JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **13** No 6, 06001(4pp) (2021)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **13** № 6, 06001(4cc) (2021)

Deep Impact of the *n*-c-Si Defect Density on Heterojunction with Intrinsic Thin Layer Solar Cells

Z. Dahlal[1], F. Hamdache[1], D. Rached[1], W.L. Rahal[2,3,*]

[1] *Laboratoire de Physique des Plasmas, Matériaux Conducteurs et Leurs Applications, U.S.T.O.M.B. – B.P. 1505, El M'naouar, Oran, Algérie*
[2] *Laboratoire d'Analyse et d'Application des Rayonnements, U.S.T.O.M.B. – B.P. 1505, El M'naouar, Oran, Algérie*
[3] *Département de Physique, Faculté des Sciences Exactes et de l'Informatique, Université Abdelhamid Ibn Badis de Mostaganem, Algérie*

(Received 16 January 2021; revised manuscript received 01 December 2021; published online 20 December 2021)

In this work, a Heterojunction with Intrinsic Thin layer (HIT) *n*-c-Si solar cell: Indium Tin Oxide (ITO)/hydrogenated *p*-doped amorphous silicon (*p*-a-Si:H)/hydrogenated intrinsic polymorphous silicon (i-pm-Si:H)/*n*-doped crystalline silicon (*n*-c-Si)/Aluminum (Al) has been optimized. Using solar cell capacitance simulator (SCAPS-1D), we have studied the effect of defect density in the bulk (N_t) and at the surface (N_{ss}) of the *n*-c-Si active layer on the current density-voltage (*J-V*) characteristic (open-circuit voltage, short-circuit current density, Fill Factor and efficiency). To calculate the values of N_{ss}, we have taken the average between the density of states G_{mg} located in the band gap (*U*-shaped model) and the total density of states N_{tot} (Urbach tails) that we have multiplied by the thickness of the defective layer. We have shown that for a defective surface thickness of 32 Å between hydrogenated polymorphous silicon and crystalline silicon (i-pm-Si:H/*n*-c-Si), the density of states G_{mg} located in the band gap and the density of states N_{tot} at Urbach tails must be equal to $3.5 \cdot 10^{17}$ cm^{-3} and $2.8 \cdot 10^{17}$ cm^{-3}, respectively (using *U*-shaped model). We conclude that the surface of the active layer must be passivated so as to have N_{ss} less than 10^{11} cm^{-2}. Then, the lifetime of the minority carriers in the active layer (*n*-c-Si) must be greater than 1 ms. Indeed, an efficiency of 22.08 % was obtained for $N_{ss} = 10^{10}$ cm^{-2}, $\tau = 5$ ms.

Keywords: HIT solar cells, Silicon, Defect density, SCAPS-1D, Current density-voltage (*J-V*) characteristic.

DOI: 10.21272/jnep.13(6).06001 PACS numbers: 73.61.Jc, 71.20.Mq, 88.40.jj, 88.40.hj

1. INTRODUCTION

Heterojunctions with amorphous hydrogenated silicon and crystalline silicon (a-Si:H/c-Si) are a very active research area for photovoltaic applications. Indeed, HIT (Heterojunction with Intrinsic Thin layer) solar cells have been the subject of much attention through theoretical and empirical studies due to their high energy conversion efficiency and relatively simple structure [1-6]. HIT solar cells have advantages over other crystalline silicon photovoltaic technologies in terms of low cost and low temperature (200 °C) process of a-Si:H [7-9]. Sanyo (Japan) reported that a conversion efficiency of up to 24.7 % for HIT solar cells was achieved in 2013 [10]. In 2019, a record efficiency of up to 26 % was achieved [11]. However, the energy efficiency of silicon-based solar cells under unconcentrated solar radiation could reach 30 %. In order to produce high efficiency HIT solar cells, several parameters must be understood and carefully optimized. Our study focused on the impact of defect density in the bulk (N_t) and at the surface (N_{ss}) of the crystalline silicon active layer on the current density-voltage *J-V* characteristic. A numerical modelling was carried out using solar cell capacitance simulator SCAPS-1D, which is a one-dimensional solar cell simulation software developed at the Department of Electronics and Information Systems (EIS), University of Gent, Belgium, and used for numerical analysis of solar cells [12-14]. This software examines the performance of semiconductor device structures under steady state in one dimension by simultaneously solving the Poisson equation and the continuity equations for free electrons and free holes using finite differences and the Newton-Raphson method [15].

2. PRESENTATION OF THE HIT *N*-C-SI SOLAR CELL

The studied HIT *n*-c-Si solar cell consists of the following stack: Indium Tin Oxide (ITO)/hydrogenated *p*-doped amorphous silicon (*p*-a-Si:H)/hydrogenated intrinsic polymorphous silicon (i-pm-Si:H)/*n*-doped crystalline silicon (*n*-c-Si)/Aluminum (Al) represented in Fig. 1.

This cell consists of a substrate of *n*-doped crystalline silicon (*n*-c-Si), on the front face of which, intrinsic polymorphous silicon (i-pm-Si:H) is deposited. This intrinsic layer is specific to HIT cells. It allows the modelling of surface defects existing at the *p*-a-Si:H/*n*-c-Si interface. Then, a layer of *p*-doped amorphous silicon is deposited to constitute the emitter (*p*-a-Si:H) with a thickness of 50 Å. An anti-reflective layer (Transparent Conductive Oxide (TCO)) based on ITO is deposited on *p*-doped amorphous silicon to form the front contact. Finally, a layer of metal consisting of aluminum is deposited on the active *n*-c-Si layer to form the rear face. Our study focused on the impact of defect density in the bulk (N_t) and at the surface (N_{ss}) of the crystalline silicon active layer on the photovoltaic parameters (short-circuit current density, open-circuit voltage, Fill Factor and efficiency).

The principal parameters of each layer are summarized in Table 1.

---

[*] leila.rahal@univ-mosta.dz

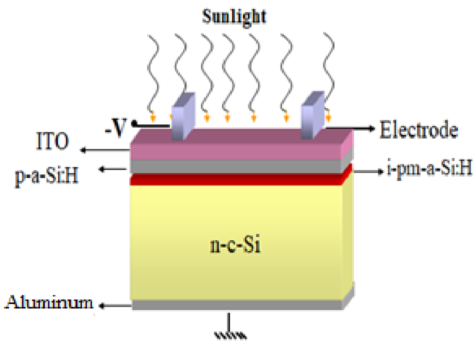


Fig. 1 – Structure of a HIT *n*-c-Si (ITO/*p*-a-Si:H/i-pm-Si:H/*n*-c-Si/Al) solar cell

Table 1 – Principal parameters of different layers use for the simulation

Parameters	*p*-a-Si:H	i-pm-Si:H	Defective *n*-c-Si	*n*-c-Si
d (μm)	0.005	0.005	0.0032	300
χ (eV)	3.90	3.90	4.22	4.22
E_μ (eV)	1.72	1.96	1.12	1.12
N_A (cm^{-3})	10^{19}	0	0	0
N_D (cm^{-3})	0	0	10^{17}	10^{17}
N_t (cm^{-3})	10^{21}	10^{13}	variable	variable
E_D (eV)	0.01	0.01	0.01	0.01
E_A (eV)	0.01	0.01	0.01	0.01
μ_n (cm^2/Vs)	20	30	1450	1450
μ_p (cm^2/Vs)	5	10	450	450
N_C, N_V (cm^{-3})	10^{20}	2 10^{20}	10^{19}	10^{19}

3. RESULTS AND DISCUSSION

We have plotted the recombination rate under 100 mWcm^{-2} of AM1.5 light, as a function of the position in the device for two defect density values ($N_t = 10^{10}$ cm^{-3} and 10^{13} cm^{-3}) in the active layer (*n*-c-Si). The surface defect density N_{ss} is taken equal to 10^{10} cm^{-2} ($N_{tot} = 3.5 \cdot 10^{17}$ cm^{-3}, $G_{mg} = 2.8 \cdot 10^{17}$ cm^{-3}, $d = 32$ Å).

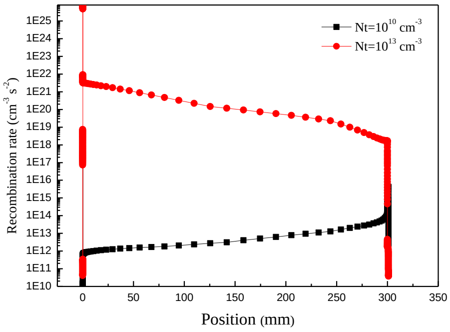


Fig. 2 – The recombination rate as a function of the position in the device for $N_t = 10^{10}$ cm^{-3} and 10^{13} cm^{-3}. The surface defect density $N_{ss} = 10^{10}$ cm^{-2}

We can see from Fig. 2 that the recombination rate increased in the active layer of our device when we increased the defect density N_t. This increase is directly linked to the reduction of the carrier lifetime τ in the active layer. Indeed, according to Eq. (1) [16], the recombination rate is inversely proportional to the carrier lifetime τ:

$$\tau_{n,p} = \frac{n,p - n_0,p_0}{R}, \qquad (3.1)$$

p (n) represents the density of free holes (electrons) under 100 mWcm^{-2} of AM1.5 light, p_0 (n_0) represents the density of holes (electrons) at thermodynamic equilibrium, R represents the recombination rate in the active *n*-c-Si layer.

We have varied the defect density N_t as a function of the carrier lifetime τ in the active layer. In agreement with Eq. (3.1), the obtained results (from Fig. 3) show that an increase in N_t decreases the carrier lifetime τ. This decrease will have a detrimental effect on the output parameters of the studied *n*-c-Si solar cells.

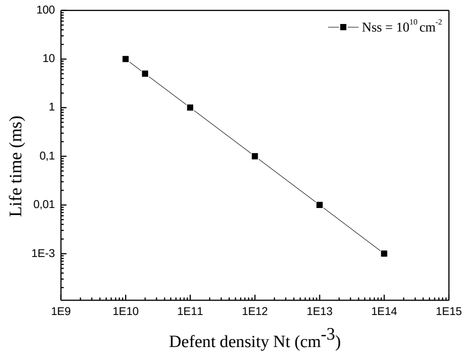
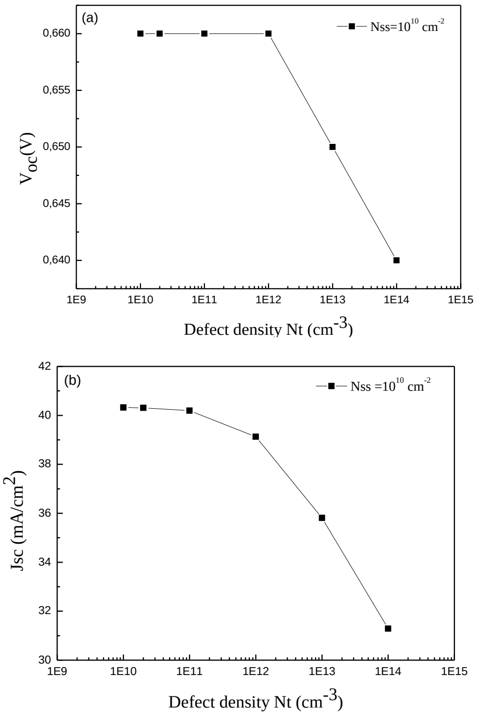


Fig. 3 – The carrier lifetime τ as a function of the defect density N_t. The surface defect density $N_{ss} = 10^{10}$ cm^{-2}

Fig. 4 represents the photovoltaic parameters under illumination of the ITO/*p*-a-Si:H/i-pm-Si:H/*n*-c-Si/Al structure as a function of the defect density N_t. The surface defect density N_{ss} is taken equal to 10^{10} cm^{-2}.

Indeed, from Fig. 4, all photovoltaic parameters decrease with the increasing of defect density N_t in the active layer of the studied cell. The V_{oc} drops from 0.66 to 0.64 V, the J_{sc} from 40.32 to 31.29 mA/cm^2, the FF from 82.60 to 82.51 % and η from 22.04 to 16.71 %. The degradation of the efficiency can be explained by the



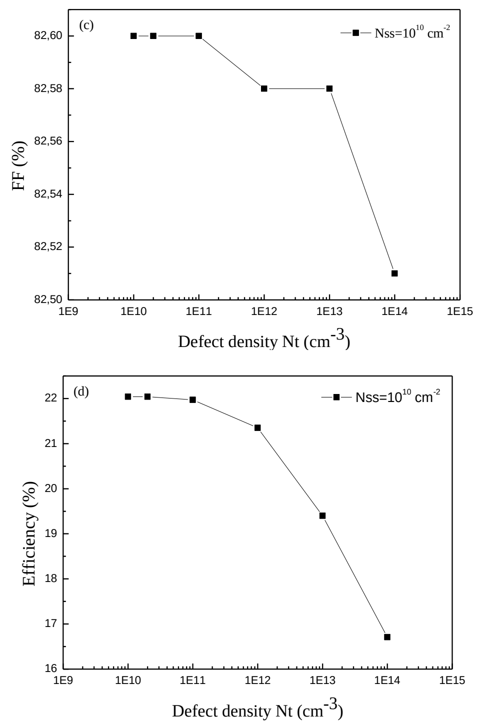


Fig. 4 – Plots of the open-circuit voltage V_{oc} (a), short-circuit current density J_{sc} (b), Fill Factor FF (c) and efficiency η (d) of the HIT *n*-c-Si solar cell as a function of N_t with $N_{ss} = 10^{10}$ cm^{-2}

Table 2 – Calculation of the efficiency of the HIT *n*-c-Si solar cell as a function of N_t and τ. $N_{ss} = 10^{10}$ cm^{-2} ($N_{tot} = 3.5\cdot10^{17}$ cm^{-3}, $G_{mg} = 2.8\cdot10^{17}$ cm^{-3}, $d = 32$ Å)

N_{ss} (cm^{-2})	N_t (cm^{-3})	τ (ms)	η (%)
10^{10}	10^{10}	10	22.09
	2.10^{10}	5	22.08
	10^{11}	1	22.01
	10^{12}	0.1	21.37
	10^{13}	0.01	19.40
	10^{14}	0.001	16.71

Table 3 – Calculation of the efficiency of the HIT *n*-c-Si solar cell as a function of N_t and τ. $N_{ss} = 10^{11}$ cm^{-2} ($N_{tot} = 3.5\cdot10^{17}$ cm^{-3}, $G_{mg} =2.8\cdot10^{17}$ cm^{-3}, $d = 32$ Å)

N_{ss} (cm^{-2})	N_t (cm^{-3})	τ (ms)	η (%)
10^{11}	10^{10}	10	19.57
	2.10^{10}	5	19.56
	10^{11}	1	19.49
	10^{12}	0.1	19.94
	10^{13}	0.01	17.22
	10^{14}	0.001	14.91

fact that an increase in N_t causes a decrease in the minority carrier lifetimes. Thus, these charge carriers will recombine because they do not have enough time to be collected. We then analyzed the variation of N_{ss} (surface defect density), N_t and τ compared to the efficiencies of our *n*-type HIT structure. To obtain the values of N_{ss}, we have taken the average between the density of states G_{mg} located in the band gap (*U*-shaped model) and the total density of states N_{tot} (Urbach tails) that we have multiplied by the thickness of the defective layer [18]. We obtained the five tables below.

Table 4 – Calculation of the efficiency of the HIT *n*-c-Si solar cell as a function of N_t and τ. $N_{ss} = 10^{12}$ cm^{-2} ($N_{tot} = 3.5\cdot10^{17}$ cm^{-3}, $G_{mg} = 2.8\cdot10^{17}$ cm^{-3}, $d = 32$ Å)

N_{ss} (cm^{-2})	N_t (cm^{-3})	τ (ms)	η (%)
10^{12}	10^{10}	10	17.09
	2.10^{10}	5	17.08
	10^{11}	1	17.03
	10^{12}	0.1	16.54
	10^{13}	0.01	15.03
	10^{14}	0.001	13.01

Table 5 – Calculation of the efficiency of the HIT *n*-c-Si solar cell as a function of N_t and τ. $N_{ss} = 10^{13}$ cm^{-2} ($N_{tot} = 3.5\cdot10^{17}$ cm^{-3}, $G_{mg} = 2.8\cdot10^{17}$ cm^{-3}, $d = 32$ Å)

N_{ss} (cm^{-2})	N_t (cm^{-3})	τ (ms)	η (%)
10^{13}	10^{10}	10	14.78
	2.10^{10}	5	14.77
	10^{11}	1	14.72
	10^{12}	0.1	14.30
	10^{13}	0.01	12.98
	10^{14}	0.001	11.22

By analyzing Table 2-Table 5, we can conclude that to have a good efficiency, the surface of the active layer must be passivated so as to have a defect density N_{ss} less than 10^{11} cm^{-2}. Then, the lifetime of the minority carriers in the active layer (*n*-c-Si) must be greater than 1 ms. Indeed, an efficiency of 22.08 % was obtained for $N_{ss} = 10^{10}$ cm^{-2}, $\tau = 5$ ms.

4. CONCLUSIONS

In this article, we have studied the deep impact of the defect density in the bulk (N_{ss}) and at the surface (N_t) of the crystalline silicon active layer on the short-circuit current density, open-circuit voltage, Fill Factor and efficiency. The studied solar cell is a HIT *n*-c-Si (ITO/*p*-a-Si:H/i-pm-Si:H/*n*-c-Si/Al). We have shown that to have high-quality HIT solar cells, it is important to:

1. Reduce the recombination rate at the interface (i-pm-Si:H/*n*-c-Si), and this by reducing the surface defect density N_{ss} of this defective layer. The surface of the active layer must be passivated so as to have a N_{ss} less than 10^{11} cm^{-2}. For this, the density of states G_{mg} located in the band gap must be equal to $3.5\cdot10^{17}$ cm^{-3} and the density of states N_{tot} must be equal to $2.8\cdot10^{17}$cm^{-3}.
2. Reduce the recombination rate in the bulk of the active layer (*n*-c-Si), and this by increasing the lifetime of the minority carriers (τ must be greater than 1 ms).

All these optimized parameters can be obtained during the experimental elaboration of the *n*-c-Si active layer.

REFERENCES

1. L. Zhao, C.L. Zhou, H.L. Li, H.W. Diao, W.J. Wang, *Sol. Energy Mater. Sol. C.* **92**, 673 (2008).
2. M. Taguchi, K. Kawamoto, S. Tsuge, T. Baba, H. Sakata, M. Morizane, K. Uchihashi, N. Nakamura, S. Kiyama, O. Oota, *Prog. Photovolt.* **8**, 503 (2000).
3. K. Yamamoto, D. Adachi, H. Uzu, M. Ichikawa, T. Terashita, T. Meguro, N. Nakanishi, M. Yoshimi, J.L. Hernández, *Jpn. J. Appl. Phys.* **54**, 08KD15 (2015).
4. D. Adachi, J.L. Hernández, K. Yamamoto, *Appl. Phys. Lett.* **107**, 233506 (2015).
5. M.A. Green, Y. Hishikawa, W. Warta, E.D. Dunlop, D.H. Levi, J. HohlEbinger, A.W.H. Ho-Baillie, *Prog. Photovolt.* **25**, 668 (2017).
6. Cao Yu, Miao Yang, Gangqiang Dong, Fuguo Peng, De-Cheng Hu, Wei Long, Chengjian Hong, Ge Cui, Jianqiang Wang, Yongcai He, *Jpn. J. Appl. Phys.* **57** 08RB15 (2018).
7. S. De Wolf, A. Descoeudres, Z.C. Holman, C. Ballif, *Green* **2**, 7 (2012).
8. T. Ishii, K. Otani, T. Takashima, S. Kawai, *Sol. Energy Mater. Sol. C.* **95**, 386 (2011).
9. N. Aste, C. Del Pero, F. Leonforte, *Sol. Energy* **109**, 1 (2014).
10. M. Taguchi, A. Yano, S. Tohoda, K. Matsuyama, Y. Nakamura, T. Nishiwaki, K. Fujita, E. Maruyama, *IEEE J. Photovolt.* **4**, 96 (2014).
11. M.A. Green, E.D. Dunlop, D.H. Levi, J. Hohl-Ebinger, M. Yoshita, A.W.Y. Ho-Baillie, *Prog. Photovolt.: Res. Appl.* **27** No 7, 565 (2019).
12. M. Burgelman, J. Verschraegen, S. Degrave, P. Nollet, *Prog. Photovolt.: Res. Appl.* **12**, 143 (2004).
13. J. Verschraegen, M. Burgelman, *Thin Solid Films* **515**, 6276 (2007).
14. K. De Cock, S. Khelifi, M. Burgelman, *Thin Solid Films* **519**, 7481 (2011).
15. K. Bendjebbar, W.L. Rahal, D. Rached, S. Bahlouli, *Optik* **212**, 164741 (2020).
16. A. Kanevce, W.K. Metzger, *J. Appl. Phys.* **105** No 9, 094507 (2009).
17. Madhumita Nath, P. Chatterjee, J. Damon-Lacoste, P. Roca i Cabarrocas, *J. Appl. Phys.* **103**, 034506 (2008).
18. D. Rached, W.L. Rahal, *Optik* **223**, 165575 (2020).

Вплив густини дефектів на сонячні елементи *n*-*c*-Si на основі гетеропереходу з внутрішнім тонким шаром

Z. Dahlal[1], F. Hamdache[1], D. Rached[1], W.L. Rahal[2,3]

[1] *Laboratoire de Physique des Plasmas, Matériaux Conducteurs et Leurs Applications, U.S.T.O.M.B. – B.P. 1505, El M'naouar, Oran, Algérie*
[2] *Laboratoire d'Analyse et d'Application des Rayonnements, U.S.T.O.M.B. – B.P. 1505, El M'naouar, Oran, Algérie*
[3] *Département de Physique, Faculté des Sciences Exactes et de l'Informatique, Université Abdelhamid Ibn Badis de Mostaganem, Algérie*

У роботі оптимізовано сонячний елемент *n*-c-Si на основі гетеропереходу з внутрішнім тонким шаром (HIT): оксид індію і олова (ITO)/гідрогенізований *p*-легований аморфний кремній (*p*-a-Si:H)/гідрогенізований власний поліморфний кремній (i-pm-Si:H)/*n*-легований кристалічний кремній (*n*-c-Si)/алюміній (Al). За допомогою симулятора ємності сонячних елементів (SCAPS-1D) ми вивчили вплив густини дефектів в об'ємі (N_t) і на поверхні (N_{ss}) активного шару сонячного елемента *n*-c-Si на характеристику густини струму від напруги (*J*-*V*) (напруга холостого ходу, густина струму короткого замикання, коефіцієнт заповнення та ефективність). Для обчислення значень N_{ss} ми взяли середнє між густиною станів G_{mg}, розташованих у забороненій зоні (*U*-подібна модель), і загальною густиною станів N_{tot} (хвости Урбаха), яку ми помножили на товщину дефектного шару. Ми показали, що для товщини дефектної поверхні 32 Å між гідрогенізованим поліморфним кремнієм і кристалічним кремнієм (i-pm-Si:H/*n*-c-Si) густина станів G_{mg}, розташованих у забороненій зоні, і густина станів N_{tot} в хвості Урбаха повинні дорівнювати відповідно $3{,}5\cdot 10^{17}$ см$^{-3}$ і $2{,}8\cdot 10^{17}$ см$^{-3}$ (використовуючи *U*-подібну модель). Можна зробити висновок, що поверхню активного шару необхідно пасивувати так, щоб отримати N_{ss} менше 10^{11} см$^{-2}$. Тоді час життя неосновних носіїв в активному шарі (*n*-c-Si) має бути більше 1 мс. Дійсно, для $N_{ss} = 10^{10}$ см$^{-2}$ та $\tau = 5$ мс отримано ККД 22,08 %.

Ключові слова: Сонячний елемент на основі гетеропереходу з внутрішнім тонким шаром (HIT), Кремній, Густина дефектів, SCAPS-1D, Характеристика густини струму від напруги (*J*-*V*).