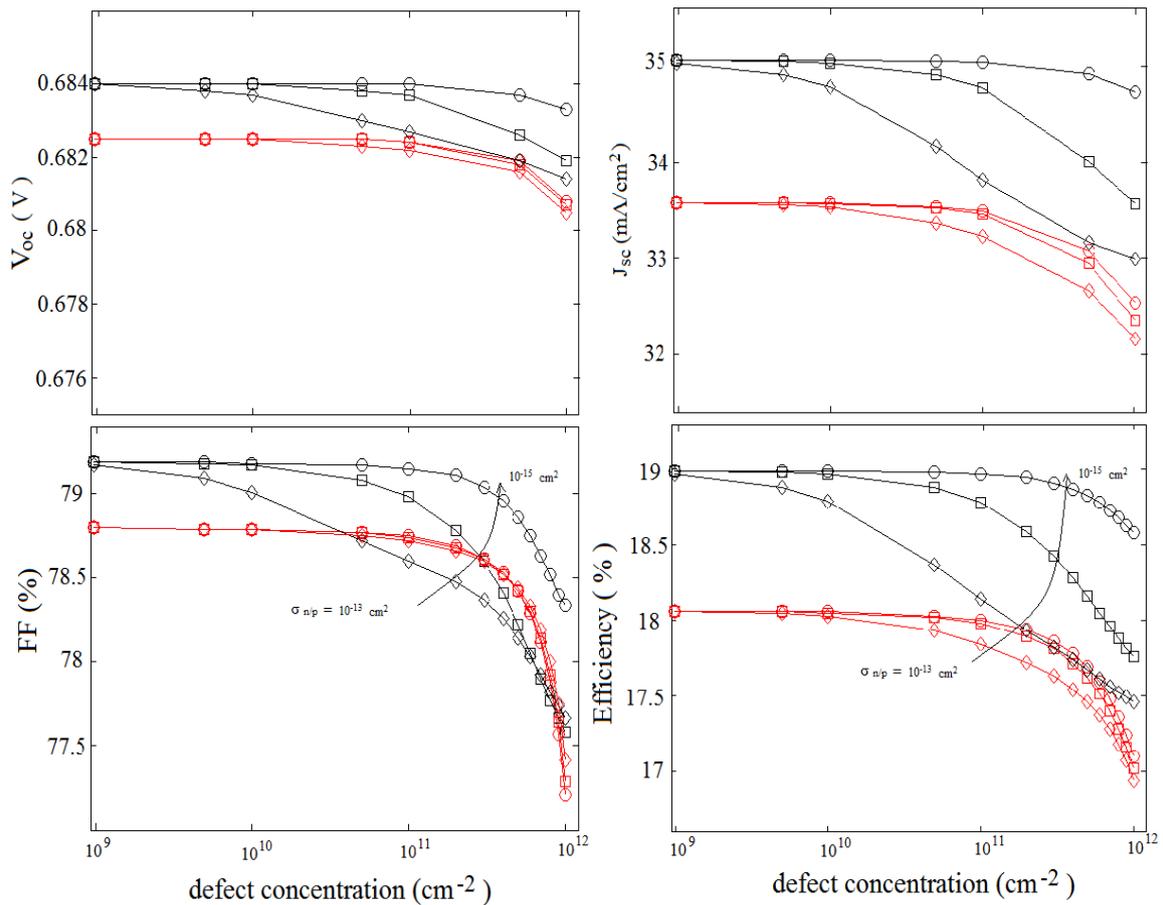


Fig.3. Simulated dependence of the efficiency η , short circuit current density J_{sc} , open circuit voltage V_{oc} , and fill factor FF on the defect concentration at the CdS/SDL interface. The pinning model (black lines) and doping model (red lines) capture cross-sections $\sigma_{n/p}$ for electrons and holes are chosen $\sigma_n = \sigma_p = 10^{-13}/10^{-14}/10^{-15}$ cm² (diamonds, squares, circles).

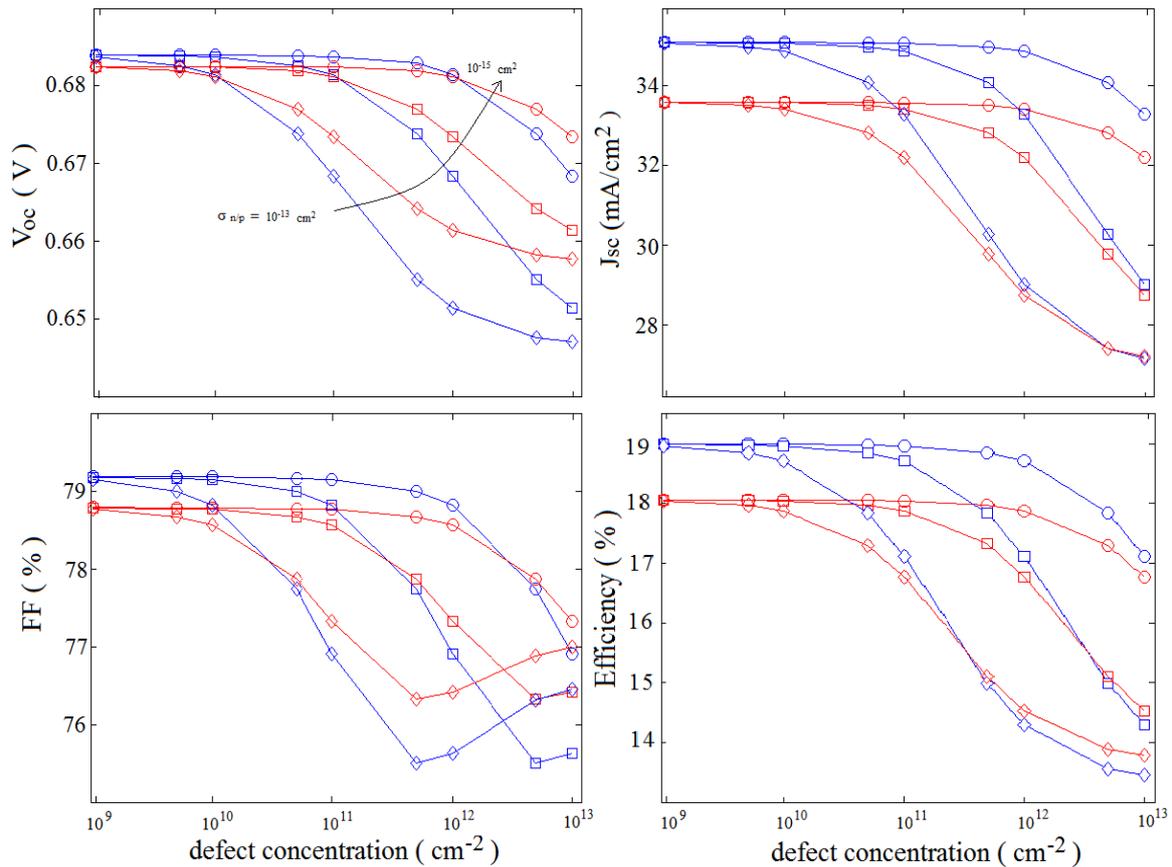


Fig.4. Simulated dependence of the efficiency η , short circuit current density J_{sc} , open circuit voltage V_{oc} , and fill factor FF on the defect concentration at the SDL/CIGS interface. The pinning model (bleu lines) and doping model (red lines). capture cross-sections $\sigma_{n/p}$ for electrons and holes are chosen $\sigma_n = \sigma_p = 10^{-13}/10^{-14}/10^{-15} \text{ cm}^2$ (diamonds, squares, circles).

3.3. Influence of the band-gap widening

A major role in the suppression of interface recombination is played by the Cu-poor surface defect layer (SDL) that forms in Cu-poor chalcopyrite and leads to surface band-gap widening [20]. This layer is expected to play an important role in the performance of the high efficiency Cu $\text{In}_{1-x}\text{Ga}_x\text{Se}_2$ based solar cells [10,11]. So, evaluating its effect on the performances of the solar cells is important. The optical of surface defect layer (SDL) is similar to that of CIGS [21]. So, only the SDL electron affinity was adjusted according to the band-gap variation in the SDL, keeping valence band offset between the surface region and the bulk region of CIGS layers at 0.1 eV. The capture cross-section is fixed to $\sigma_{n/p} = 10^{-13} \text{ cm}^2$, and the defect concentration in both models, is varied in the range from 10^9 - 10^{12} cm^2 . The band-gap of the SDL layer is varied from 1.2 to 1.5 eV. Fig.5 shows calculated efficiency with defect concentration and band-gap energy Fig.5a present the results at the SDL/CIGS interface and Fig.5b at the CdS/SDL ones, the doping model (bleu lines) and the pinning model (black lines). For a both models, increasing the defects beyond 10^{11} cm^2 the impact of band-gap widening becomes more pronounced where efficiency increase by about 3% when passed from 1.2 to 1.5 eV because increasing the SDL band-gap reduces the conduction band offset at CdS/SDL interface which leads to an improvement of the performance of solar cells.

4. Conclusion

In the present study, the effect of excess defect at the CdS/CIGS interface on the performance of solar cell is investigated numerically by using one dimensional SCAPS-1D computer software. In the simulation studies, the defects concentration in a both SDL/CIGS and CdS/SDL interfaces, the capture cross-sections $\sigma_{n/p}$ and the SDL band-gap are varied to study their influence on the performance of CIGS solar cells. We have shown that the impact of this excess is crucial. Increasing defect concentration or large capture cross-sections, both at CdS/SDL and SDL/CIGS interfaces, for the models studied: doping model and pinning model, deteriorate the device efficiency from 19% to levels of 14%, depending on the model and the capture cross section.

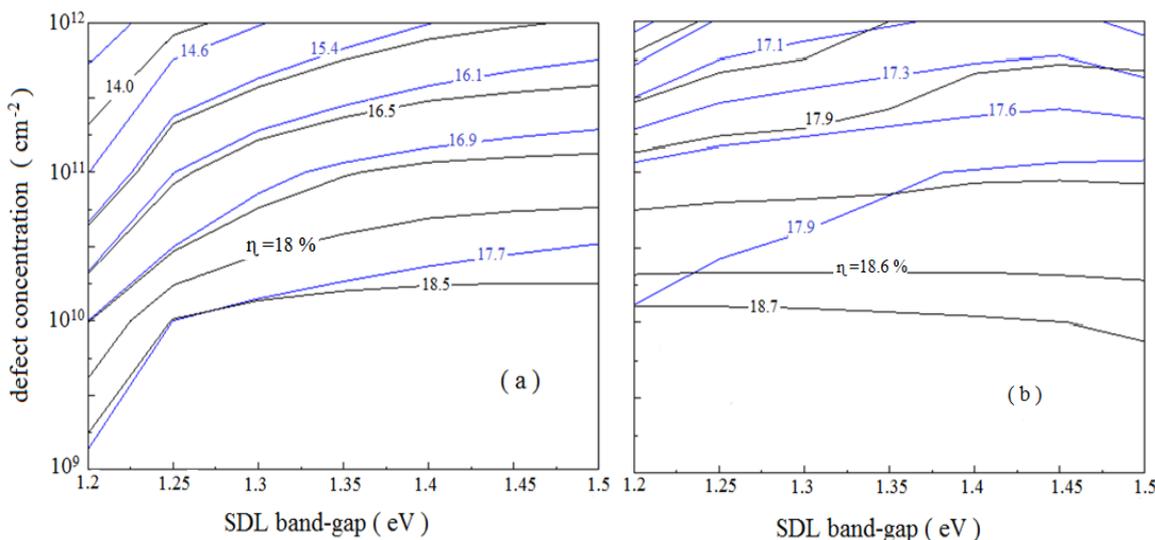


Fig.5. The conversion efficiency of the solar cell as function of the SDL band gap variation and the defect concentration (a) at the SDL/CIGS interface (b) at the CdS/SDL interface. Pinning model (black lines) and doping model (bleu lines).

Increasing the defect concentration beyond 10^{10} cm⁻² the performance drops especially for the pinning model. The pinning model is more sensitive to the variation of the capture cross-sections where the efficiency drops by about 1.2% at the CdS/SDL interface and 4-5% at the SDL/CIGS ones compared to the doping model which shows a decrease of 0.2% for the CdS/SDL interface and between 3 and 3.5% for the SDL/CIGS interface. We conclude from our numerical results that the surface band-gap widening in CIGS photovoltaic absorbers provides a certain tolerance to excess defects at the both junction interfaces where the efficiency increases by about 3% when passed from 1.2 to 1.5 eV.

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