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Numerical Simulation to Study The Effect Of Reflection Layers on Solar Cell Efficiency $CH_3NH_3Pbx_3$

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Abstract :

This research deals with the study and simulation of a perovskite-based solar cell ($CH_3NH_3PbX_3$) using SCAPS-1D software, to analyze and improve their conversion efficiency by introducing multiple back-reflection layers, and to test the effect of the type and thickness of these layers on the cell's photovoltaic performance. The simulations were performed using a conventional cell structure, then gradually modified by adding materials such as Sb_2Se_3, Si, SnS, CIGS, Sb_2S_3, and ZnTe, and the results of each were compared with the original cell.

The results showed that some materials were more effective than others in improving cell performance, with the layer outperforming ZnTe is clearly shown to have the highest conversion efficiency of about 28.4% at an optimal thickness (1.42 µm). It was also shown that the improvement of open voltage (Voc), short-circuit current (Jsc) and fullness factor (FF) was possible by using materials with a wide bandgap and optical and electrical compatibility with the perovskite layer.

The study also demonstrated that the thickness of the back-reflection layer plays a significant role in enhancing the absorption of long-wavelength photons, reducing optical loss, and improving carrier collection. However, it was noted that there is an optimal limit to this thickness, as increasing it beyond a certain level does not lead to significant additional improvement and may even cause increased resistance or internal losses.

Keywords: Perovskite, Solar Cells, SCAPS-1D Simulation, Back Surface Reflector (BSR), Photovoltaic Efficiency Enhancement, Thin Film Optoelectronics.

محاكاة عددية لدراسة تأثير طبقات الانعكاس الخلفي على كفاءة الخلية الشمسية $CH_3NH_3Pbx_3$

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مستخلص:

تناول هذا البحث دراسة ومحاكاة خلية شمسية ذات أساس بيروفسكايت ($CH_3NH_3PbX_3$) باستخدام برنامج SCAPS-1D، بهدف تحليل وتحسين كفاءتها التحويلية من خلال إدخال طبقات انعكاس خلفي متعددة، واختبار تأثير نوع وسماكة هذه الطبقات على الأداء الكهروضوئي للخلية. تمت المحاكاة باعتماد بنية خلية تقليدية، ثم تعديلها تدريجيًا بإضافة مواد مثل Sb_2Se_3، Si، SnS، CIGS، Sb_2S_3، وZnTe، مع مقارنة نتائج كل منها مع الخلية الأصلية.

أظهرت النتائج أن بعض المواد كانت أكثر فعالية من غيرها في تحسين أداء الخلية، حيث تفوقت طبقة ZnTe بشكل واضح، مسجلة أعلى كفاءة تحويلية بلغت حوالي 28.4٪ عند سماكة مثالية (~1.42 µm) كما تبين أن تحسين الجهد المفتوح (Voc) والتيار القصير (Jsc) وعامل الامتلاء (FF) كان ممكنًا من خلال استخدام مواد ذات فجوة طاقية واسعة وتوافق بصري وكهربي مع طبقة البيروفسكايت.

كذلك، أوضحت الدراسة أن سماكة طبقة الانعكاس الخلفي تلعب دورًا كبيرًا في تعزيز امتصاص الفوتونات الطويلة الموجة، وتقليل الفقد الضوئي، وتحسين جمع الحاملات. ولكن لوحظ أن هناك حدًا أمثل لهذه السماكة، إذ إن زيادتها بعد مستوى معين لا تؤدي إلى تحسن إضافي ملموس، بل قد تسبب زيادة في المقاومة أو الخسائر الداخلية.

الكلمات المفتاحية: البيروفسكايت، الخلايا الشمسية، محاكاة SCAPS-1D، السطح الخلفي (BSR)، كفاءة الخلايا الكهروضوئية، الإلكترونيات الضوئية للأغشية الرقيقة.

1-Introduction

Global interest in renewable energy sources has grown in recent decades due to the environmental challenges associated with fossil fuels, which has stimulated the search for clean and efficient alternatives. Among these alternatives, perovskite-based solar cells have emerged.($CH_3NH_3PbX_3$) is considered one of the most promising technologies due to its high efficiency and relatively low manufacturing cost compared to conventional cells such as monocrystalline silicon [1,2].

Perovskites exhibit remarkable optical and electrical properties, including a tunable bandgap, high light absorbance, and efficient electron and hole transport. This has led to record power conversion efficiencies exceeding 25% in less than a decade, an unprecedented growth rate in the history of solar cell technologies [3,4]. However, improving the efficiency of these cells remains an open area of research, particularly through improved layer structure design and the addition of functional layers such as back-reflection layers [5].

Numerical simulation plays a pivotal role in accelerating the development of solar cells, with tools such as theSCAPS-1D is an effective method for studying the impact of different parameters on the ultimate cell performance without the need for expensive or complex experiments [6,7]. This helps explore the potential effects of changing thicknesses, material types, and structural modifications without compromising the main active material.

In this research, the program was used (SCAPS-1D) is used to simulate a perovskite solar cell with the addition of multiple back-reflection layers, in order to study its effect on the photovoltaic performance, and measure the change in parameters such as: short-circuit current (Jsc), open-circuit voltage (Voc), fullness factor (FF), and total conversion efficiency (η). The study aims to provide an improved structure that contributes to raising the cell efficiency in line with practical solar energy applications [8,9].

In addition, the effect of changing the thickness of the back-reflection layer was evaluated. ZnTe, in order to determine the optimal thickness that leads to the highest possible efficiency.

This study is an advanced simulation that contributes to a deeper understanding of the interaction of light with the layered structure of the cell, improving the collection of photo carriers , and reducing losses [10].

2-Simulation method

This study was conducted using the program (SCAPS-1D) (Solar Cell Capacitance Simulator), developed by Ghent University in Belgium, is one of the most widely used programs for simulating multilayer solar cells. The program solves three fundamental equations: the Poisson equation, the continuity equation, and the electric current equation, to model the electrical distribution, generation, and transport of charge within the cell. SCAPS-1D is capable of simulating cells with three main active layers and allows for the input of all physical, optical, and electrical properties with high accuracy, making it a powerful tool for analyzing and optimizing solar cell performance.

The simulation was prepared according to the following steps:

1. The solar cell is designed using perovskite .$CH_3NH_3PbI_3$ as a light absorbing layer.
2. It was used TiO_2 as an electron transport layer (ETL) and Spiro-OMeTAD as a hole transport layer (HTL).
3. Six different types of materials were introduced into the rear reflective layer (BSR)
4. Sb_2Se_3, Si, SnS, CIGS, Sb_2S_3, ZnTe, to compare their effect on cell performance As shown in Table (1).
5. All other parameters were held constant during the change of backing material to ensure an objective assessment of the effect of each material.
6. The physical properties entered for each layer included:
7. Energy gap (Eg), relative permittivity (εr), charge mobility (μ))Effective density of states of the stateNc, Nv), impurity concentration (ND, NA), and layer thickness (thickness).
8. Additional analysis was performed on the effect of layer thickness. ZnTe, where the thickness was changed from 1.39 μm to 1.42 μm to determine the optimum value.

9. All simulations were performed under standard solar radiation of typeAM1.5G, radial power 100 mW/cm², constant temperature 300 K.
10. The photovoltaic parameters extracted from the simulation included:

Open circuit voltage (Voc), short-circuit current (Jsc), fullness factor (FF), and conversion efficiency (η

The results showed that materials with a wide energy gap and a high reflection coefficient, such asZnTe and Sb_2S_3 showed the best performance when used as a back reflection layer.

Table (1) Parameters of back-reflection layers

Parameters	symbol (unit)	Sb2Se3	Si	SnS	CIGS	Sb2S3	ZnTe
Thickness	W(μm)	0.05	0.05	0.05	0.05	0.050	0.05
Bandgap	Eg (ev)	1.2	1.12	1.1	1.05	1,600	2.2
Electron affinity	χ (ev)	4.04	4.05	4.2	4.14	3,700	3.73
Dielectric permittivity	ϵr	18,000	11.9	12.5	10	7,080	10.3
CB effective density of states	$N_C(c)m^{-3}$	2.2E+18	E+192.580	E+191,000	E+181,000	2.630E+19	1.7E+18
VB effective density of states	$N_v(c)m^{-3}$	1.8E+19	E+192.650	E+194.130	E+181,000	2,250E+19	1.16E+19
Electron thermal velocity	V_n (cm/s)	1.000E+7	E+71,000	E+71,000	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	E+71,000	E+71,000	1.5E+7
Electron mobility	μ_n(c/vs) m^2	1.5E+1	E+31.350	E+12.500	E+13,000	5,000E+1	3.3E+2
Hole mobility	μ_p(c/vs) m^2	5.1E+0	E+24.500	E+21,000	E+11,500	1,000E+1	8E+1
Shallow uniform donor density	ND (1/cm3)	0	0	0	0	0	0
Shallow uniform acceptor density	NA (1/cm3)	1E+17	1E+17	1E+17	1E+17	1E+17	1E+17

3- Physical models and equations

To understand the working mechanism of a perovskite solar cell, it is necessary to analyze the physical aspects related to charge transport, voltage distribution, photo generation, and recombination. Therefore, a set of fundamental physical equations is used in numerical simulations to represent cell behavior.[13,12,11].

1-EquationPoisson's Equation

This equation is used to calculate the electrostatic distribution of electric potential within the layered structure of a solar cell. The net charge density at each point within the material is related to the electric potential, according to the relationship:[11]

$$\nabla^2\varphi = -\frac{q}{\varepsilon} \dots\dots\dots (1)$$

2-EquationContinuity Equations

These equations describe the relationship between the change in charge concentrations (electrons and holes) with time and the rates of generation, recombination, and transport currents.[12]

$$\frac{dn}{dt} = \left(\frac{1}{q}\right)\nabla \cdot J_n + G - R \dots\dots\dots (2)$$

$$\frac{dp}{dt} = -\left(\frac{1}{q}\right)\nabla \cdot J_p + G - R \dots\dots\dots (3)$$

3-Drift-Diffusion Equations

These equations are used to calculate the current density resulting from the movement of charges via conduction and diffusion:[13]

$$J_n = q \cdot n \cdot \mu_n \cdot E + q \cdot D_n \cdot \nabla n \dots\dots\dots (4)$$

$$J_p = q \cdot p \cdot \mu_p \cdot E - q \cdot D_p \cdot \nabla p \dots\dots\dots (5)$$

4-EquationShockley–Read–Hall Recombination

Recombination is the process by which charge carriers (electrons and holes) are lost within a solar cell, with electrons returning from the conduction band to the valence band and vanishing, preventing them from contributing to the generation of electrical current.[14]

$$R_{SRH} = \frac{np - n_i^2}{\left[\tau_{p(n+n_i)} + \tau_{n(p+n_i)}\right]} \dots\dots\dots (6)$$

5-EquationPhotosynthesis (Generation Rate)

It refers to the process of generating electrons and holes as a result of the absorption of light in the absorbing layer. When a photon penetrates the material and has an energy higher than the energy gap (Eg), is absorbed and causes an electron to move into the conduction band, leaving a hole in the valence band.

$$G(x) = \alpha \cdot I^0 \cdot e^{-\alpha x} \ldots\ldots\ldots(7)$$

6-EquationEfficiency

Count efficiency of converting solar energy into electricity.[16]

$$\eta = \frac{V_{oc} \cdot J_{sc} \cdot FF}{P_{in}} \ldots\ldots\ldots(8)$$

7-FactorFill Factor

The fill factor is an indicator of the quality of cell performance, and expresses the ratio of the actual power generated by the cell to the maximum power that can be theoretically generated (i.e. the product ofVoc and Jsc The closer FF is to 1 (or 100%), the more the cell has a low internal resistance and an ideal voltage-current curve.[11]

$$FF = \frac{V_{mpp} \cdot J_{mpp}}{V_{oc} \cdot J_{sc}} \ldots\ldots\ldots(9)$$

4- Results and discussion

Simulation results show that adding back-reflection layers to perovskite solar cells resulted in varying improvements in photovoltaic performance. These improvements were related to a set of physical factors associated with each material, most notably: energy bandgap, optical behavior, structural and electrical compatibility, reflection coefficient, and layer thickness.

4-1 Effect of back-reflection layers

1-Original cell performance for Without back reflection layer

When simulating a perovskite solar cell without introducing any back reflection layer, its performance was shown to exhibit moderate photovoltaic properties, reflecting the natural limitations of a conventional cell structure. The open-circuit voltage (Voc) is approximately (0.8478 V), which is a value that reflects the quality of the absorbing layer in terms of generating a potential difference as a result of absorbing photons.

The resulting current in the short circuit condition (Jsc) reached (17.65 mA/cm^2), which is a result of light absorption within the active layer, but it is still relatively modest, indicating that a portion of the incident light was lost as a result of passing to the rear layers without being absorbed or utilized. Also, the Fill Factor (FF) reached about (82.7%), indicating the presence of non-ideal internal resistances in the cell structure.

Based on these data, the overall conversion efficiency was calculated (η) was about (12.38%), which is a theoretically acceptable result, but it remains below the target level for high-efficiency solar cell applications. This is likely due to the absence of an effective mechanism for recovering unabsorbed photons, which could contribute to their reabsorption through the active layer [14].

These results justify the need to improve the backside structure of the cell by introducing a reflective layer that reflects light leaking from the backside, thus enhancing the chance of it being reabsorbed into the active material, thus increasing the number of photocarriers produced and raising the conversion efficiency.

2-layer Sb_2Se_3 as a back reflection layer

When adding a layer of material using Sb_2Se_3 at a suitable thickness as a back-reflection layer in the perovskite solar cell structure, a significant improvement in cell performance was observed compared to the original state. The open-circuit voltage (Voc) increased to a value of approximately 0.9094 V, indicating improved electron-hole separation and reduced back-recombination.

The resulting current in the short circuit condition (Jsc) remained close to the original value, which was (17.65 mA/cm²), indicating that most of the improvement resulted from the recovery of some light photons and the improvement of the resulting voltage, and not necessarily an increase in the total generation of electrons[15].

Moreover, the fullness factor (FF) at a good level of (82.49%), indicating that the introduction of the layer did not cause a deterioration in the internal balance of the cell or in its series resistances.

More importantly, the conversion efficiency (η) has increased to about (12.20%), which is a slight increase compared to the original case, but it shows the positive role of the Sb_2Se_3 layer in enhancing the overall performance of the cell.

3-layer Si as a back reflection layer

In an attempt to employ the silicone material (Using Si as a back-reflection layer, the results showed that the cell performance did not show a significant improvement compared to the original case. The open voltage (Voc) after layer insertion was approximately 0.8380 V, which is lower than the voltage obtained when using the Sb_2Se_3 layer, and even slightly lower than the original case, indicating the possibility of an interface mismatch between the silicon and perovskite, or the occurrence of photo carrier recombination.

As for the short current (Jsc) remained almost the same at 17.65 mA/cm², indicating that silicon was not effective in reflecting photons or improving absorption.

As for the fullness factor (FF), it was fixed at about (82.49%) without change, which reflects the stability of the general electrical properties of the cell in terms of its resistances and limiting voltage[16].

But in return, the conversion efficiency decreased (η) to approximately (12.20%), which is slightly lower than the original efficiency. This can be explained by the fact that silicon, despite being a well-known semiconductor material, its relatively narrow energy bandgap (Eg ≈ 1.12 eV) and its imperfect matching with perovskites may have led to it absorbing part of the light instead of reflecting it, causing additional losses.

These results suggest that using silicon as a back-reflection layer in perovskite cells may not be the best option, and that the focus should be on materials with larger bandgaps and better interface compatibility.

4-layer SnS as a back reflection layer

The results showed that introducing a layer of material SnS within the back structure of the solar cell led to a significant improvement in photovoltaic performance compared to the original state. The open voltage (Voc) increased to a value of approximately 0.9545 V, an indication of improved charge separation and reduced recombination rates in the back region of the cell.

The short current also increased (Jsc) to reach about (17.74 mA/cm²), which reflects an improvement in photon collection, and perhaps a higher ability of the SnS layer to reflect a larger portion of the light passing without absorption.

The fullness factor was recorded (FF) slightly increased to (83.39%), indicating an improvement in the quality of the cell's internal communications and a slight decrease in series resistances, which are good indicators of more stable performance[17].

As for the conversion efficiency (η) witnessed a significant jump, reaching about (14.12%), which is a clear improvement compared to previous values, and reflects the effectiveness of the SnS layer in redirecting photons towards the active layer.

This improvement is attributed to the structural and electrochemical compatibility between the layer.SnS and the perovskite layer, in addition to their favorable energy gap (Eg ≈ 1.1 eV), prevent light absorption and allow it to be reflected effectively inward. The excellent optical properties of SnS, such as a high reflectance coefficient at long wavelengths, also contribute to reducing loss and increasing the overall absorption efficiency.

5-layer CIGS as a back reflection layer

The results showed that using a layer of material CIGS (copper-indium-gallium-selenide) on the back side of the solar cell resulted in a further and significant improvement in photovoltaic performance. The open circuit voltage (Voc) rose to a value of approximately 1.0095 V, which is higher than all previous values, indicating high efficiency in preventing back recombination and improving the quality of charge separation[17].

The resulting current in the short circuit condition (Jsc) recorded a value of approximately (17.97 mA/cm²), which indicates an increase in the total absorption thanks to the ability of the CIGS layer to reflect long-wave photons, which increases the possibility of their reabsorption within the perovskite.

The fill factor also increased (FF) to a good level of (83.92%), which reflects stable electrical performance and improvement in the quality of internal connections between layers[18].

As for the conversion efficiency (η) witnessed a clear increase to reach (15.22%), which is one of the highest values recorded so far in this study.

This improvement is attributed to the distinct properties of the material.CIGS, which has a suitable energy gap (Eg ≈ 1.05 eV) and good optical properties, is also relatively structurally compatible with other semiconductor materials in terms of refractive index and permittivity. The high ability of this layer to reduce backlight losses also plays an important role in enhancing charge collection.

6-layer Sb_2S_3 as a back reflection layer

When inserting a layer of material using Sb_2S_3 on the back side of the perovskite solar cell, the results showed a significant improvement in photovoltaic performance, reflecting the material's effectiveness as a light-reflecting layer. The open-circuit voltage (Voc) rose to a relatively high value of approximately 1.1696 V, one of the highest values recorded in the study, demonstrating a significant reduction in the back recombination rate and enhanced electron-hole separation.

The resulting current in the short circuit condition (Jsc) reached (21.76 mA/cm^2), which is a significant increase compared to previous cases, indicating that the Sb_2S_3 layer was very effective in redirecting unabsorbed photons towards the active layer, which led to an enhancement in the photo generation rate[18].

The fullness factor also increased . (FF) to a good value of approximately (82.82%), which indicates that the electrical properties remain stable without negative effects from the new layer.

All this was clearly reflected in the conversion efficiency (η) which reached about (21.08%), which is a qualitative leap compared to the original state, and proves that Sb_2S_3 is a very promising material in this context.

This improvement is due to the unique optical and electrical properties of the material .Sb_2S_3, which has a favorable energy gap ($Eg \approx 1.6$ eV) and suitable optical behavior to reflect light without absorbing it, as well as being easy to integrate with other cell layers without creating a large lattice or electrostatic mismatch.

7-layer ZnTe as a back reflection layer

Simulation results showed that introducing a layer of ZnTe on the backside of the cell led to exceptional improvements in photovoltaic performance, with the cell recording its best results under this condition. The open-circuit voltage (Voc) rose to a high of approximately 1.3961 V, the highest voltage recorded in all formulations, indicating a significant reduction in recombination and a significant enhancement in photovoltaic stability[19].

The resulting current at the short circuit was also recorded ((Jsc) had a very high value of about (22.26 mA/cm²), which reflects ZnTe's great ability to reflect photons and improve internal absorption, especially in the medium and long wavelength range.

As for the fullness factor (FF) has reached (85.37%), which is one of the highest values recorded, reflecting a decrease in internal resistances and an improvement in the quality of connections between layers.

The most obvious effect was on conversion efficiency (η) which jumped to a remarkable value of about (26.53%), making ZnTe the best choice among all the materials tested.

These results are attributed to the fact that ZnTe has a relatively wide bandgap (Eg ≈ 2.2 eV) and a good match in permittivity and refractive index with the absorbing layer, making it non-absorbent in the visible range but highly reflective, thus redirecting unabsorbed photons towards the perovskite layer for reabsorption. Its electronic compatibility also makes it a good transition layer that contributes to improving carrier collection efficiency[19].

Table (2) Cell results adding the back reflection layer

%Ŋ	FF%	Jsc(mA/Cm2)	Voc(v)	Layers
12.1994	82.4932	17.646684	0.909445	Sb2Se3
12.1994	82.4932	17.646684	0.838024	Yes
12.3779	82.7036	17.65400364	0.847775	original cell
14.1164	83.3864	17.736698	0.954454	SnS
15.2239	83.9174	17.970455	1.009516	CIGS
21.0808	82.8212	21.762976	1.169572	Sb2S3
26.5299	85.3742	22.25775	1.396136	ZnTe

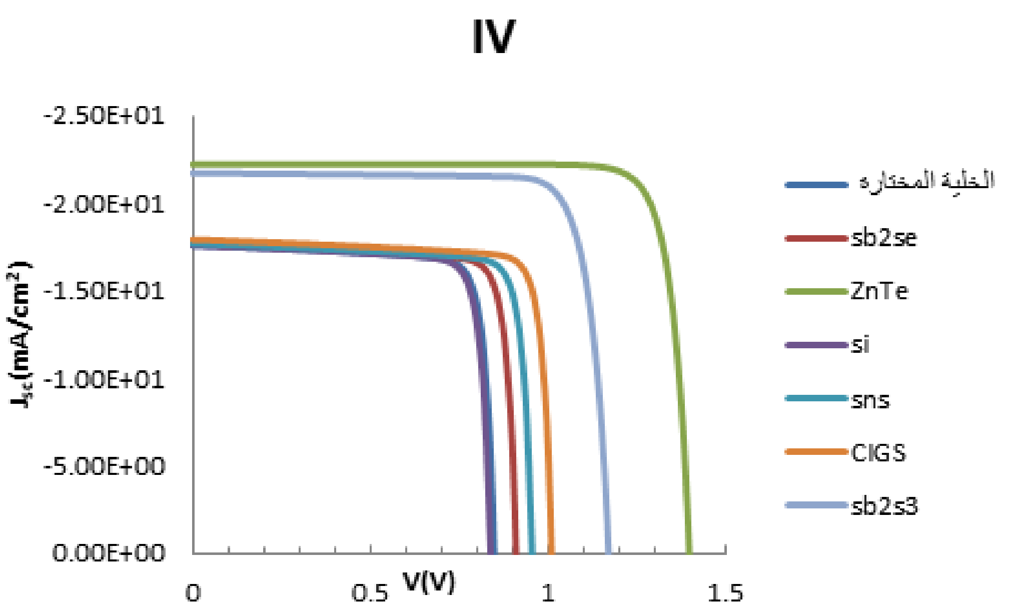

Figure (1) Current-voltage diagram after adding a back reflection layer

4-2 Impact Change layer thickness ZnTe on cell performance

After showing the layer ZnTe has high efficiency when used as a back-reflection layer. Additional simulations were performed to test the effect of varying its thickness on solar cell performance, with the goal of determining the optimal thickness that achieves the highest possible conversion efficiency.

The results showed that the gradual increase in the thickness of the layer ZnTe provided a continuous improvement in all photovoltaic parameters. As the thickness increased, the layer's ability to reflect long-wavelength photons increased, resulting in improved light absorption in the active layer. For example, when the thickness increased to values close to 1.419 µm, the open voltage (Voc) reached approximately 1.4194 V, while the short-circuit current (Jsc) rose to 22.33 mA/cm², with a fill factor (FF) of 89.65%. This resulted in a high conversion efficiency of approximately 28.41%, as shown in Table 3.

This remarkable improvement is attributed to improved backscattering, reduced optical loss, and enhanced photon reabsorption, especially at longer wavelengths that require a longer absorption path. However, it is noted that the improvement reaches a saturation point beyond a certain thickness, where the performance gains become minimal and not economically or technically feasible.

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

%Ƞ	FF%	Jsc(mA/Cm2)	Voc(v)	layer thickness
27.1034	87,114	22,2633	1.397486	0.01μm
27,772	88,657	22.2891	1.405404	0.03μm
28.0552	89,135	22.3065	1.411029	0.05μm
28.2718	89,489	22.3185	1.415533	0.07μm
28.4098	89,648	22.3272	1.419357	0.09μm

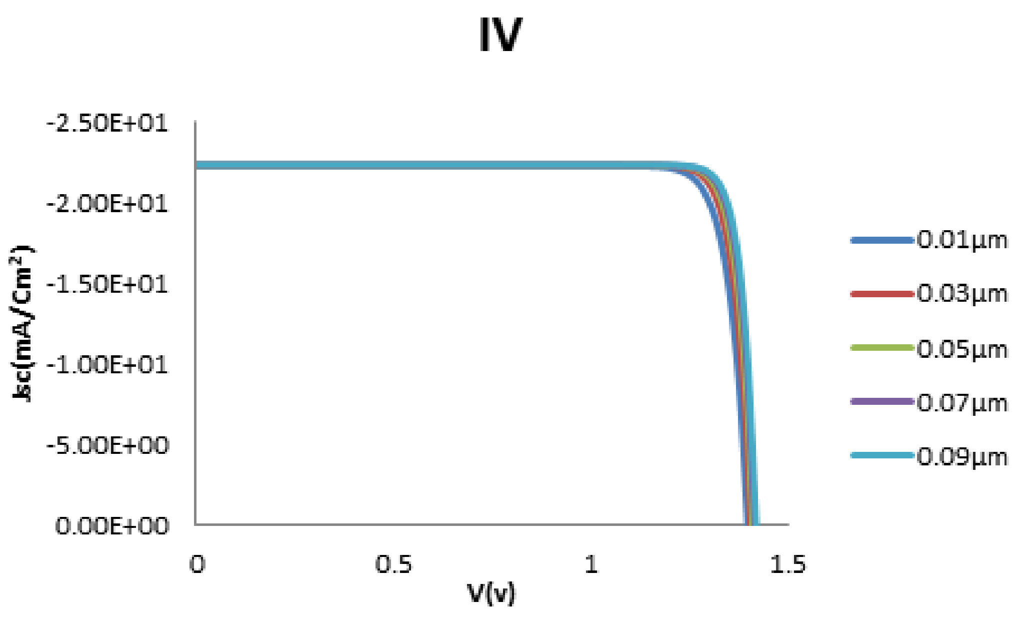

Figure (2) Current-voltage diagram when changing the thickness of the reflection layer (ZnTe)

Conclusions

Through this numerical study that was carried out using the program for SCAPS-1D, the choice of material used for this layer was shown to play a crucial role. Materials such as ZnTe, Sb_2S_3, and CIGS demonstrated superior performance in terms of increased open voltage, short-circuit current, fill factor, and, consequently, overall efficiency. ZnTe emerged as the most effective material, contributing to an efficiency increase of over 28% at optimal thickness, indicating the potential for performance exceeding the theoretical limit of conventional perovskite cells.

The study also showed that the thickness of the reflective layer is a very important variable, as increasing it within a certain range led to improved light absorption, while exceeding this range led to stable or even slight decline in performance due to increased resistance or optical loss.

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