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Simulation Back Reflection Layer Effect Znte on Solar Cell Performance a Study Using SCAPS-1D

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Abstract :

In this study, a theoretical simulation was conducted to improve the performance of a solar cell with a structure. ZnSnS/Cu by analyzing the effect of the back-reflection layer, varying its thickness, and doping. The results showed that introducing a back-reflection layer is an effective strategy for increasing solar cell efficiency by enhancing the internal reflection of unabsorbed photons and redirecting them toward the absorber layer.

Several materials have been tested as back reflective coatings such as:Si, Sb_2Se_3, Zn_2P_3, CIGS, and ZnTe. ZnTe showed superior performance across all cell parameters, with higher open-circuit voltage (Voc), short-circuit current (Jsc), and fill factor (FF), achieving a maximum photovoltaic efficiency of 29.26% compared to the reference value of 11.23%.

The results of changing the layer thickness also showed thatZnTe has an ideal thickness of 1.60 µm that achieves the optimal balance between optical and electrical properties, contributing to improved carrier extraction and reduced losses due to interference or random reflections.

ZnTe was preferable because it has high reflectivity and a wide energy gap, which returns unabsorbed photons to the absorber layer and reduces charge loss, resulting in a significant improvement in cell efficiency.

As for doping the reflection layer, it has been shown that it contributes to tuning the electronic properties at the backside of the cell, by improving conductivity and reducing recombination rates. Doped ZnTe is the most compatible in terms of electronegativity, carrier speed, and state density, making it the ideal choice for backscattering layers.

These results confirm the importance of careful layer design for thin-film solar cells, and the need to fine-tune the reflective layer properties in terms of material, thickness, and doping, to achieve high and stable conversion efficiencies.

Keywords: ZnTe, backscatter, solar cell efficiency, simulation using SCAPS-1D, photovoltaic performance.

محاكاة تأثير طبقة الانعكاس الخلفي ZnTe على أداء الخلية الشمسية: دراسة باستخدام SCAPS-1D

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مستخلص:

تم في هذه الدراسة إجراء محاكاة نظرية لتحسين أداء الخلية الشمسية ذات البنية ZnSnS/Cu من خلال تحليل تأثير طبقة الانعكاس الخلفي (Reflection layer) وتغيير سمكها وتشويبها (Doping). أظهرت النتائج أن إدخال طبقة انعكاس خلفي يُعد من الاستراتيجيات الفعالة لرفع كفاءة الخلية الشمسية، وذلك عبر تعزيز الانعكاس الداخلي للفوتونات غير الممتصة وإعادة توجيهها نحو طبقة الامتصاص.

تم اختبار عدة مواد كطبقات انعكاس خلفي مثل Si، Sb_2Se_3، Zn_2P_3، CIGS، وZnTe. وقد أظهرت مادة ZnTe أداءً متفوقًا من حيث جميع مؤشرات الخلية، حيث ارتفع جهد الدائرة المفتوحة (Voc) وتيار الدائرة القصيرة (Jsc) ومعامل الامتلاء (FF)، لتصل الكفاءة الكهروضوئية القصوى إلى ٪29.26 مقارنة بالقيمة المرجعية ٪11.23.

كما بينت نتائج تغيير سمك طبقة ZnTe أن هناك سمكًا مثاليًا بحدود 1.60 ميكرومتر يحقق التوازن الأمثل بين الخصائص البصرية والكهربائية، حيث ساهم في تحسين استخراج الحوامل وتقليل الفواقد الناتجة عن التداخل أو الانعكاسات العشوائية.

كانت ZnTe الأفضل لأنها تمتلك انعكاسية عالية وفجوة طاقة واسعة، مما يعيد الفوتونات غير المتصة إلى طبقة الامتصاص ويقلل فقد الشحنات، مما أدى إلى تحسين كبير في كفاءة الخلية (Efficiency).

أما تشويب طبقة الانعكاس، فقد أظهر أنه يساهم في ضبط الخواص الإلكترونية على مستوى الواجهة الخلفية للخلية، من خلال تحسين التوصيلية وتقليل معدلات إعادة الاتحاد (Recombination). وقد أثبتت ZnTe المشوبة أنها الأكثر توافقًا من حيث الكهروسالبية، وسرعة الحوامل، وكثافة الحالات، مما يجعلها الخيار الأمثل ضمن طبقات الانعكاس الخلفي.

تؤكد هذه النتائج أهمية التصميم الطبقي الدقيق للخلايا الشمسية الرقيقة، وضرورة ضبط خصائص الطبقة العاكسة من حيث المادة، السمك، والتشويب، للوصول إلى كفاءة تحويل عالية ومستقرة.

الكلمات المفتاحية: ZnTe، الانعكاس الخلفي، كفاءة الخلية الشمسية، المحاكاة باستخدام SCAPS-1D، الأداء الكهروضوئي.

1-Introduction

In recent years, solar cell technologies have witnessed remarkable development driven by the need for clean and renewable energy sources, and improving solar cell performance is a major goal for researchers and engineers [1]. Among the promising materials used in the manufacture of thin-film solar cells, a compound appears ZnSnS is an environmentally friendly and efficient absorber, thanks to its suitable direct energy gap and the abundance of its components in nature [2][3]. In addition, copper (Cu) is used to improve electrical conductivity and enhance the generation of photoelectron pairs, which contributes to raising the cell efficiency [4].

The thickness of the absorber layer plays a crucial role in determining the amount of light absorbed and, consequently, the number of electrons generated. Increasing thickness initially results in greater absorption, but it may also increase the recombination rates of the carriers, reducing efficiency [5]. It is important to achieve the ideal balance between thickness and material properties to ensure optimal photovoltaic performance.

In addition, the back reflection layer (Back Surface Reflector (BSR) is a key factor in improving light absorption, especially in thin-film cells. It reflects unabsorbed photons back toward the absorber layer, increasing the likelihood of generating electron-hole pairs [6][7]. Studies show that materials such as ZnTe, CIGS, and Si are effective as reflection layers in many solar structures [8].

Doping of active layers (either absorption or reflection layer) is used to adjust the energy levels within the material and improve conductivity and charge transport. The density of donor or tunable impurities can be controlled to adjust the energy gap levels and the voltage generated by the cell [9]. Fine doping also reduces structural defects that lead to carrier loss, which improves the fill factor (Fill Factor) and overall conversion efficiency [10].

This research aims to study the effect of absorption layer thickness, back reflection layer addition, and doping modification on the performance of solar cell made of Cu and ZnSnS using theoretical simulation, with analysis of key performance parameters such as: Voc, Jsc, FF, and Efficiency.

2-Simulation method

The theoretical simulation in this research was done using the programSCAPS-1D is a performance simulation tool for ZnSnS/Cu thin-film solar cells. This software enables modeling the effect of various variables, such as layer thickness, back reflection layer type, and doping level, on photovoltaic performance parameters.

The physical properties of each layer (such as energy gap, electronegativity, permittivity, effective density, etc.) have been precisely entered, with operating conditions such as temperature and solar radiation intensity fixed. It explains the table (1) Parameters of back-reflection layers

Then one variable was modified in each experiment (such as thickness, type of reflective material, or doping level) to study its direct effect on cell performance.

1) Software used:SCAPS-1D for simulation of multilayer solar cells.

2) Basic structure of the cell: ZnO/ZnSnS/Cu, with a back reflection layer inserted where required.

3) The following properties were entered for each layer:

4) Energy gap (Eg), electronegativity (Electron affinity), relative permittivity (εr), effective density of states (Nc and Nv), carrier velocity (electrons and holes), mobility (Mobility), and doping density (NA or ND).

5)Variables tested:

a) layer thickness ZnSnS (0.1 to 3 µm)

b) layer thickness reflective ZnTe (0.01 to 1.5 µm)

c) Change the reflection layer type (ZnTe, Si, CIGS, …)

d) Changing the doping density of the absorbing and reflecting layer

5) Operating conditions: constant temperature (300K), AM1.5 spectrum, with continuous illumination.

Table (1) Parameters of back-reflection layers

Parameters	symbol (unit)	Sb2Se3	Yes	CIGS	ZnTe
Thickness	W(µm)	0.05	0.05	0.05	0.05
Bandgap	Eg (ev)	1.2	1.12	1.05	2.2
Electron affinity	χ (ev)	4.04	4.05	4.14	3.73
Dielectric permittivity	ϵr	18,000	11.9	10	10.3
CB effective density of states	N_C(c)m^{-3}	2.2E+18	E+192.580	E+181,000	1.7E+18
VB effective density of states	N_V(c)m^{-3}	1.8E+19	E+192.650	E+181,000	1.16E+19
Electron thermal velocity	V_n(cm/s)	1.000E+7	E+71,000	E+71,000	3.2E+7
Hole thermal velocity	V_P(cm/s)	1.000E+7	E+71,000	E+71,000	1.5E+7
Electron mobility	μ_n(c/vs)m^2	1.5E+1	E+31.350	E+13,000	3.3E+2
Hole mobility	μ_p(c/vs)m^2	5.1E+0	E+24.500	E+11,500	8E+1
Shallow uniform donor density	ND (1/cm3)	0	0	0	0
Shallow uniform acceptor density	NA (1/cm3)	1E+17	1E+17	1E+17	1E+17

3- Models physical and mathematical simulation of solar cells

1. Poisson's equation

Describe this equation represents the distribution of electrical potential within a solar cell as a result of the distribution of charges (electrons, holes, and donor or acceptor impurities). It is essential for calculating the internal electric field that stimulates the movement of carriers through the different layers [11].

$$\frac{d^2\psi(x)}{dx^2} = -\left(\frac{q}{\varepsilon}\right) * [p(x) - n(x) + N_D^+ - N_A^-] \ldots\ldots..(1)$$

2. Continuity equations

It is used these equations calculate the change in electron and hole concentration over time due to electric current, photo generation, and recombination. They represent the law of charge conservation for carriers within a solar cell [12].

Equation electrons:[12]

$$\frac{\partial n}{\partial t} = \left(\frac{1}{q}\right)\frac{\partial J_n}{\partial x} + G(x) - R(x) \ldots\ldots (2)$$

Equation gaps:[12]

$$\frac{\partial p}{\partial t} = -\left(\frac{1}{q}\right)\frac{\partial J_p}{\partial x} + G(x) - R(x) \ldots\ldots (3)$$

3. Drift diffusion equations

It is used these equations calculate the current resulting from the movement of electrons and holes within the solar cell, whether due to the electric field (drift) or the concentration gradient (diffusion). They are essential for understanding the distribution of the resulting current within the layers[13].

Equation current for electrons:[13]

$$J_n = q\,\mu_n\, n\frac{d\psi}{dx} + q\,D_n\frac{dn}{dx} \ldots\ldots (4)$$

Equation current to gaps:[13]

$$J_p = q\,\mu_p\, p\frac{d\psi}{dx} - q\,D_p\frac{dp}{dx}$$

4. Shockley–read–hall recombination model (SRH recombination)

describes this model describes the recombination mechanism of carriers (electrons and holes) through intermediate energy levels located within the energy gap, resulting from crystal defects or impurities. It is considered one of the most important models of carrier loss in solar cells[14].

$$R_{SRH} = \frac{(np - n_i^2)}{[\tau_p(n + n_i) + \tau_n(p + n_i)]} \ldots\ldots (5)$$

4- Results and discussion

4-1Results of zeroing series and parallel resistors

In the first phase of the study, a simulation was performed of the solar cell situation under ideal conditions by zeroing the series resistance (Rs) and parallel resistance (Rsh), in order to isolate the effects of internal and external electrical losses. This step is necessary to determine the maximum theoretical performance of the solar cell and provide a reference against which any subsequent improvements to the cell structure or material properties can be evaluated.

The simulation results showed that the open circuit voltage (The voltage (Voc) reached 0.654 V, representing the no-load voltage and reflecting the separation quality of photo carriers at equilibrium. The short-circuit current (Jsc) was recorded at 20.5329 mA/cm², indicating good photon absorption and conversion efficiency in the absence of conductive barriers. The fill factor also reached a high percentage of 83.57%, indicating that the voltage-current curve is close to the ideal shape, meaning that the cell is capable of maintaining high voltage and current in the maximum operating region.

The photovoltaic conversion efficiency in this case reached 11.23%, which is reasonable and satisfactory in the absence of the effects of losses associated with resistors. This theoretical evaluation provides a clear framework for assessing the impact of any subsequent modification to the solar cell, whether by adding new layers such as backscattering, or by adjusting the thickness and doping.[15].

Table (1) Cell outputs after zeroing the series and parallel resistors

Cell outputs	Value it
open circuit voltage	0.654262 v
short circuit current	20.5329 mA/cm2
milli factorand	83.5651%
Conversion efficiency	11.2261%

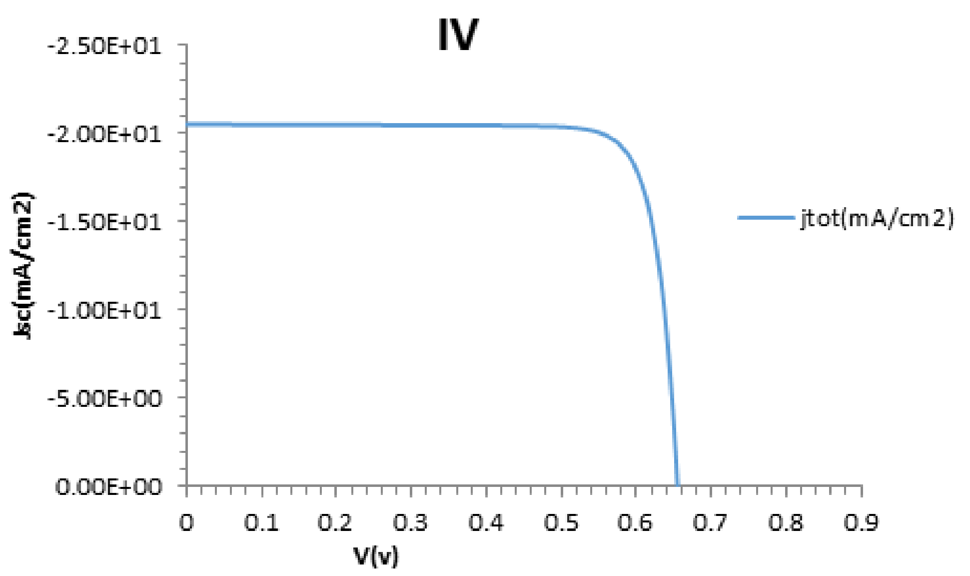

Figure (1) The relationship between voltage and current after zeroing the series and parallel resistors

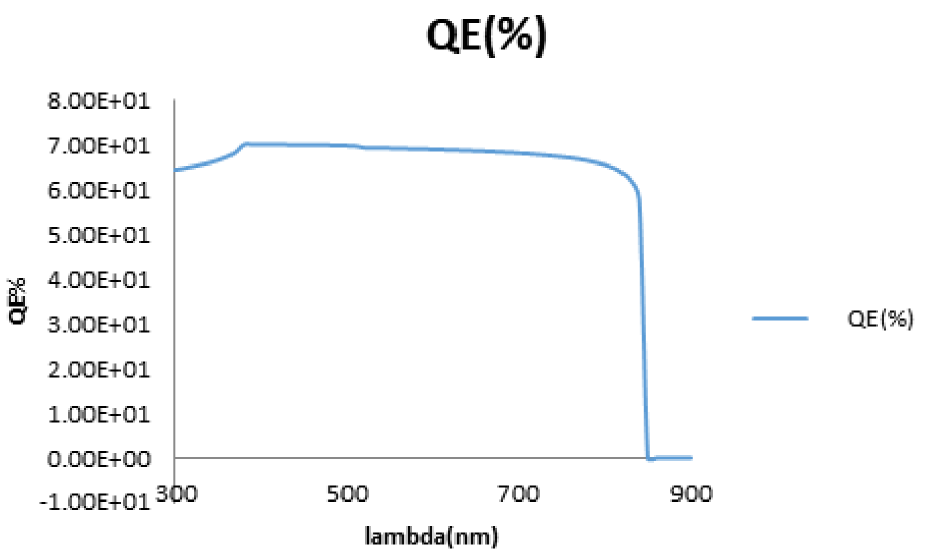

Figure (2) Quantum efficiency after zeroing the series and parallel resistors

4-2 Results of adding a reflection layer

After determining the performance of the solar cell under ideal conditions (with zero series and parallel resistors), we moved on to study the effect of introducing a back reflection layer (Back Surface Reflector (BSR) is used to improve light absorption and increase cell efficiency. This layer is an effective means of reducing light loss by reflecting unabsorbed photons back toward the absorber layer, increasing the potential for generating additional electron-hole pairs.

Several materials were tested as back-reflective coatings, including : Si, Sb_2Se_3, Zn_2P_3, CIGS, and ZnTe. The results showed significant variation in cell performance depending on the type of material used. For example, when ZnTe was used as the reflective layer, the open circuit voltage (Voc) increased to 1.592 V, compared to the baseline value of 0.654 V, a significant jump in voltage that indicates a clear improvement in charge transport and reduced losses. The short circuit current (Jsc) also increased to 21.163 mA/cm², and the fill factor to 86.83%.

These improvements were reflected in the photovoltaic conversion efficiency, which reached 29.26% when using ZnTe had the highest efficiency among all tested materials, compared to 11.23% in the original state without a reflection layer. Other materials, such as CIGS, Zn_2P_3, Sb_2Se_3, and Si, were also efficient, but ZnTe outperformed in all indicators (Voc, Jsc, FF, η).

This remarkable improvement demonstrates the importance of engineering the back-cell interface and selecting materials with suitable optical and electrical properties, especially in terms of high energy gap, electronegativity, and conductivity, which enhance photon reflection and reduce non-radiative recombination.[16].

Table (2) Cell outputs after adding the reflection layer

Reflection layers	Voc(v)	Jsc(mA/cm2)	FF%	%
Original after zeroing the resistors	0.654262	20.5329	83.5651	11.2261
so	0.682671	20.69662577	80.2348	11.3364
Sp2Se3	0.78604	21.087749	80.9536	13.4187
Zn2P3	0.823532	20.59277912	84.7003	14.3642
CIGS	0.859979	20.559552	86.3683	15.2706
ZnTe	1.592214	21.163409	86.8277	29,258

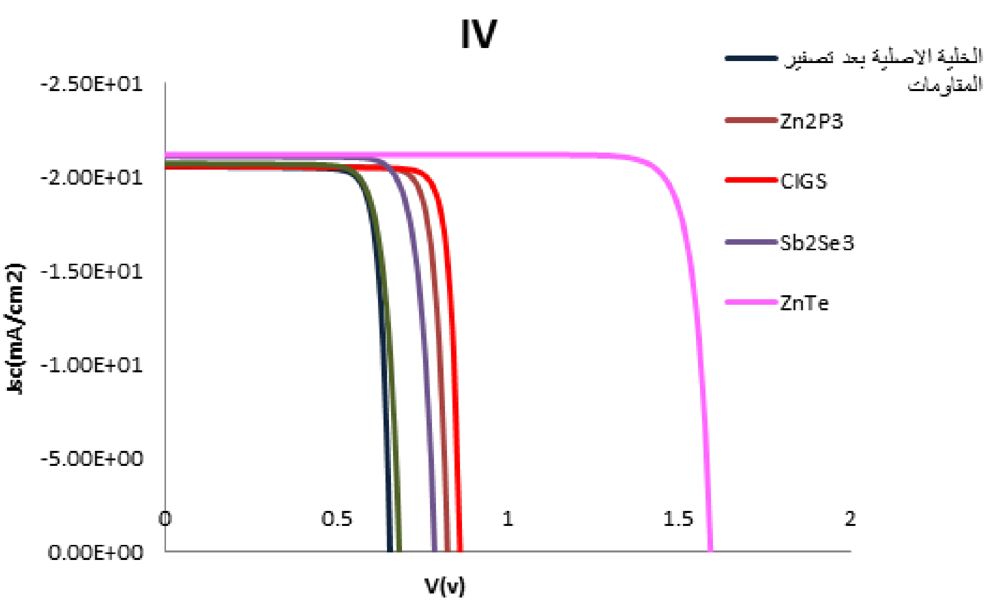

Figure (3) Current-voltage relationship after adding the back reflection layer

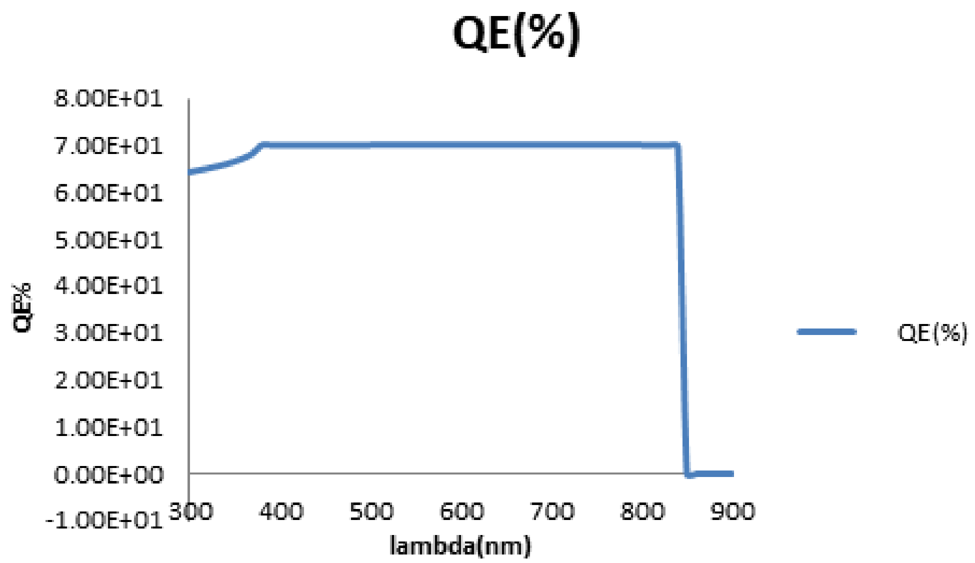

Figure (4) Quantum efficiency of the best back reflection layer (ZnTe)

4-3 Results of changing the thickness of the reflection layer ZnTe

After finding out that the material ZnTe represents the ideal choice as a backscatter layer. A series of simulations were conducted to analyze the effect of varying the thickness of this layer on solar cell performance. This analysis aimed to determine the optimal thickness that achieves the highest possible efficiency without causing optical losses or unwanted optical interference effects.

The study included modifying the thickness of the layer. ZnTe in a very fine range (between 1.602 and 1.608 μm). The results showed high stability in current ($J_{sc} \approx 21.163$ mA/cm²) and voltage ($V_{oc} \approx 1.602$–1.608 V), reflecting ZnTe's ability to maintain effective reflection within this range. The fill factor (FF) also showed a slight improvement with increasing thickness, reaching a peak value of 86.91%.

More importantly, the conversion efficiency (η) reached its highest value at 29.5121% when the thickness was 1.607827 μm, which is the maximum efficiency recorded in this study. Beyond this value, the efficiency showed a slight tendency towards decreasing despite constant current and voltage, indicating that excessive thickness may lead to unfavorable optical interference effects, or to weakening of electrical transport from the back layer towards the contacts[17].

Based on these results, it can be concluded that there is an optimum thickness for the layer.ZnTe, ranging approximately from 1.60 to 1.61 µm, ensures the highest possible conversion efficiency without negatively affecting other photovoltaic properties.

Table (3) Cell outputs when changing the thickness of the reflection layer (ZnTe)

%	FF%	Jsc(mA/cm2)	Voc(v)	layer thickness
29.5121	86,731	21.163408	1.607827	0.01µ*m*
29,463	86.8914	21.163409	1.602193	0.03µ*m*
29.4638	86.8975	21.163409	1.602123	0.05µ*m*
29.4662	86.9045	21.163409	1.602126	0.07µ*m*
29.4684	86.9107	21.163409	1.602132	0.09µ*m*

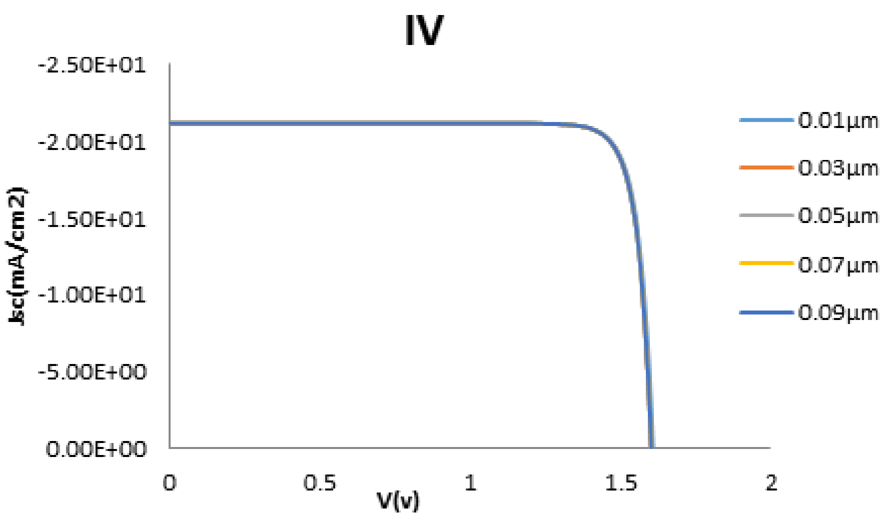

Figure (5) Current-voltage relationship when changing the thickness of the reflection layer (ZnTe)

4-4 Reflection layer doping results

In this phase of the study, the effect of doping the back-reflection layer on solar cell performance was analyzed.

The electronic structure of the reflective layer was modified by introducing acceptor or donor impurities in specific proportions. The goal of this step is to improve electrical conductivity and control the energy compositions at the interface between the reflective layer and the absorber layer, leading to improved carrier transport and reduced recombination rates.

Four materials used as back reflection layers were compared:Si, Sb_2Se_3, CIGS, and ZnTe, with the thickness uniform for all samples at 0.05 μm. The results showed that the doped ZnTe material has the highest energy gap (Eg = 2.2 eV), a feature that allows it to act as an effective barrier that prevents electron leakage to the back layer and enhances internal reflection.

Also ZnTe has excellent electronic properties in terms of electronegativity (3.73 eV), high electron velocity (3.2×10^7 cm/s), and high mobility (μ_e = 330 cm²/V·s and μ_h = 80 cm²/V·s), all of which support fast and efficient carrier transport and reduce the probability of recombination in the back layer[20].

Compared to other materials such as compared to Si or CIGS, doped ZnTe showed better matching in terms of effective density of states in the conduction band (CB) and valence band (VB), which contributes to improved voltage stability and easier charge extraction.

Table (4)Performance results of reflection layers after doping

The material	Voc (V)	Jsc (mA/cm²)	FF (%)	η (%)
Without reflection layer	0.654262	20.5329	83.5651	11.2261
Yes	0.682671	20.6966	80.2348	11.3364
Sb_2Se_3	0.786040	21.0877	80.9536	13.4187
Zn_2P_3	0.823532	20.5928	84.7003	14.3642
CIGS	0.859979	20.5596	86.3683	15.2706
ZnTe	1.592214	21.1634	86.8277	29.2580

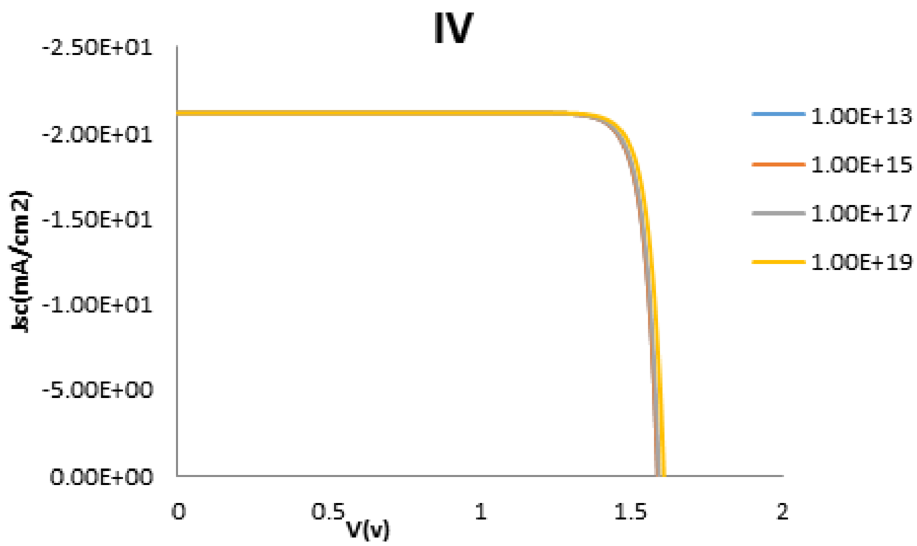

Figure (6) Current-voltage relationship when doping the reflection layer (ZnTe)

Conclusions

The study showed that introducing a back-reflection layer is a key factor in improving solar cell efficiency, as it contributed to increasing voltage, current, and fill factor. It was found that the material ZnTe was the most effective of the materials tested, achieving the highest efficiency of 29.26%. Variable thickness results also demonstrated that there is an optimal thickness that achieves the best performance without introducing additional losses. Doping the reflective layer confirmed its role in improving electronic properties and reducing losses. Therefore, controlling the reflective layer properties in terms of material, thickness, and doping is key to improving the efficiency of thin-film solar cells.

References

1. Green, MA, et al. (2020). Solar cell efficiency tables (version 56). Progress in Photovoltaics: Research and Applications, 28(7), 629–638

2. Parida, B., Iniyan, S., & Goic, R. (2011). A review of solar photovoltaic technologies. Renewable and Sustainable Energy Reviews, 15(3), 1625–1636.

3. Nair, M. T. S., & Nair, K. K.

(2001). ZnSnS thin films as a window layer in solar cells. Semiconductors and Semimetals, 65, 247–297.

4. Islam, M. T., et al. (2022). Simulation-based performance enhancement of Cu-based absorber solar cells. Journal of Materials Science: Materials in Electronics, 33(4), 2560–2573.

5. Krishnan, B., et al. (2018). Thickness optimization of absorber layers in thin film solar cells. Solar Energy, 176, 263–271.

6. Wang, W., et al. (2017). Optical management with back reflectors in thin-film solar cells. Journal of Applied Physics, 121(6), 063102.

7. Islam, R., & Hossain, M. (2021). Enhancement of solar cell performance using ZnTe as BSR. Optik - International Journal for Light and Electron Optics, 242, 167230.

8. Kumar, M., et al. (2019). Analysis of different back surface reflectors for thin-film solar cells. Materials Today: Proceedings, 18, 3902–3908.

9. Chen, S., et al. (2012). Doping strategies for thin-film solar cells. Advanced Energy Materials, 2(5), 591–596.

10. Mallick, S., et al. (2023). Effect of doping concentration on solar cell performance: A numerical study. Journal of Physics: Conference Series, 2438, 012003.

11. Jehad, A. K., & Hamammu, I. M. (2013). Computer simulation on solving Poisson’s equation for the silicon solar cell. ICECE 2013, Benghazi, Libya. https://www.researchgate.net/publication/329192018

12. Würfel, P., & Würfel, U. (2016). Physics of Solar Cells: From Basic Principles to Advanced Concepts (3rd ed.). Wiley-VCH. ISBN: 978-3-527-41203-2

13. Vedel, C. D., Gunst, T., Smidstrup, S., & Georgiev, V. P. (2023). Shockley–Read–Hall recombination and trap levels in $In_{0.53}Ga_{0.47}As$ point defects from first principles. Physical Review B, 108(9), 094113. https://doi.org/10.1103/PhysRevB.108.094113

14.Suthar, D., et al. (2022). An overview on the role of ZnTe as an efficient interface in CdTe thin film solar cells. Materials Advances, 3(10), 2022.

15.Khosroabadi, S., & Keshmiri, S. H. (2014). Design of a high efficiency ultrathin CdS/CdTe solar cell using back surface field and backside distributed Bragg reflector. Optical Express, 22(A921–A929).

16.Chaure, N.B., et al. (2023). Copper doping effect in the back surface field layer of CdTe thin film solar cells. Results in Physics, 42, 105985.

17.Padmanabhan, B., Ashok, A., Vasileska, D., & Zhang, Y.-H. (2009). Drift diffusion modeling of solar cells. AIP Conference Proceedings, 1199(1), 501–502. https://doi.org/10.1063/1.3273449