



Modeling and Numerical Simulation of a Sb_2Se_3 Solar Cell Device Considering the Photovoltaic Effect on the Absorber Layer

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Abstract

Solar cells are considered photovoltaic devices regardless of the light wavelength they absorb. Electromagnetic energy in the visible spectrum, such as visible light, is detected by photodetectors (for example, infrared detectors). In distant areas of developing nations, tiny solar cells may power anything from household appliances to satellites, outdoor lighting, and even refrigeration for medicines. Evaluations of the proposed Sb_2Se_3 -based solar cell technology have been conducted quantitatively and in terms of yield. Fluorine Doped Tin Oxide (FTO), zinc oxide (ZnO), cadmium telluride (CZTSe), and gold make up a solar cell based on Sb_2Se_3 (Au). The photovoltaic effect of the proposed Sb_2Se_3 -based solar cell device on its Sb_2Se_3 layer is also explored (i.e., absorber layer).

The research also discusses how the thickness of the absorber layer or the Sb_2Se_3 layer impacts the Performance of solar cells. The Performance of Sb_2Se_3 -based solar cells with bulk Sb_2Se_3 defects has also been documented, and it has been demonstrated that the thickness of the absorber layer in Sb_2Se_3 -based solar cell devices impacts the quantum efficiency of the suggested device. The proposed Sb_2Se_3 -based solar cell's open-source voltage is 8.62mV, short circuit current is 2.47mA/cm², fill factor is 656.9, and power conversion efficiency is 20.94%, it can be concluded.

Keywords: Photovoltaics (PV), Power Conversion Efficiency (PCE), Chemical Bath Deposition (CBD), antimony selenide (Sb_2Se_3), Sodium-Ion Battery (SIB).

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1. Introduction

Researchers in photovoltaics (PV) face difficulties with both the power conversion efficiency (PCE) and the selection of a wide variety of inexpensive, environmentally friendly materials for mass production. Silicon solar cells continue to dominate the commercial markets despite having the highest PCE in 2017 [1]. Due to the material's high melting point and little tolerance for production mistakes, processing silicon requires a high-priced environment. Concerns include declining domestic use due to traditional solar cells' fragility and escalating wafer-based silicon solar cell production prices. Scientists looked into simple production methods and new materials to aid in the evolution of cells. Several solar cells have recently become popular due to their high efficiency [2]. Among the many renewable energy options, a PV system has a lot of untapped potentials to meet the growing global need for electricity. When the sun's rays hit a PV device, also known as a solar cell, they are converted into electricity. Since the discovery of the PV effect in 1839, scientists have focused on developing PV technology that uses solar cells to improve PCE at a cheaper cost. Recent years have seen significant progress made in the study of both organic and inorganic solar cells. Four generations of solar cells have been manufactured, each distinguished by the semiconductor materials used in their manufacture and the timeline of their introduction to the market. Silicon (Si) cells were one type of first-generation solar cell. Compared to later generations, first-generation solar cells perform better in efficiency and durability [3]. Antimony chalcogenide solar cells are increasingly popular because of their superior physical properties and environmentally benign attributes (high element availability and low toxicity).

Environmental deterioration and energy constraints have worsened due to rapid population growth and robust industrial activity. There has been a lot of focus on green renewable energy and water pollution technology. Compared to other methods, such as biological therapy, adsorption, ozonation, and electrochemical oxidation, semiconductor-based photocatalysis is more effective, cheaper, and less harmful to the environment [4]. The effectiveness of photocatalysis is measured by how well photoinduced electron-hole pairs are

separated and transported. Most research suggests that developing a single semiconductor photocatalyst with good photocatalytic activity is challenging due to its limited light absorption capacity and high photogenic charge pair recombination rate. Hybrid heterostructures can be quickly and effectively created to boost photocatalytic activity. PV devices have attracted a lot of attention in the research and development of future global energy sources [5] due to their many advantages, such as their ability to provide constant electricity at a low operating cost, their long lifespan, the fact that they produce almost no pollution, their ease of operation, the absence of emissions or radiations, and their low maintenance requirements. For many reasons, including its high PCE, soft material cost, and suitability with mass manufacturing via vacuum deposition processes, thin-film solar cells (TFSCs) has emerged as one of the most attractive PV alternatives.

In recent decades, environmental preservation and global energy depletion issues have emerged as front and center. The future of humanity must discover renewable and environmentally friendly energy sources. Many scientists are looking into solar power because it has the potential to be a reliable, cheap, and sustainable source of clean energy for everyday usage [6]. Solar energy cannot be directly utilized in most situations without being converted into more usable energy like electricity and chemical to compensate for its low energy density and uneven distribution when it reaches Earth. The sun's rays, for instance, could power electrical devices through the use of solar cells. Scientists studying PV have difficulty deciding between various low-cost, environmentally friendly materials. Wafer-based silicon solar cells, the traditional solar technology, are becoming increasingly expensive, and their decreasing domestic use discourages investors. Researchers have been focusing on simpler production processes and new types of materials for use in cell evolution [7]. Many types of solar cells with various components and manufacturing methods have recently gained popularity due to their superior efficiency.

Sb_2Se_3 has gained attention as a potential light absorber for use in photovoltaics. In the future, thin-film solar cells will rely heavily on Sb_2Se_3 due to their unique properties, such as their low toxicity, worldwide abundance, and low cost [8]. Despite significant progress, Sb_2Se_3 thin-film solar cells' PV conversion efficiency remains considerably below theoretical norms. The accumulation of severe defects in the Sb_2Se_3 absorption layer, which act as non-radiation recombination sites and carrier traps, is a contributing factor. Because of the reduced transfer and separation rates of photogenerated non-equilibrium charges at these spots, the PV conversion efficiency of solar cell designs is decreased. Today's information age could not function without the photodetector, which finds widespread use in optical communication, imaging, and other fields. The optoelectronic sector may meet the urgent requirement for smaller devices in today's technology by developing a self-power detector [9]. However, the fabrication costs for self-biased devices are higher than for non-biased ones because of the processes involved in making the devices. Making devices that can run on their power is quick and easy with p-n junctions and heterostructures.

Because of differences in work functions, photogenerated carriers are swept by an intrinsic electric field in heterojunctions of the same or different semiconductor types [10]. Because of simple, commercialized technology, their use has expanded, and people's standard of living has increased. To prevent the recombination of photo-excited carriers, heterostructures (with varying bandgaps and closely matched lattice characteristics) are particularly useful. Recent years have seen a surge in interest in hybrid heterostructures that combine organic and inorganic (hybrid) components and inorganic and organic components. This heterostructure excels in autonomy, responsiveness, detectivity, speed, and stability of response. Tin selenide's versatility has made it the chemical of most demand. Despite its diminutive stature, the gadget proved quick to respond and recover [11].

2. Related Background

The semiconductor orthorhombic antimony selenide (Sb_2Se_3) has a smoky p-type bandgap.

It is different from anything else that is currently known due to the straight band gap, high absorption coefficient, and adjustable band holes. Because of their accessibility, affordability, and safety, Se and Sb are widely prized. Sb_2Se_3 might be beneficial as a photovoltaic (PV) material [12]. Sb_2Se_3 , an absorber layer for solar cells, was successfully produced in 2009 using a chemical bath deposition (CBD) procedure. Highly effective FTO/ TiO_2 / Sb_2Se_3 /Au heterojunction solar cells were made possible by spin-coating and low-temperature sintering. In the same year, extremely effective CdS/ Sb_2Se_3 solar cells were produced via thermal evaporation. A selenium vacancy reduction phase has been suggested to help reduce the severe defect density of selenium vacancies brought on by Se loss during the average thermal deposition of Sb_2Se_3 thin films [13]. 2015 saw the rapid thermal evaporation (RTE) of Sb_2Se_3 sheets to produce a one-dimensional crystal structure. A hole transport layer (HTL), developed in 2017 using PbS colloidal quantum dots, significantly increased performance and decreased carrier recombination loss. Utilizing vapor transport deposition (VTD), Sb_2Se_3 film deposition effectiveness and carrier transport were enhanced in 2018. In 2019, Sb_2Se_3 nanorod arrays were successfully created on a Mo electrode utilizing a close-spaced sublimation technique in the [001] direction. (CSS). Although improvements have been achieved, Sb_2Se_3 solar cells still do not have optimal open-circuit voltage or short-circuit current density [14].

2014 saw the start of research on TiO_2 -sensitized solar cells and thin-film solar cells based on TiO_2 , Sb_2Se_3 , and CdS. The result is that this material is being used by PVs more and more. It has been suggested [15] that Sb_2Se_3 ribbons arranged vertically across a one-dimensional Sb_2Se_3 sheet can improve carrier transmission. Sb_2Se_3 solar cells, the most effective solar cells currently on the market, are created using close-space sublimation. Thin-film solar cells made of Sb_2Se_3 or other Sb-containing materials demonstrate a high-power conversion efficiency (PCE). These developments have led to the Sb_2Se_3 solar cell being the de facto industry standard, demonstrating the effectiveness of Sb-containing thin-film absorbers in PV systems. Sb_2Se_3 is gaining popularity, as evidenced by

several recent academic publications. Numerous techniques, including spin coating and electrodeposition (ED), atomic layer deposition (ALD), magnetron sputtering (MS), and close-spaced sublimation (CSS), have been used successfully to manufacture Sb_2Se_3 .

In many cases, chemical deposition techniques have proven more effective than their physical counterparts [16]. Sb_2Se_3 solar cells can be made using a variety of substrates and cell designs. This superstrate structure is seen in most champion cells. The buffer/absorber interface has received particular attention in studies on the quality of heterojunctions and interfaces. In the short-wavelength market, wide-bandgap materials like ZnO and TiO_2 have replaced conventional CdS due to good band alignment lattice mismatch and reduced Cd interdiffusion. Recent research has shown that Sb_2Se_3 thin-film solar cells may be made to appear semi-transparent, making them ideal for application in energy-efficient window glazing [17].

Iodine and tin were injected into Sb_2Se_3 nanoparticles using a hot-injection technique, as reported by Lojpur V et al. [18]. It was shown that the nanoparticles could take on a spherical shape. It has been shown that even slight differences in bandgaps are not reliable markers of doping when comparing the reflectance spectra of doped and non-doped materials. Along with studying amorphous materials, researchers also analyze crystalline examples to understand the difficulties better.

Thin films of antimony sulfide selenide ($Sb_2S_xSe_3x$) were tested in heterojunction solar cells by Messina S et al. and colleagues [19] to determine if they might be used as optical absorbers. Argon was heated, and chemical deposition was used to create thin crystalline layers. A material's optical transmittance and reflectance spectra are used to calculate its refractive index and high-frequency relative permittivity. According to the optical absorbance coefficient of the film, the linear bandgap with the electrical transition is forbidden.

Mao X et al. [20] found that antimony selenosulfide ($Sb_2(S, Se)_3$) has excellent material and optoelectronic characteristics, making it a promising candidate for use in thin-film PVs. Merge the benefits of (Sb_2Se_3) alloys with the flexibility of Sb_2Se_3 alloys to alter the

bandgap. CdS are commonly employed as an electron transport layer in solar cells, allowing photogenerated electrons to be transferred from absorbers to conductive substrates. Poor contact between the ETL and absorber often leads to interface recombination. Adding an ultrathin SnO_2 buffer layer can improve the Performance of a high-roughness fluorine-doped tin oxide substrate. Solar cells based on SnO_2/CdS ETL ($Sb_2(S, Se)_3$) have a high open-circuit voltage and high efficiency. Emission efficiency can be improved by adjusting the interface contact and band offset.

According to Zhang YH et al. [21], antimony sulfide is a dangerous electrode material for sodium-ion battery (SIB) electrodes because of its low toxicity, low cost, and high theoretical specific capacity. However, electrochemical Performance is a long way off. Using a solvothermal method, a group of Sb_2Se_3 nanoneedles and nanorods self-assembled from Sb_2Se_3 microspheres. Structural characterization suggests that enlarging the distance between the planes of a material (interplanar spacing, or (1 1 0)) can significantly increase its electrochemical activity. The site's micro-nano structure synergizes on several fronts, allowing for a notable increase in salt storage efficiency.

According to Dai C et al. [22], the ideal bandgap structure and light-matter solid interaction of Sb_2Se_3 and graphene oxide (GO) make them excellent photoelectric materials for optical modulators, broadband ultrafast optical switches, and other photoelectric applications. Increased modulation depth highlights the nonlinear features of GO and Sb_2Se_3/GO measurements. Fiber lasers based on GO can simultaneously produce light at two distinct wavelengths via their harmonic dual-wavelength (HDW) mode. In addition to a wide range of wavelengths, ultrashort pulse generators may also have a wide range of frequencies. An SA mode-locked pulse is generated when Sb_2Se_3/GO is introduced into the laser cavity.

Antimony sulfide (Sb_2Se_3) photodetectors (PDs), as reported by Lai Y et al. [23], are suitable for usage in national-economic and military applications due to their high absorption coefficient. It has been possible to develop a novel form of depleted Sb_2Se_3 thin-film photoconductive detector with a TiO_2

interlayer by using the construction Au/glass/TiO₂/Sb₂Se₃/Au. Increases in responsiveness and selectivity over standard Au/Sb₂Se₃/Au PDs are a result of using depleted Sb₂Se₃ PDs. Due to the electric field in the depletion region, the response time is drastically reduced. Sb₂Se₃ films with a solid horizontal orientation can also detect polarised light when it is anisotropic.

According to Wang Z et al. [24], Sb₂Se₃ crystals with dumbbell- and bundle-like morphologies were made by employing various amorphous-to-crystalline phase transitions. The researchers identified the most crucial factor in defining the material's shape by analyzing the solvent/surfactant ratio, reaction temperature, and reaction time. Electrochemical impedance spectroscopy, transient photocurrent-time curves, and linear sweep voltammetry are all used to evaluate charge separation. Since bundle-like Sb₂Se₃ is better at collecting light and separating charges, it was able to speed up the photodegradation of malachite green (MG). According to the intermediates into small molecules photodegradation pathway proposed for MG, the bundle-like Sb₂Se₃ was more easily changed into small molecules. The photodegradation of MG was successful when performed on Sb₂Se₃ that resembles bundles.

Zhu SH et al. [25] found that, as pressure is increased, mechanical characteristics become unstable and fail to meet mechanical stability requirements. At ambient pressure, the phonon dispersion spectrum of Sb₂Se₃ has no virtual screen. A wobbly virtual screen seems to characterize the phonon. The findings provide a theoretical basis for further investigation of Sb₂Se₃ at extreme pressure.

For an efficient photoelectrochemical (PEC) cell, an Sb gradient-doped SnO₂/Sb₂Se₃ heterostructure is discussed by Han J et al. [26], who detail the steps involved in developing this structure using an integrated, synergistic technique known as quadruple optimization. Ultrahigh electron mobility, aided by the intense visible light absorption of Sb₂Se₃ combined with SnO₂ anti-reflection, facilitates the crystallization of Sb₂Se₃ and is consistent with its crystalline structure. In photoelectrochemistry, comprehensive methods are used to create photoelectrodes.

Transition metal sulfides (TMSs) have been widely employed as photocatalytic materials

due to their high light absorption and low work function, as stated by Wang CY et al. [27] and his colleagues. However, photo activity associated with photo corrosion is often very volatile. Antimony sulfide (Sb₂Se₃) is a highly stable TMS semiconductor due to its massive microstructure. The considerable time it takes for carriers to get from the body to the surface makes photocatalysis inefficient. Ultrafine MoS₂ is synthesized on the covers of Sb₂Se₃ nanorods using a green hydrothermal process, leading to a TMS-based photocatalyst with high photoactivity for hydrogen production also, durability and stability. The heterostructure catalyst's light-harvesting capabilities are enhanced since both materials have a low bandgap. The combined electric field synergistically accelerates the motion of photocarriers in the depletion zone. This new catalyst exhibits enhanced photoactivity for hydrogen evolution under solar-like conditions compared to bare Sb₂Se₃ and MoS₂.

In their paper [28], Zhao W et al. offer a novel ultrasonic sonochemical synthesis process that can generate extreme conditions at room temperature. At first, bimetallic sulfide linked to graphene nanosheets was developed via ultrasonic processing for use in sodium-ion batteries. The produced nanocomposites exhibit exceptional electrochemical properties. Heterostructures with different bandgaps can be grown on graphene using in-situ ultrasonic irradiation, which significantly increases the material's electrochemical conductivity and salt storage capacity.

3. Proposed design of Sb₂Se₃-solar cell, working, modeling, and numerical simulation

Recent years have increased the popularity of numerical modeling of solar cell design and operation. In this case, the absorber layer is made of Sb₂Se₃, the hole transport layer is made of CZTSe, and the electron transport layer is made of ZnO. Despite this, the values of the HTL and ETL parameters did not change at any point during the simulation [29, 30].

3.1 Working on Solar Cell

Light quickly travels through the p-type layer and enters the p-n junction upon arrival. Intense photons create many electron-hole pairs in the light energy. Light impairs thermal equilibrium

[31]. As electrons are liberated in the depletion region, they can easily cross to the n-type side. Depletion holes can also quickly go to the p-type end of a wire. The barrier potential of the junction prevents newly created free electrons from crossing to the n-type side. When the intersection is close to the n-type side, the p-type side's barrier potential becomes too high for holes to overcome. The n-type side of the p-n corner in semiconductors, where electrons congregate but holes do not, serves as small battery cells. Photovoltaics is the term used to describe the resulting voltage. It has been shown that if a small load is put across the junction, just a tiny amount of current will flow [32].

3.2 Modeling of Solar Cell

The figure:1 shows the solar cell's layers from top to bottom [33-35].

- **Fluorine-coated Indium tin oxide (FTO)** acts as an anode, or light enters the cell through a window layer.

- **Zinc Oxide (ZnO)** acts as an electron transport layer.
- **Antimony Selenide (Sb_2Se_3)** acts as an active layer or absorber layer.
- **$Cu_2ZnSnSe_4$ (CZTSe)** acts as a hole transport layer. It is a quaternary compound with a Kesterite structure that works as a hole transport layer. Cu_2ZnSnS_4 (CZTSe) semiconductors are gaining popularity as light-absorbing materials in thin-film solar cells. Because their constituent components are abundant and ecologically friendly, their band gaps are close to the optimal bandgap of the light-absorber semiconductor for single-junction solar cells. They absorb a lot of visible light. In this phase, Cu, Zn, Sn, Se, and a KL-KCL combination are present.
- **Gold (Au)** is a back contact or cathode + substrate layer.

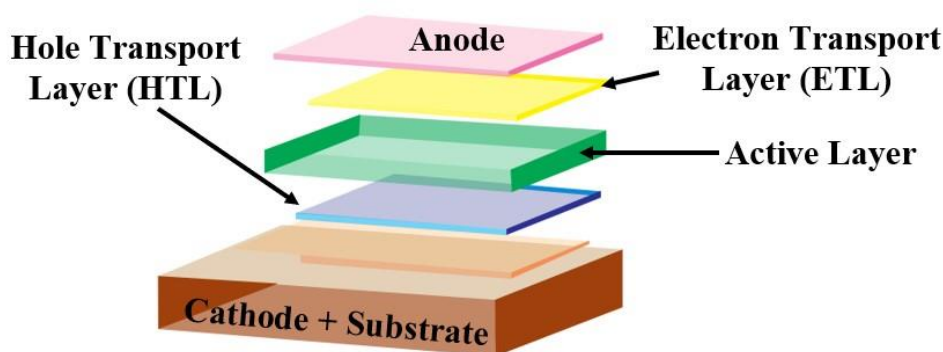


Figure:1 Proposed Design of Sb_2Se_3

4. Results and Discussions

The overall defect count, carrier concentration, and absorber layer thickness of BSF-free solar cells are evaluated. Figure: 2 demonstrates how the efficiency of solar cells, the density of defects, and the concentration of acceptors change as a function of the thickness of the

Sb_2Se_3 absorber layer. Increasing the thickness of the Sb_2Se_3 absorber layer increases photovoltaic efficiency across the board. A more significant number of electron-hole pairs (EHP) can be generated when the absorber layer is thickened. For a given absorber layer thickness of Sb_2Se_3 , there is a decreasing open-circuit voltage (VOC).

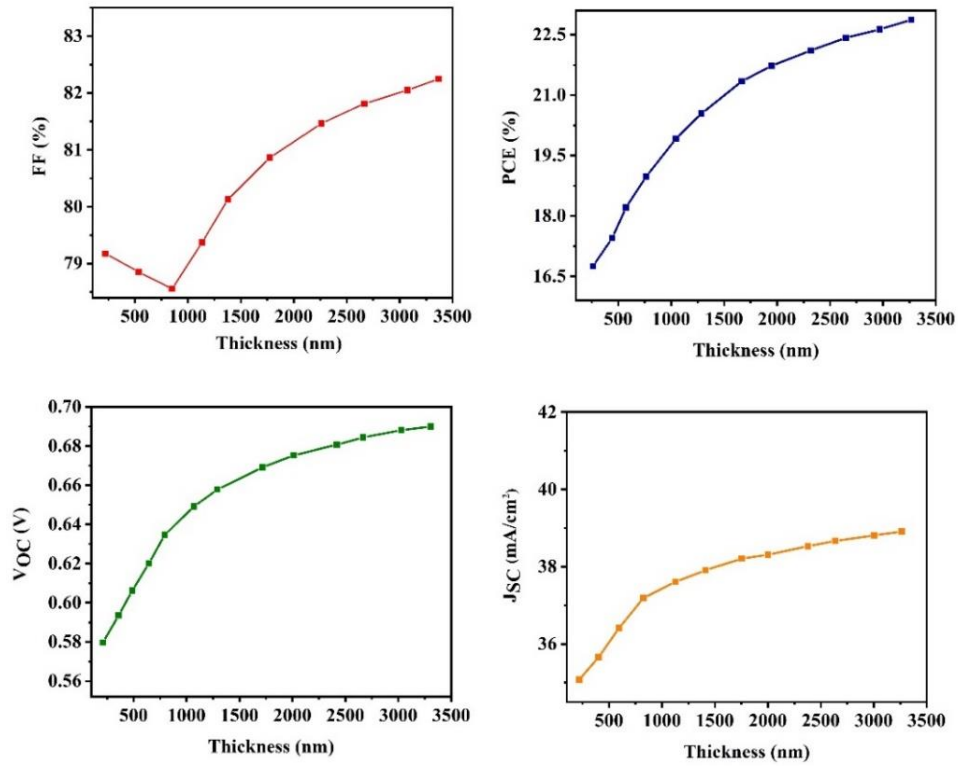


Figure:2 The Performance of solar cells is influenced by Sb_2Se_3 thickness.

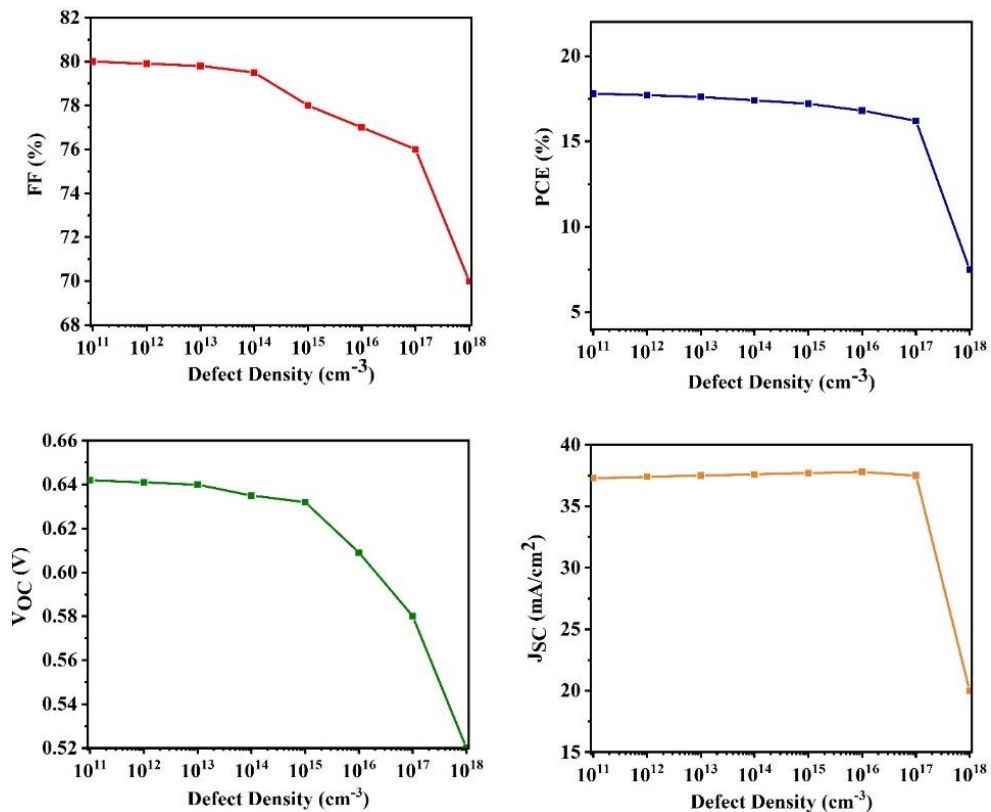


Figure:3 Performance of solar cells with Sb_2Se_3 bulk flaws

A solar cell's Performance can be impacted by several things, including manufacturing flaws. The formation energy and transition levels of Sb₂Se₃ defects have been investigated. Figure 3 displays, as an illustration, PV characteristics and bulk defects in the Sb₂Se₃ absorber layer. The output parameters were assumed to be connected to defects in the Sb₂Se₃ absorber layer via single donor-type faults. The fact that most measurements are flawed impacts all of them. Reverse saturation current rises, and device VOC falls due to Shockley-Read-Hall (SRH) recombination, which takes over at high defect levels. In solar cells with growing Sb₂Se₃ layer bulk defects, parameters decrease, and the PCE sharply decreases. A recent study shows that the ZnO window layer hardly affects the output characteristics. Researchers took the BSF layer off the Sb₂Se₃ solar cell to find the optimal PCE.

very consistent using the SCAPS-1D method. As shown in Figure:4, the J-V of a Sb₂Se₃ solar cell was in perfect agreement with the experimental J-V after accounting for modeling faults. We first optimized the defect trap value to replicate the practical outcomes before introducing defects at the FTO/ZnO/Sb₂Se₃/CZTSe/Au interface.

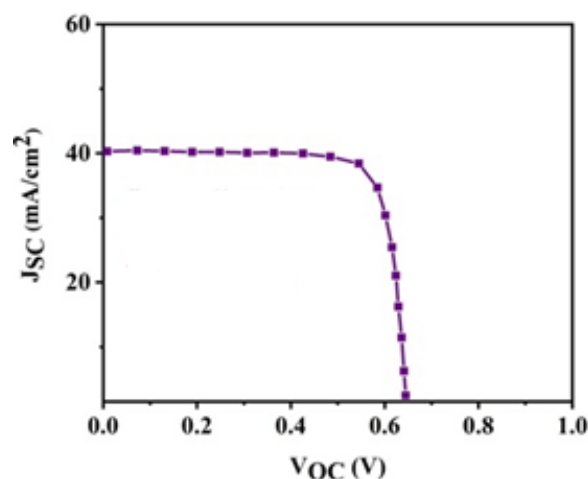


Figure:4 proposed J-V properties of solar cell devices

Designers used SCAPS-1D software to recreate the data from the experimental solar cell so that we could compare and test our proposed methodology against the original. Results from the simulation and experiment were found to be

Table:1 Result comparison with existing solar cell structure with this work

| Reference | Device Structure | V _{oc} (V) | J _{sc} (mA/cm ²) | FF (%) | PCE (%) |
|------------------|---|---------------------|---------------------------------------|--------|---------|
| 2017 [36] | ITO/CdS/Sb ₂ Se ₃ /PbSCQD/Au | 0.427 | 27.7 | 58 | 6.87 |
| 2018 [37] | FTO/CdS/ Sb ₂ Se ₃ /Au | 0.410 | 38.15 | 74.08 | 11.52 |
| 2019 [38] | ITO/In ₂ Se ₃ /Sb ₂ Se ₃ /Cu ₂ O/CNT | 0.420 | 25.9 | 58.7 | 6.32 |
| 2020 [39] | FTO/Zn (Sn, O)/Sb ₂ Se ₃ /CZTSe/Au | 0.320 | 26.88 | 45.33 | 3.59 |
| 2021 [40] | FTO/WS ₂ /Sb ₂ Se ₃ /HTL/Au | 0.364 | 27.68 | 52.54 | 5.29 |
| This Work | FTO/ZnO/Sb ₂ Se ₃ /CZTSe/Au | 0.086 | 2.47 | 70.38 | 14.95 |

In the table:1, these are the chemical formulas that have been used.

FTO – Fluorine Doped Tin Oxide

CdS – Cadmium Sulfide

Sb₂Se₃ – Antimony Selenide

Au – Gold

Zn (Sn, O) – Tin doped with Zinc Oxide

CZTSe – (Cu₂ZnSnSe₄) phase from elemental Cu, Zn, Sn, and Se with the addition of KI-KCl mixture

ITO - Indium Tin Oxide

In₂Se₃ – Indium Selenide

Cu₂O – Copper Oxide

CNT – Carbon Nanotube

ZnO – Zinc Oxide

WS₂ – Tungsten Bisulfide

PbSCQD – Lead (II) sulfide carbon quantum dots

HTL – Hole Transport Layer

5. Conclusion

FTO/ZnO/Sb₂Se₃/CZTSe/Au-based solar cell device with a VOC of 0.086V, JSC of 2.47mA/cm², FF of 982.09%, and PCE of 20.94% was proposed in this study using SCAPS-1D. The device's Performance was then improved by adjusting physical parameters such as absorber and buffer layer doping density and thickness. After turning the device's Performance, it was discovered that the band alignment between the absorber/buffer layer interface had a significant impact. Co-evaporation of Se and Sb₂Se₃ produces thin-film absorber layers. The evaporation of Se in Sb₂Se₃ thin-film solar cells increased orientation preference and compensated for the loss of Se during thermal evaporation, reducing recombination loss and improving heterojunction quality. It was found that the VOC, JSC, and conversion efficiency of solar cells fabricated with Sb₂Se₃ thin films were lower than those manufactured with Se-free absorbers.

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