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III-V MULTIJUNCTION SOLAR CELLS CONTRIBUTIONS IN THE RENEWABLE ENERGY ENGINEERING

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TESE DE DOUTORAMENTO

**III-V MULTIJUNCTION SOLAR CELLS
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ENERGY ENGINEERING**

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**PROGRAMA DE DOUTORAMENTO EN ENERXÍAS RENOVABLES E
SUSTENTABILIDADE ENERXÉTICA**

SANTIAGO DE COMPOSTELA

*(Lee en el nombre de tu Señor que creó,
creó al hombre de un coágulo. Lee, que tu
Señor es el más generoso, el que enseñó
por el cálamo, enseñó al hombre lo que no
sabía)*

Holy Quran- Sura AlAlaq (1-5)

*(Read in the name of your Lord who cre-
ated, created man from a clinging sub-
stance. Read, and your Lord is the most
Generous - Who taught by the pen -
Taught man that which he knew not)*

Holy Quran - Sura AlAlaq (1-5)

Dedication

To my beloved mother, a firm yet gentle soul who taught me the value of hard work and showed me that even the most minor means could achieve great things.

To my father, whose unwavering support and dedication to an honest living inspired me to believe in myself and pursue my dreams.

To my beloved wife, who holds a special place in my heart, offering love, strength, and encouragement throughout this journey.

To my dear children, whose laughter, love, and endless curiosity bring joy and purpose to my life.

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Abstract

Renewable energy is rapidly replacing fossil fuels due to the urgent need to reduce greenhouse gas emissions and minimize the environmental impact of fossil fuels. In addition to their abundance, cleanliness, and cost-effectiveness, solar photovoltaic systems stand out among renewable energy technologies. The focus of this research is the advancement of vertical multijunction (VMJ) gallium arsenide (GaAs) solar cells that are essential for ultra-high concentration photovoltaic (UHCPV) systems. The advantages of VMJ solar cells are their high energy conversion efficiency, robustness against space radiation, and suitability for CubeSats. Several key parameters, ranging from doping density to layer thickness and solar concentration, are addressed in this study using the ATLAS Silvaco simulation platform. An advanced modeling technique investigated the interaction between intrinsic parameters (e.g., doping and thickness of the P and N layers) and extrinsic conditions (e.g., sun concentration levels under AM0 and AM1.5 spectrums). Based on simulations covering a range of doping concentrations from 10^{12} to 10^{17} cm^{-3} , optimal configurations were identified that maximized short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), and fill factor. Our study found that thicker layers increased J_{sc} and FF when doping levels were higher in both P and N regions. Nevertheless, carrier recombination effects are more complex in V_{oc} , and require careful optimization. The study found that the N-layer thickness should be $7.0 \text{ }\mu\text{m}$, and the P-layer doping should be optimized to improve solar cell efficiency. At one sun, the maximum J_{sc} and V_{oc} were 2.74 mA/cm^2 and 2.1 V , respectively, while at 10,000 suns, they increased to 27.43 mA/cm^2 and 2.34 V . Efficiency rose from 23.93% under one sun to 30.2% under 10,000 suns. As light intensities increased, recombination losses increased, and FF declined, but the optimized design maintained a favorable performance balance. At one sun, the optimized VMJ solar cell showed a linear increase in V_{oc} , and at 10,000 suns, it reached 2.4 volts with an overall structure width of $20.33 \text{ }\mu\text{m}$ and a height of $1.25 \text{ }\mu\text{m}$. Various performance trade-offs

were evaluated, including Auger, Shockley-Read-Hall (SRH), and radiative recombination. This study demonstrates that predictive modeling can result in cost-effective, high-efficiency solar cells by reducing prototyping costs, fine-tuning experimental designs, and accelerating the development of these devices. Finally, this work advances our understanding and optimization of VMJ GaAs solar cells for UHCPV systems, providing a pathway for their broader application in space and terrestrial energy.

Resumen extendido

A situación enerxética de todo o mundo están a cambiar drasticamente, xa que se deben reducir as emisións de gases de efecto invernadoiro e facer a transición cara ás fontes de enerxía renovable. O impacto ambiental dos combustibles fósiles, que alimentaron as economías durante séculos, converteuse nunha preocupación cada vez máis urxente. Isto impulsou o crecemento e a relevancia das fontes de enerxía renovable. A enerxía solar destaca fronte a outras alternativas pola súa natureza limpa, abundante e cada vez máis rendible. A tecnoloxía fotovoltaica (FV) emerxeu como a forma máis barata de electricidade en moitas rexións debido á diminución dos custos e ao aumento da capacidade. Os beneficios da enerxía renovable van máis aló dos impactos ambientais, pois tamén crean oportunidades económicas. Foron os esforzos constantes dos investigadores os que deron lugar a melloras xeración tras xeración das diversas tecnoloxías fotovoltaicas. Segundo os avances tecnolóxicos e a composición material das células fotovoltaicas, existen catro xeracións principais: a primeira xeración de fotovoltaicas; o silicio e o arseniuro de galio (GaAs) son os semicondutores empregados nesta xeración inicial. As células de GaAs de alta eficiencia son unha elección popular para aplicacións de multiunión. En aplicacións especializadas, como a xeración de enerxía solar no espazo, as células de GaAs poden acadar niveis de eficiencia superiores ao 28 % en condicións estándar. Debido á súa elevada pureza e calidade, as células fotovoltaicas de primeira xeración resultan relativamente caras de producir. Na segunda xeración de células fotovoltaicas, empréganse tecnoloxías de película fina para reducir os custos, diminuindo o consumo de material a uns poucos micrómetros. Existen varios tipos destas células, incluíndo o silicio amorfo (a-Si), o telurio de cadmio (CdTe) e o seleniuro de cobre, indio e galio (CIGS). Non obstante, estas células adoitan degradarse máis rapidamente e presentan eficiencia máis baixa. A terceira xeración de fotovoltaicas, a través de novos materiais e de técnicas de deposición de capas delgadas, busca acadar maior eficiencia. Entre as diver-

As células solares desta xeración inclúense as células sensibilizadas por colorante (DSSC), as células solares orgánicas e poliméricas, as células de perovskita, os puntos cuánticos e as células solares de multiunión. A pesar do seu maior custo, estas tecnoloxías son altamente eficientes e resistentes a nivel mecánico. Baixo luz solar concentrada, as células de multiunión, que combinan múltiples materiais semicondutores, poden superar o 40% de eficiencia. Aínda que as células de terceira xeración precisan materiais e procesos de fabricación máis caros, poden ofrecer rendementos máis elevados e novas aplicacións, compensadas por un incremento no rendimento e na produción enerxética. A cuarta xeración de fotovoltaicas, coñecida como células fotovoltaicas “inorgánicas-en-orgánicas” debido ao seu baixo custo e flexibilidade, combina a durabilidade de nanestructuras inorgánicas como nanopartículas metálicas e óxidos metálicos con nanomateriais orgánicos. O obxectivo desta xeración é reducir os custos de fabricación, incrementar a eficiencia e mellorar a estabilidade. É evidente, a través da evolución das xeracións fotovoltaicas, que existe un equilibrio entre eficiencia e custo: a primeira xeración ofrece alta eficiencia pero elevado custo, a segunda reduce os custos sacrificando algo de eficiencia, a terceira persegue unha maior eficiencia con materiais avanzados, e a cuarta combina baixo custo e alta eficiencia mediante materiais híbridos innovadores. Declaración do Problema: As células solares, que son moi eficientes e rendibles, están a adquirir unha importancia crecente a medida que as fontes de enerxía renovable e a tecnoloxía espacial evolucionan rapidamente. Ademais das aplicacións terrestres, as misións espaciais con CubeSats ou outros pequenos satélites dependen especialmente desta necesidade. A xeración actual de células solares, baseada principalmente en configuracións horizontais monolíticas, enfronta limitacións inherentes ao uso de semicondutores compostos, especialmente III-V. Varios factores limitan a eficiencia máxima destas células baixo condicións de alta concentración, como os efectos de sombreado provocados pola malla metálica que cobre a superficie da célula e que impide que a luz solar chegue ás rexións activas, ou a resistencia en serie (R_s), que restrinxe o fluxo de corrente. Unha alternativa prometedora a estas limitacións son as células solares de multiunión vertical (VMJ) feitas con arseniuro de galio (GaAs). Unha vantaxe destacada das células VMJ con GaAs é a súa superioridade material, incluíndo unha excelente mobilidade electrónica e un salto de banda. A configuración vertical tamén evita que os fotóns se acoplen co fluxo de corrente, o que reduce problemas como o sombreado e a resistencia en serie. As concentracións de dopaxe nas rexións P e N das células solares deben optimizarse con precisión. Axustar adecuadamente os niveis de dopaxe resulta fundamental para acadar as propiedades eléctricas desexadas sen introducir perdas excesivas

por recombinación. Ademais de maximizar a absorción de luz solar, é importante minimizar as perdas resistivas e garantir unha recollida eficiente de portadores de carga mediante o axuste do espesor das capas P e N. Os pequenos satélites, como os CubeSats, teñen unha superficie moi limitada para paneles solares, polo que o desenvolvemento de células solares altamente eficientes é necesario para proporcionar xeración de enerxía fiable nun espazo e peso moi reducidos. As células solares VMJ baseadas en GaAs son adecuadas para estas aplicacións pola súa alta eficiencia de conversión enerxética e a súa resistencia á radiación espacial e ás fluctuacións de temperatura. Para que os próximos sistemas de CPV sexan economicamente viables e teoricamente eficientes, precísase comprender a interacción de varios parámetros de deseño, incluída a densidade de dopaxe, o espesor das capas e a concentración solar. Desenvolver células solares de multiunión vertical (VMJ) de arseniuro de galio (GaAs) de baixo custo e alta eficiencia é fundamental para os sistemas fotovoltaicos de ultra-alta concentración (UHCPV). Estes sistemas concentran a luz solar por un factor superior a 1000 soles, sendo cruciais para futuras misións espaciais e aplicacións terrestres. Esta investigación céntrase en optimizar o deseño de células solares empregando ferramentas de simulación avanzadas para afrontar retos significativos. Entre estes desafíos inclúese o axuste da concentración de dopaxe e a adaptación do espesor das capas en condicións de alta concentración con masas de aire (AM) de 0 e 1.5. Neste traballo, empregárase software avanzado para optimizar as células VMJ de GaAs en sistemas UHCPV, cun foco especial na ampliación da súa aceptación en contornos diversas. Resulta prometedor que as células solares de multiunión feitas con arseniuro de galio (GaAs) poidan aumentar radicalmente a eficiencia de conversión. As células solares de multiunión vertical (VMJ) baseadas en GaAs son especialmente axeitadas para aplicacións en satélites, grazas á súa alta eficiencia de conversión, á súa robustez fronte á radiación e á súa capacidade de funcionar de forma efectiva a baixas temperaturas. A optimización do deseño das células solares require un enfoque sistemático, que pode acadarse de xeito eficaz empregando ferramentas de simulación avanzadas como ATLAS Silvaco. Estas ferramentas permiten que os investigadores analicen factores críticos como a densidade de dopaxe, o espesor das capas ou os niveis de concentración solar nun contorno controlado. Mediante a modelización detallada e a experimentación virtual, é posible axustar estes parámetros para mellorar a eficiencia e o rendemento das células solares. Estas simulacións empréganse para atopar estruturas de células solares que maximicen a eficiencia e minimicen os custos de produción, o que conduce, en última instancia, a unha maior adopción das tecnoloxías de enerxía renovable. Os principais obxectivos son:

1. Presentar o estudo e o rendemento de recursos de enerxía renovable en aplicacións espaciais e terrestres mediante células solares verticais GaAs homo-multiunión de alta eficiencia e baixo custo.
2. Caracterizar, simular e analizar estes dispositivos empregando o simulador ATLAS-SILVACO (TCAD) para acadar a máxima eficiencia de conversión e factor de enchido en varios sistemas fotovoltaicos de ultra-alta concentración, a diferentes niveis de irradiación solar.
3. Estudar e desenvolver estruturas de multiunión para maximizar a eficiencia usando unións túnel verticais, coa fin de reducir perdas resistivas en condicións de alta concentración fronte a deseños estándar.
4. Analizar o efecto da variación de parámetros intrínsecos como o espesor das capas e a concentración de dopaxe na eficiencia global das células solares. Deseñamos unha célula solar homo-multiunión de GaAs adaptada para satélites miniaturizados (Cube-Sat) e outras aplicacións terrestres, cunha alta eficiencia de conversión enerxética e robustez.
5. Comparar o rendemento destas células solares baixo distintos espectros solares (AM0 e AM1.5) e avaliar a súa adecuación para aplicacións espaciais e terrestres.
6. Propoñer melloras nas propiedades dos materiais e optimizacións no deseño das células para minimizar as perdas por resistencia, mellorar a xestión térmica e incrementar o factor de enchido. Integrar as células solares con sistemas de almacenamento de enerxía para aumentar a preparación comercial destas tecnoloxías e reducir os custos de produción.

As células solares son, na súa base, unións PN expostas á luz. O proceso de absorción de fotóns xera pares electrón-ocúpaa, e as unións p-n separan estes portadores, dando lugar a unha corrente coñecida como fotocorrente. A densidade de corrente de curto-circuíto, a tensión de circuíto aberto e o factor de enchido son parámetros importantes para estimar o rendemento dunha célula solar. Nun circuíto aberto sen corrente, a tensión é a máxima posible; o factor de enchido é a relación entre a potencia máxima e a potencia teórica. Silvaco utiliza simulacións e análises para calcular o factor de enchido (FF) das células solares en condicións específicas. As características corrente-tensión (I-V) das células solares determínanse resolvendo ecuacións complexas de semicondutores. O factor de enchido dunha

célula solar calcúlase comparando a potencia de saída coa potencia de entrada. As células solares de multiunión (MJSCs, polas súas siglas en ingles, Multi-junction solar cells) representan unha tecnoloxía punteira en fotovoltaica, xa que ofrecen eficiencias moito maiores que as células solares dunha única unión tradicionais. Están compostas por capas de distintos materiais semicondutores, cada unha co seu propio salto de banda. Estas células poden acadar eficiencias superiores ao 45 % baixo luz solar filtrada. As MJSCs empréganse en aplicacións de alto rendemento, como en misións espaciais, e están a gañar popularidade para aplicacións terrestres. Estes sistemas poden superar os 1000 soles de concentración e considéranse unha das vías máis prometedoras para combinar baixo custo e alta eficiencia nos sistemas de CPV. Para acadar sistemas de CPV de alta eficiencia e baixo custo, cómpre unha nova xeración de tecnoloxía. Os investigadores están a explorar a fotovoltaica de ultra-alta concentración (UHCPV), que emprega lentes ou espellos para concentrar a luz solar nas células. Este método mellora de maneira notable a eficiencia e reduce os custos do material, contribuíndo á competitividade da enerxía solar. As células solares multiunión de GaAs son dispositivos fotovoltaicos moi eficientes, axeitados tanto para aplicacións espaciais como terrestres. Presentan alta eficiencia e son resistentes a doses elevadas de radiación, ademais de poder operar moi ben baixo espectros tipo AM0. O GaAs emprégase amplamente en CubeSats, que son satélites miniaturizados deseñados para numerosas misións, incluíndo exploracións interplanetarias. Atlas Silvaco é unha potente e completa plataforma de software de simulación, moi empregada en fotovoltaica (FV). Desenvolvida por Silvaco, Inc., líder global en automatización de deseño electrónico (EDA), Atlas ofrece ferramentas robustas para modelar e simular dispositivos semicondutores. No ámbito da fotovoltaica, resulta fundamental para optimizar o deseño e o rendemento das células solares, permitindo que investigadores e enxeñeiros simulen e analicen fenómenos físicos complexos dentro destes dispositivos FV. As células solares poden ser simuladas a nivel eléctrico, óptico e térmico, converténdose así nunha ferramenta esencial para quen busque mellorar a eficiencia dos sistemas FV. A principios dos anos 2000, coa crecente importancia global de solucións enerxéticas sostibles, Atlas Silvaco acadou gran relevancia na investigación fotovoltaica tanto académica como industrial. Permitiu a análise e optimización detallada de novos materiais e estruturas de célula, contribuíndo de forma destacada aos avances do sector. As actualizacións e melloras continuas de Silvaco mantiveron Atlas na vangarda da tecnoloxía de simulación FV. As súas capacidades de modelización detallada axudan a comprender e mellorar o rendemento dos dispositivos, ampliando os límites da eficiencia e da innovación no sector da enerxía solar. Neste

traballo, o código ATLAS Silvaco proporcionado simula unha célula solar de multiunión vertical fabricada en arseniuro de galio (GaAs), con dúas células e catro capas. As estruturas semiconductoras optimízanse mediante modelización numérica baseada en fenómenos físicos, e o salto de banda pódese axustar ás necesidades de cada aplicación. Este estudo modela unha estrutura de banda única e aplica un procedemento de optimización para estimar a súa eficiencia máxima. Ademais, ofrece directrices para futuras melloras na fabricación de células solares. Neste traballo, optimizamos unha célula con unión túnel vertical (VTJ) de arseniuro de galio (GaAs), composta por dúas sub-células idénticas, cada unha delas con catro capas, unidas a través dunha unión túnel. Este dispositivo ilumínase de xeito vertical segundo as especificacións da norma ASTM E-490, que define o espectro AM0 para aplicacións espaciais, variando en magnitude en función da distancia ao Sol. A norma ASTM G-173-03 define dous espectros estándar de uso terrestre para módulos fotovoltaicos con 1000 W/m² de potencia integrada e unha temperatura de célula de 25 °C. As células acadaron elevados valores en parámetros clave como a densidade de corrente, a tensión de circuío aberto, o factor de enchido e a eficiencia. Primeiro, comparamos o noso modelo con células establecidas que contan con datos de rendemento e características ben documentadas; despois, optimizamos a estrutura para mellorar o seu rendemento. Axustamos parámetros intrínsecos (espesor e niveis de dopaxe) e modificamos parámetros extrínsecos (niveis de concentración). O proceso de optimización comeza axustando o espesor das capas P para maximizar a eficiencia, logo axústase o espesor da capa N sen cambiar os niveis de dopaxe e, por último, axústanse as dopaxes das capas P e N para acadar o mellor rendemento posible.

As simulacións exploraron un rango de concentracións de dopaxe entre 10^{12} e 10^{17} cm⁻³, variando o espesor das rexións P e N para identificar a estrutura óptima que maximice a eficiencia das células solares. Unha maior dopaxe nas capas P e N xeralmente mellora o rendemento do dispositivo, sendo as capas máis grosas as que producen maiores densidades de corrente de curto-circuíto (J_{sc}) e factores de enchido (FF). Non obstante, a resposta da tensión de circuío aberto (V_{oc}) é máis complexa. Baixo as condicións de masas de aire AM0, AM1.5 e 4000 soles, as eficiencias variaron entre o 25,42 % e o 29,78 %, acadando o máximo cunha dopaxe de 10^{14} cm⁻³.

As células solares VMJ destacan por vantaxes únicas, como o desacoplamento de fotóns e correntes, mitigando problemas de compensación observados nas células convencionais. O espesor da capa absorbente tipo P inflúe significativamente no rendemento: as capas máis finas melloran o FF, pero poden reducir o J_{sc} debido a unha menor xeración de portadores;

as capas máis grosas, pola contra, aumentan a xeración de portadores, pero reducen o FF. Do mesmo xeito, incrementar o espesor da capa tipo N aumenta o Jsc, pero diminúe o Voc debido a unha maior recombinación de portadores. A optimización experimental determinou que un espesor de 7,0 μm na capa N é óptimo para altas concentracións solares.

A dopaxe tipo P axeitada incrementa o Jsc e o FF ao mellorar a concentración de electróns libres, pero unha dopaxe excesiva pode reducir o potencial interno da unión P-N, afectando negativamente ao FF. O equilibrio entre Jsc, Voc e FF determina a eficiencia total. A unha intensidade solar de un sol, os valores máximos de Jsc e Voc foron 2,74 mA/cm^2 e 2,1 V, respectivamente, aumentando a 27,43 mA/cm^2 e 2,34 V a 10.000 soles. A eficiencia mellorou do 23,93 % ao 30,2 %, aínda que o FF diminuíu lixeiramente debido ás maiores perdas por recombinación. Equilibrar os incrementos de corrente coas perdas no FF é esencial para manter unha alta eficiencia. A célula solar VTJ optimizada, cun ancho de 20,33 μm e unha altura de 1,25 μm , mostrou un incremento lineal de Voc, de 1,86 V a un sol ata 2,4 V a 10.000 soles. As análises detalladas dos mecanismos de recombinación, incluíndo Auger, SRH e radiativa, proporcionaron información valiosa sobre os compromisos de rendemento baixo diferentes condicións. Empregando a ferramenta avanzada de simulación Silvaco ATLAS, este estudo subliña como a modelización predictiva pode reducir os custos de prototipado e mellorar os deseños experimentais futuros. Esta tese consta de seis capítulos, cada un estruturado para ofrecer un fío condutor coherente da investigación. O capítulo de Introducción aborda o contexto, os avances nas tecnoloxías fotovoltaicas, a formulación do problema, as motivacións da investigación e os obxectivos. O capítulo de Antecedentes explora os principios fundamentais da fotovoltaica, destacando a evolución das tecnoloxías solares e o papel das unións PN. A Revisión Bibliográfica analiza estudos previos sobre células solares multixuntión, as súas configuracións (homo e heteromultixuntión), a fotovoltaica de concentración e a aplicación das células multixuntión verticais de GaAs (VMJ) para contornos terrestres e satélites. O capítulo de Metodoloxía detalla o proceso de simulación mediante o software ATLAS Silvaco, explicando a modelización das células VMJ e os pasos esenciais para sistemas fotovoltaicos de ultra-alta concentración en aplicacións CubeSat e terrestres. O capítulo de Resultados e Discusión analiza os resultados das simulacións, incluíndo modelos de recombinación, o rendemento dos dispositivos baixo diversas condicións e as súas implicacións prácticas. Finalmente, o capítulo de Conclusións resume os achados clave, subliña a súa relevancia e proporciona recomendacións para futuras investigacións. Os apéndice inclúen materiais complementarios, o código de simulación ATLAS Silvaco e referencias.

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CHAPTER 1

INTRODUCTION

1.1 Background

Energy landscapes worldwide are changing dramatically, as greenhouse gas emissions must be reduced and renewable energy sources must be transitioned. The environmental impact of fossil fuels, which have powered economies for centuries, is becoming an increasingly pressing concern. This has driven the growth and importance of renewable energy sources. Solar energy stands out among alternatives for its clean, abundant, and increasingly cost-effective nature. Solar photovoltaic (PV) technology has emerged as the cheapest form of electricity in many regions due to falling costs and growing capacity [1, 2].

Solar energy helps reduce carbon footprints, enhances energy security, and provides electricity access to remote communities. Renewable energy's benefits extend beyond its environmental impacts, creating economic opportunities.

However, it's essential to acknowledge the environmental impacts associated with renewable technologies. Solar energy systems, for instance, can have land use and habitat implications, depending on the scale and technology used. Despite these challenges, the overall environmental benefits of transitioning to renewable energy sources are substantial, as they produce far fewer emissions and pollutants than fossil fuels. In the face of climate change and energy access challenges, solar energy is becoming more prevalent around the globe [1, 2]. Electricity is generated directly from sunlight by solar cells. Photovoltaic cells, which convert light energy into electrical energy, were invented by Alexander-Edmond Becquerel in 1839. The first solar cells were built in 1883, using selenium to form cells that were about 1% efficient. A modern solar cell was patented by Russell Ohl in 1946, ushering in a new era in solar

1.2. Advancements in Photovoltaic Technologies

power technology. This cell was improved by Bell Laboratories to about 6% efficiency [3,4]. As a result of modern cell design, efficiency has increased significantly.

1.2 Advancements in Photovoltaic Technologies

Solar technology has offered a sustainable alternative, and various solar cell structures have been discovered in the quest to achieve efficient and sophisticated designs. Despite this, the first solar cells were not commercialized on a large scale due to several factors. These factors include the massive installation area, high cost, limited durability, and associated losses [5,6]. These factors have caused researchers to explore various research routes to address these shortcomings. The diligent efforts of researchers have resulted in generation-by-generation improvements. According to the technological advancements and material composition of photovoltaic cells, there are four main generations:

1.2.1 The first generation of photovoltaics

Silicon (monocrystalline and polycrystalline) and gallium arsenide (GaAs) are the semiconductor materials used in the first generation of photovoltaic cells. Because silicon-based solar cells are abundant, nontoxic, and compatible with silicon-based electronic products, they are the most popular on the market. High-efficiency GaAs cells are a popular choice for multi-junction applications. Because monocrystalline silicon cells utilize a single crystal structure, they typically achieve efficiency levels between 15% and 20% [7, 8]. Due to the multiple silicon crystals creating boundaries, polycrystalline silicon cells have efficiencies between 13% and 16%. In specialized applications such as space solar power generation, GaAs cells can achieve efficiency levels up to 28% under standard conditions, thanks to their superior light absorption and electronic properties [9]. Due to their high purity and quality, first-generation photovoltaic cells are relatively expensive to produce. The production of monocrystalline silicon wafers is more complicated than polycrystalline, while GaAs wafers have specialized manufacturing processes and material costs, making them more expensive than polycrystalline silicon cells.

1.2.2 The second generation of photovoltaics

In the second generation of photovoltaic cells, thin-film technologies are used to minimize costs by reducing material consumption to a few microns. There are several types of these

cells, including amorphous silicon (a-Si), cadmium telluride (CdTe), and copper indium gallium selenide (CIGS). They are more cost-effective than first-generation cells due to their lower production costs [10]. Due to their thin-film construction, thin-film technologies use less semiconductor material, reducing production costs as well as energy consumption. Nonetheless, these cells tend to degrade more quickly and have lower efficiencies. Over time, amorphous silicon cells deteriorate significantly and have efficiencies between 6% and 10%. Commercially, cadmium telluride cells attain efficiency levels of 11% to 12%, with laboratory efficiency levels exceeding 20% [11]. According to various manufacturing processes and material qualities, copper indium gallium selenide cells are capable of 15% to 20% efficiency [12, 13]. Cost-effectiveness can be affected by the lower efficiency of second-generation cells despite their lower production costs.

1.2.3 The third generation of photovoltaics

Third-generation photovoltaics aim to achieve higher efficiency through novel materials and thin-layer deposition techniques. There are several types of solar cells in this generation, including dye-sensitized solar cells (DSSCs), organic and polymeric solar cells, perovskite cells, quantum dots, and multijunction solar cells [14]. Despite the higher cost, these technologies are highly efficient and mechanically tough. In dye-sensitized solar cells, efficiency ranges from 7% to 11%, depending on dye stability and electrolyte composition. These lightweight, flexible solar cells are extremely efficient, typically between 5% and 11% [15, 16]. However, organic and polymeric cells are typically less efficient and have shorter lifespans than inorganic solar cells. The performance of perovskite cells has improved rapidly over the past few years, with efficiencies exceeding 25% in laboratory settings, though stability and toxicity are still issues [17]. In quantum dot cells, efficiencies may range from 11% to 16%, and tunable electronic properties can result in high efficiency. Under concentrated sunlight, multijunction cells, which combine multiple semiconductor materials, achieve more than 40% efficiency [18, 19]. While third-generation cells require more expensive materials and manufacturing processes, they have the potential to provide higher efficiencies and new applications, offset by increased performance and energy yield.

1.3. Problem Statement

1.2.4 The fourth generation of photovoltaics

It is known as “inorganic-in-organics” photovoltaic cells because of their low cost and flexibility, and it combines the durability of inorganic nanostructures like metal nanoparticles and metal oxides with organic nanomaterials [20]. The purpose of this generation is to reduce manufacturing costs, increase efficiency, and enhance stability [21, 22]. In fourth-generation cells, hybrid materials improve efficiency by improving charge dissociation and transport mechanisms to combine the best elements of previous generations. Due to the synergy between the combinations of materials, the efficiency of these cells is expected to surpass that of the second and third generations. The materials and manufacturing costs of these cells are lowered because they combine flexible, inexpensive polymers and durable inorganic nanostructures. Solar energy deployment may be cost-effective because these materials are scalable and flexible, making them suitable for various applications [23, 24].

It is evident from the evolution of photovoltaic generations that efficiency and cost are being balanced, with the first generation offering high efficiency but high cost, the second generation reducing costs at the expense of efficiency, the third generation striving to achieve high efficiency with advanced materials, and the fourth generation combining low cost and high efficiency through innovative hybrid materials. Table 1.1 show how technologies, efficiencies, and costs have changed with each generation of photovoltaic cells. NREL maintains a chart of the highest confirmed conversion efficiencies for research cells across various photovoltaic technologies, updated continuously since 1976 [25].

1.3 Problem Statement

Solar cells, which are highly efficient and cost-effective, are becoming increasingly important as renewable energy sources and space technology evolve rapidly. In addition to terrestrial applications, space missions using CubeSats or other small satellites mainly depend on this demand. The current generation of solar cells, primarily composed of monolithic horizontal configurations, faces inherent limitations due to compound semiconductors, particularly III-V. Several factors limit the maximum efficiency of solar cells when they are exposed to high-concentration conditions, including shadowing effects caused by a metal grid pattern on the cell surface, which prevents sunlight from reaching the active regions of the cell, and series resistance (R_s), which restricts current flow [26–29]. A promising alternative to these limitations is vertical multijunction solar cells (VMJ) using gallium arsenide (GaAs). A sig-

Table 1.1: Summary of Photovoltaic Generations.

Generation	Technology	Efficiency	Cost
First Generation	Crystalline film technology using silicon (monocrystalline and polycrystalline) and GaAs	Monocrystalline Silicon: 15% - 27.6% Polycrystalline Silicon: 13% - 24.4% GaAs: Up to 30.8%	High production costs due to high purity and quality materials. GaAs cells are the most expensive.
Second Generation	Thin-film technologies using a-Si, CdTe, and CIGS	Amorphous Silicon: 6% - 14.0% CdTe: 11% - 23.08%, CIGS: 15% - 23.6%	Lower production costs due to reduced material usage and energy consumption. Less efficient, affecting cost-effectiveness.
Third Generation	Novel materials and thin-layer deposition techniques (DSSCs, organic/polymeric, perovskite, quantum dot, multi-junction)	DSSCs: 7% - 13% Organic/Polymeric: 5% - 19.2% Perovskite: 26.7% Quantum Dot: 11% - 19.1% Multi-Junction: >40%	Higher production costs due to advanced materials and complex manufacturing. Potential for high efficiencies and unique applications.
Fourth Generation	Hybrid materials combining polymer thin films with inorganic nanostructures (e.g., graphene, carbon nanotubes)	Projected to surpass second and third generations due to combined material synergy.	Goal to achieve low-cost production while maintaining/improving efficiency. Scalable and flexible, reducing overall solar energy deployment costs.

nificant advantage of GaAs-based VMJ solar cells is their superior material properties, including excellent electron mobility and a direct bandgap, which make them ideal for photovoltaic applications [30]. The silicon-based solar cells capture a broader spectrum of photons and convert them more efficiently into electrical energy [31]. The vertical configuration also prevents photons from coupling with the current flow, reducing shadowing and series resistance issues.

1.3. Problem Statement

In addition to the challenges presented by optimizing VMJ solar cells for ultra-high concentration photovoltaic (UHCPV) systems, particularly for CubeSat applications. Doping concentrations in solar cells' P and N regions must be precisely optimized. Calibrating the doping levels is critical to achieving the desired electrical properties without introducing excessive recombination losses [32, 33]. In addition to maximizing sunlight absorption, it is essential to minimize resistive losses and ensure efficient charge carrier collection by adjusting the thickness of the P and N layers. Additionally, the high concentration levels, often exceeding 1000 suns, pose significant challenges to thermal management. Overheating can degrade the performance of solar cells, which requires efficient heat dissipation mechanisms [34, 35]. Advanced simulation tools like ATLAS Silvaco are essential to address these challenges. These tools allow researchers to model and simulate solar cell structures, enabling them to perform virtual experiments and optimize design parameters [36]. Small satellites like CubeSats have limited surface area for solar panels, so developing highly efficient solar cells is necessary to generate reliable power in limited space and weight. VMJ solar cells based on GaAs are well-suited for these applications because of their high energy conversion efficiency and ruggedness against space radiation and temperature fluctuations. For these next-generation CPV systems to be economically viable and theoretically efficient, they require an understanding of the interaction of various design parameters, including doping density, layer thickness, and sun concentration [37, 38]. A new generation of solar cells that meet the stringent efficiency requirements for space applications and offer economic benefits for terrestrial deployment can be developed if these challenges are addressed using advanced simulation and optimization techniques. UHCPV technologies can help lower dependence on fossil fuels and mitigate climate change impacts by overcoming technological barriers associated with renewable energy technologies [39].

Developing low-cost, high-efficiency VMJ gallium arsenide (GaAs) solar cells is essential for UHCPV systems, which are pivotal for future space missions and terrestrial applications. This research focuses on optimizing solar cell design using advanced simulation tools to tackle significant challenges. These challenges include refining doping concentration and adjusting layer thickness with high concentrations under air masses (AM) of 0 and 1.5. Addressing these factors is crucial for achieving superior performance and economic feasibility in these advanced solar cells.

1.4 Research Motivations

Researchers are driven to develop highly efficient and cost-effective solar cells tailored to meet the specific requirements of both terrestrial and satellite applications. This endeavor involves overcoming the limitations of conventional designs. By focusing on innovative approaches and advanced technologies, researchers aim to enhance the performance and affordability of solar cells, ensuring they can efficiently serve diverse and demanding environments. In this study, advanced simulation tools will be utilized to optimize VMJ GaAs solar cells for UHCPV systems, and a focus will be placed on increasing their acceptance in diverse environments [7, 40].

1.4.1 Renewable Energy Efficiency

The global shift towards renewable energy sources is driven by the urgent need to reduce greenhouse gas emissions and mitigate climate change. The abundance and decreasing cost of photovoltaic technology make solar energy an attractive renewable energy source [41, 42]. For solar energy to become economically viable and widespread, solar cells must be maximized for efficiency. It is promising that multijunction solar cells using GaAs can dramatically increase conversion efficiency [43, 44].

1.4.2 Overcoming Limitations of Traditional Solar Cells

The traditional horizontal solar cell structure is limited by metal grid patterns that can cast shadows and series resistances that impede the flow of current. Especially under high concentration conditions, these factors limit the efficiency of solar cells. The VMJ solar cell offers a potential solution to shadowing problems through its ability to decouple photons and currents, reduce resistance losses, and eliminate shadowing [45–47]. To overcome these inherent limitations and achieve higher efficiency, this research explores and optimizes VMJ solar cells.

1.4.3 Terrestrial and Space Applications

As the deployment of CubeSats and other small satellites increases, the development of highly efficient and lightweight solar cells that can endure harsh terrestrial and space environments becomes essential [48, 49]. VMJ solar cells based on GaAs are particularly well-suited for satellite applications due to their high energy conversion efficiency, robustness against radi-

1.5. Outline of the thesis structure

ation, and ability to operate effectively at low temperatures. This research focuses on optimizing these solar cells for space missions, ensuring consistent power generation despite the limited surface area available on small satellites.

1.4.4 Photovoltaic Systems with Ultra-High Concentration

A promising strategy for enhancing sunlight conversion efficiency and reducing electricity generation costs is the use of UHCPV systems. These systems concentrate sunlight by a factor of over 1000 suns [50, 51]. By employing high-efficiency VMJ-GaAs solar cells, UHCPV systems can significantly cut costs by minimizing the required cell area. To fully realize the potential of UHCPV systems, this research tackles key technological challenges such as managing thermal effects and optimizing doping concentrations and layer thicknesses [32, 52].

1.4.5 Advanced Simulation Tools

Optimizing solar cell designs requires a systematic approach, which can be effectively achieved using advanced simulation tools like ATLAS Silvaco [53, 54]. These tools enable researchers to explore critical factors such as doping density, layer thickness, and sun concentration levels in a controlled environment. Through detailed modeling and virtual experimentation, researchers can fine-tune these parameters to enhance the efficiency and performance of solar cells. These simulations find solar cell structures that maximize efficiency and minimize production costs, resulting in broader adoption of renewable energy technologies.

1.5 Outline of the thesis structure

This thesis consists of six chapters, each structured to provide a cohesive narrative of the research. **The Introduction** outlines the background, advancements in photovoltaic technologies, the problem statement, research motivations, objectives of the study, and an overview of the thesis structure. **The Background** chapter explores the fundamental principles of photovoltaics, including the evolution of solar technologies, the physical and chemical foundations of photovoltaic systems, and the role of PN junctions. **The Literature Review** examines previous studies on multi-junction solar cells, with a focus on their configurations (homo and hetero-multijunction), concentrated photovoltaics, and the applicability of GaAs-based VMJ for satellite and terrestrial use. **The Methodology** chapter describes the process of simulation

using ATLAS Silvaco software, detailing the modeling of VMJ solar cells, essential simulation steps, and the specific adaptations for ultra-high concentration photovoltaic systems in CubeSats and terrestrial environments. **The Results and Discussion** chapter presents a thorough analysis of the simulation outcomes, including recombination models, device performance under varying conditions, and their practical implications. The final chapter, **Conclusions and Future Work**, summarizes the findings, discusses their relevance, and provides recommendations for further research. Additionally, the thesis includes **appendices** with supplementary materials, such as the ATLAS Silvaco code, alongside references and lists of figures and tables to enhance clarity.

1.6 Publications Based on this Research

This research has resulted in two publications showcasing contributions to advanced solar cell technologies. These publications are categorized based on the author's role, as detailed below: These two peer-reviewed publications form the scientific core of this doctoral thesis. They constitute the original contributions of the candidate and provide the main results, analysis, and conclusions developed throughout this research. Full documentation and licensing terms are provided in accordance with publisher policies. The following publications highlighting primary contributions to the development and analysis of solar cell systems:

1. **Ahmad A. Abushattal**, Antonio García Loureiro, Nour El I. Boukortt, "Ultra-High Concentration Vertical Homo-Multijunction Solar Cells for CubeSats and Terrestrial Applications," *Micromachines*, vol. 15, no. 2, pp. 204, 2024.

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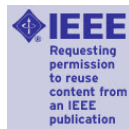
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1.6. Publications Based on this Research

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2. **Ahmad A. Abushattal**, Antonio García Loureiro, Nour El I. Boukortt, Sattam Almatarneh, “Simulation-Enhanced Insights for High-Concentration Solar Cells for Nano-Satellites,” *2023 2nd International Engineering Conference on Electrical, Energy, and Artificial Intelligence (EICEEAI)*, pp. 1–7, 2023.

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1.6. Publications Based on this Research

This section highlights the significant contributions in advancing high-efficiency solar cells, focusing on tandem and homo-multijunction designs and their applications in Cube-Sats and terrestrial systems. These publications underline the researcher's role in addressing challenges in efficiency, stability, and application-specific requirements for solar cell technologies.

1.7 Objectives of the thesis

- To present the study and performance for renewable energy resources in space and terrestrial applications through high-efficiency, low-cost vertical GaAs homo-multijunction solar cells.
- To characterize, simulate, and analyze such devices using the ATLAS-SILVACO simulator (TCAD) to achieve maximal conversion efficiency and fill factor under various ultra-high concentrator photovoltaic systems at different sun concentrations.
- To study and develop multi-junction structures to maximize efficiency using vertical tunnel junctions in reducing resistive losses at high concentration levels compared to standard designs.
- To study the effect of variation of intrinsic parameters such as layer thickness and doping concentration on the overall efficiency of the solar cells. We have designed a GaAs homo-multijunction solar cell adaptation for miniaturized satellites (CubeSat) and other terrestrial applications via high energy conversion efficiency and robustness.
- To compare the performances of these solar cells under various solar spectra (AM0 and AM1.5) and evaluate their suitability for space and terrestrial applications.
- To propose improvements in material properties and cell design optimizations for minimizing resistance losses, improving thermal management, and enhancing the fill factor. Integrate solar cells with energy storage systems to scale up technologies' commercial readiness and do the same for production cost reduction.

CHAPTER 2

BACKGROUND

2.1 Introduction to Photovoltaics

2.1.1 Overview of Solar Energy

In ancient civilizations, sunlight was used for heating and drying, and modern solar technology uses solar energy in various ways. Over the last few decades, solar energy utilization has advanced significantly in technology, and its potential to provide clean energy has become increasingly apparent [55,56]. Today, solar energy is a critical component of the global energy landscape, offering tremendous potential for sustainable development. Continuing innovation and supportive policies will make solar energy a cleaner and more resilient energy source for the future. In the 21st century, solar energy is one of the most abundant and environmentally friendly forms of energy. A significant role of solar energy is not only to reduce dependence on fossil fuels but also to mitigate climate change and promote sustainable development [57,58].

2.1.2 Solar Radiation

The sun emits electromagnetic waves that constitute solar radiation, the source of solar energy. Among the wavelengths of this radiation are visible light, ultraviolet light, and infrared light. To capture and convert solar energy, we must understand the solar spectrum [59,60]. Solar irradiance refers to the power transmitted by the sun's radiation per unit area, and it determines the amount of solar energy that can be generated. The solar constant represents the average irradiance received at the top of Earth's atmosphere, approximately 1361 watts per square meter. As a result of atmospheric conditions, geography, and time of year, the amount of solar

2.1. Introduction to Photovoltaics

radiation reaching the Earth's surface varies [61,62]. There is an uneven distribution of solar radiation globally, with more solar energy being received by regions closer to the equator than those further north and south. Several factors influence this variation, including angle of incidence, atmospheric scattering, and weather patterns. Solar energy systems should be placed and optimized based on an understanding of these variations [63,64].

2.1.3 The advantages of solar energy

Many advantages of solar energy make it a viable option for generating sustainable energy:

- **A renewable and sustainable resource:** solar energy is inexhaustible, unlike fossil fuels. Energy will continue to flow from the sun as long as it exists.
- **Benefits to the environment:** A solar power plant produces electricity without emitting greenhouse gases or other pollutants into the atmosphere. This approach reduces air pollution, mitigates climate change, and protects natural ecosystems. By optimizing solar cell designs and utilizing advanced simulation tools, researchers can create more efficient and environmentally friendly energy solutions [65,66].
- **Achieving energy independence and security:** Achieving energy independence and security can be closely linked to the use of solar energy. Solar power provides a sustainable and abundant energy source, reducing reliance on traditional energy grids and fossil fuels. Solar energy ensures a stable and reliable supply when combined with efficient storage systems like hydrogen production or batteries. This lowers environmental impact and promotes self-sufficiency, offering a practical pathway to a secure and sustainable energy future [67].
- **Economic Benefits:** The solar industry has experienced rapid growth, creating numerous jobs and boosting the economy. Investing in solar energy infrastructure offers long-term financial benefits, making it a wise and sustainable economic choice [68].

2.1.4 The future of solar energy

Continuing advancements and innovations are set to make solar energy more efficient, affordable, and seamlessly integrated into existing energy systems. Key developments include:

- **Technological Advancements:** Solar technologies such as photovoltaic (PV) cells, concentrated solar power (CSP) systems, and solar thermal energy are continually improving in efficiency and effectiveness [68].
- **Smart grids and energy storage integration:** To manage the intermittency of solar power effectively, innovative grid technologies and advanced energy storage solutions are crucial. Innovations in batteries and grid management are enhancing the reliability and flexibility of solar energy systems [69].
- **Role in Mitigating Climate Change:** As the world transitions to a low-carbon economy, solar energy is vital in reducing carbon emissions and combating climate change. It is central to climate action strategies, providing clean, sustainable power [70].
- **Support for policies and incentives:** The adoption of solar energy is significantly driven by government policies and incentives. Regulatory frameworks, subsidies, and tax incentives are essential to promote solar investments and accelerate their deployment [71].

2.2 History and Evolution of Photovoltaics

Photovoltaic technology has revolutionized how we harness solar energy thanks to significant discoveries and innovations. Solar power has evolved remarkably since the first observation of the photovoltaic effect over a century ago. The modern solar energy industry is built on a series of landmark milestones and technological advancements [72]. This section highlights key achievements and contributions from scientists and researchers who have been instrumental in developing this transformative technology. It has taken every step on this journey to transform solar power from a scientific curiosity into one of the most significant components of global energy [73]. This is from Alexander Edmond Becquerel's discovery of the photovoltaic effect in 1839 to the sophisticated solar cells used in today's cutting-edge applications. An overview of key events and technological advancements in photovoltaic technology is provided in the Table (2.1). It highlights the pioneering efforts of individuals who have significantly contributed to this field. It also highlights the historical progression of solar cell development [12, 27, 74].

2.3. The Foundations of Photovoltaics

Table 2.1: Timeline of Photovoltaics.

Year	Event	Details
1839	Discovery of Photovoltaic Effect	Alexandre Edmond Becquerel observed the effect on silver and platinum electrodes exposed to sunlight.
1873	Selenium Photovoltaic Effect	Willoughby Smith noticed resistance changes in selenium when exposed to light.
1877	First Solar Cell	Adams and Richard Day developed the first solar cell using selenium with an efficiency of 0.5%.
1878	Improved Solar Cell Efficiency	Charles Fritts doubled the efficiency of selenium solar cells.
1905	Photoelectric Theory	Albert Einstein proposed the photoelectric theory, explaining the relation between light and electron liberation.
1921	Nobel Prize	Albert Einstein was awarded the Nobel Prize for discovering the law of the photoelectric effect.
1939	Discovery of n- and p-type Silicon	Russell Ohl discovered the photoelectric effect in p-n junctions of silicon.
1940	First Silicon Solar Cell	Russell Ohl developed the first silicon solar cell at Bell Labs.
1954	Silicon Doping Process	Calvin Fuller developed a process to dope silicon, creating the first p-n junction with 6% efficiency.
1955	First Application in Telecommunications	A solar cell powered a telecommunication network in Americus, Georgia.
1958	Vanguard-1 Satellite	NASA launched the first satellite with a solar power system.
1958	Sputnik-3 Satellite	The Russian space program launched Sputnik-3 with a photovoltaic solar source.
1970s	Increased Silicon Solar Cell Efficiency	Joseph Lindmeyer developed a process to increase silicon solar cell efficiency by 50%.
1973	Solarex Foundation	Joseph Lindmeyer, and Peter Varadi founded Solarex, leading to increased photovoltaic technology adoption due to the oil crisis.
1980	Photovoltaic Market Growth	Solarex held approximately 50% of the photovoltaic industry market.
1970s-1980s	Introduction of Poly-Si and a-Si	Polycrystalline and amorphous silicon became popular due to lower manufacturing costs.
2000s-Present	New Solar Cell Generations	Development of flexible and painted solar cells, advancements in inverters, batteries, and overall system efficiency.
Present	NREL Efficiency Chart	National Renewable Energy Laboratory maintains a chart of the highest confirmed conversion efficiencies for research cells.

2.3 The Foundations of Photovoltaics

Solar energy is converted into electrical energy through semiconductors, a material that converts light energy into electricity. Understanding the fundamental principles of semiconductors and their application in photovoltaic systems is essential for understanding solar cell performance and efficiency. An atom is the physical unit of all materials, and these atoms determine how a material conducts electrical current. The electrical properties of an atom can be simplified into two parts: the valence shell and the core, which consists of the inner shells and the nucleus. This section's material is based on publications about the fundamentals of

photovoltaics and the references within [75–78].

Insulators

In normal conditions, an insulator does not conduct electrical current. Insulating materials generally are compounds rather than single-element materials, and their resistivities are incredibly high. Insulators have very few free electrons because valence electrons are tightly bound to their atoms. Rubber, plastics, glass, mica, and quartz are all insulators.

Conductors

Conductors are materials that readily conduct electrical current. Most metals are excellent conductors, especially single-element metals like copper (Cu), silver (Ag), gold (Au), and aluminum (Al). Conductors contain atoms with valence electrons, which can quickly become free electrons when the atom is loosely bound. This is called the valence electron in conductive materials.

Semiconductors

Semiconductors can similarly conduct electrical current to conductors and insulators. Semiconductors are neither good conductors nor good insulators in their pure form. A semiconductor that contains only one element, silicon (Si) and germanium (Ge). In addition to gallium arsenide and indium phosphide, gallium nitride, silicon carbide, and silicon germanium, compound semiconductors are also widely used. The most common semiconductor is silicon, which has four valence electrons.

2.3.1 Semiconductor Properties

Developing renewable energy technologies requires understanding the atomic structure and elemental composition of semiconductors like silicon and germanium. Conductors and insulators have different conductivities; semiconductors have a conductivity between them. Other semiconductors used in photovoltaics include gallium arsenide (GaAs) and cadmium telluride (CdTe). Silicon is the most commonly used semiconductor in photovoltaics, but other materials also are widely used.

Atomic structure and Energy Bands

The electrical properties of semiconductors make them ideal for solar cells, among other electronic devices—semiconductors function based on their atomic structure. Si and Ge, two semiconductors with distinct atomic structures, have different electrical properties. In contrast, gallium arsenide (GaAs) is a compound semiconductor that contains gallium (atomic number 31) and arsenic (atomic number 33). Silicon has 14 electrons, while gallium arsenide has 14 electrons. It is possible for thermal energy at room temperature to break some of the covalent bonds in a semiconductor, releasing the valence electrons. During the movement of these free electrons, holes are formed in the crystal lattice, which can be filled in by neighboring electrons that jump into these openings. The intrinsic carrier concentration n_i represents free electrons and holes in a semiconductor. Electrons can occupy continuous ranges of energy levels in semiconductors, separated by band gaps. In the valence band (VB), electrons involved in bonding are at their lowest energy levels, while in the conduction band (CB), they are at their highest. Between the conduction band minimum (E_C) and the valence band maximum (E_V) is the band gap energy (E_G):

$$E_G = E_C - E_V \quad (2.1)$$

The band gap energy of silicon at room temperature is approximately 1.12 eV, whereas that of GaAs is approximately 1.42 eV. Photovoltaic applications rely on the band gap to determine what wavelengths of light can be absorbed by the semiconductor.

Doping and Carrier Concentrations

Doping is the addition of impurity atoms to semiconductors to modify their electrical properties. A n-type semiconductor is created by introducing donor atoms with extra valence electrons, while a p-type semiconductor is made by introducing acceptor atoms with fewer valence electrons [76, 77, 79]. It is the intrinsic concentration carrier (n_i) that drives the concentrations of electrons (n) and holes (p) in doped semiconductors (**the mass-action law**):

$$np = n_i^2 \quad (2.2)$$

For an n-type semiconductor with donor concentration (N_D):

$$n \approx N_D \quad (2.3)$$

$$p = \frac{n_i^2}{N_D} \quad (2.4)$$

For a p-type semiconductor with acceptor concentration (N_A):

$$p \approx N_A \quad (2.5)$$

$$n = \frac{n_i^2}{N_A} \quad (2.6)$$

The elements in Group IV, such as silicon and germanium, are natural semiconductors. Several compounds from Group III-V, such as aluminum arsenide and gallium arsenide, and Group II-VI exhibit semiconductor properties. Doping refers to replacing an atom with an impurity in a lattice structure. Group III or Group V dopants add free carriers to the lattice structure, not disrupting electron bonds. A Group V element like arsenide can provide more electrons if added to silicon with a minimum concentration of 10^{16}cm^{-3} , much greater than the intrinsic electron density of pure silicon. The mass-action law causes an electron concentration to increase while the hole concentration decreases. A semiconductor with an n-type (n-doped) structure has 10^{16}cm^{-3} electrons per cm^3 and 10^4cm^{-3} holes per cm^3 . In contrast, a p-type (p-doped) semiconductor has a higher hole concentration because it uses Group III (acceptor) dopants. It is essential to create electronic devices and enhance their performance with the n-type semiconductor, which is dominated by negatively charged electrons, and the p-type semiconductor, which has positively charged holes.

2.3.2 Transport Properties

Transport properties play a critical role in understanding how semiconductor devices generate and control electrical currents. A net electrical current flows through the material during operational conditions, unlike equilibrium conditions, where no net current flows. Drift and diffusion are semiconductor transport mechanisms [80, 81].

- **Drift**

Drift occurs as a result of an electric field moving charge carriers. Charged electrons and holes are forced to move in an electric field when a force is applied. The electron drifts toward a positive potential, whereas the hole drifts toward a negative potential. Drift currents are determined by the mobility of carriers, their concentrations (n for electrons, p for holes),

2.3. The Foundations of Photovoltaics

their charges (q), and the electric field (E):

Drift current for electrons:

$$J_{\text{drift}} = q \cdot n \cdot \mu_n \cdot E \quad (\text{for electrons}) \quad (2.7)$$

Drift current for holes:

$$J_{\text{drift}} = q \cdot p \cdot \mu_p \cdot E \quad (\text{for holes}) \quad (2.8)$$

Here, (μ_n) and (μ_p) are the mobilities of electrons and holes, respectively. According to the electric field, mobility refers to how quickly carriers can move through the semiconductor.

• Diffusion

Charge carriers move according to electric field gradients and concentration gradients demonstrated by these equations.

Diffusion current for electrons:

$$J_{\text{diff}} = -q \cdot D_n \cdot \frac{dn}{dx} \quad (\text{for electrons}) \quad (2.9)$$

Diffusion current for holes:

$$J_{\text{diff}} = -q \cdot D_p \cdot \frac{dp}{dx} \quad (\text{for holes}) \quad (2.10)$$

where D_n and D_p are the diffusion coefficients for electrons and holes, respectively, and $\frac{dn}{dx}$ and $\frac{dp}{dx}$ are the concentration gradients of electrons and holes.

• Mechanisms of combined transport

Drift and diffusion processes often occur simultaneously in semiconductor devices. Drift and diffusion currents are added together to form the total current density in a semiconductor (J):

Total current density for electrons:

$$J_n = q \cdot n \cdot \mu_n \cdot E - q \cdot D_n \cdot \frac{dn}{dx} \quad (\text{for electrons}) \quad (2.11)$$

Total current density for holes:

$$J_p = q \cdot p \cdot \mu_p \cdot E - q \cdot D_p \cdot \frac{dp}{dx} \quad (\text{for holes}) \quad (2.12)$$

Charge carriers move according to electric field gradients and concentration gradients demonstrated by these equations.

2.3.3 Recombination Models

Semiconductors, including solar cells, rely heavily on recombination mechanisms for efficiency. Recombination occurs when electrons and holes annihilate each other, releasing heat or light. For semiconductor devices to perform optimally, it is essential to understand these mechanisms. Shockley-Read-Hall (SRH) recombination, Auger recombination, and radiative recombination are the primary mechanisms of recombination [82–84].

• Auger Recombination

The Auger recombination involves three carriers and is a non-radiative process. During this process, electrons in the conduction band combine with holes in the valence band, transferring their energy to a third carrier. As the recombination energy is converted into heat, the excited carrier eventually loses its excess energy through phonon interactions. During high injection conditions or in highly doped semiconductors, Auger recombination occurs at a higher rate with the cube of carrier concentration. The Auger recombination rate is expressed as:

$$R_{\text{Auger}} = C_n n^2 p + C_p n p^2 \quad (2.13)$$

where the Auger coefficients for electrons and holes are (C_n) and (C_p), and n and p indicate the electron and hole concentrations, respectively. Material with narrow bandgaps and high temperatures is particularly susceptible to Auger recombination.

• Radiative Recombination

During radiative recombination, electrons from the conduction band recombine with holes in the valence band, emitting a photon. A mechanism like this plays a crucial role in optoelectronic devices. Radiative recombination is calculated as follows:

$$R_{\text{rad}} = B_{\text{rad}} n p \quad (2.14)$$

B_{rad} is the radiative recombination coefficient. Based on radiative recombination, electrons and holes can have the following lifetimes:

$$\tau_{\text{rad,e}} = \frac{1}{B_{\text{rad}} p} \quad (2.15)$$

$$\tau_{\text{rad,h}} = \frac{1}{B_{\text{rad}} n} \quad (2.16)$$

2.3. The Foundations of Photovoltaics

Here, $\tau_{rad,e}$ represents the radiative recombination lifetime of electrons based on the hole concentration p . In a similar way, $\tau_{rad,h}$ is the radiative recombination lifetime of holes as a function of electron concentration n . Device efficiency is significantly affected by radiation recombination in direct bandgap semiconductors like GaAs.

• Shockley-Read-Hall (SRH) Recombination

As SRH recombination occurs non-radiatively, defect states and traps within the bandgap facilitate the process. This mechanism involves capturing a carrier by a trap and another carrier of opposite charge before the first is thermally re-emitted. The SRH recombination rate equation describes this process:

$$R_{SRH} = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad (2.17)$$

hole and electron lifetimes are given by τ_p and τ_n , respectively, electron density at trap level is given by n_1 and hole density by p_1 , and intrinsic carrier concentration is given by n_i . The recombination rate is significantly affected by the trap energy level. It is common to model SRH recombination empirically in materials with high defect densities.

• Combined Effects

Matthiessen-like rules combine all recombination mechanisms to determine minority carrier lifetimes in semiconductor devices:

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_{Auger}} + \frac{1}{\tau_{rad}} + \frac{1}{\tau_{SRH}} \quad (2.18)$$

This relationship illustrates how various recombination processes collectively affect carrier lifetimes and device performance.

2.3.4 Basic equations of device physics

There are three equations that are critical to the physics of PV devices: continuity equations, Poisson's equation, and current-density equations. Charge carriers are described by continuity equations, while electrostatic potential is explained by Poisson's equation, and electric current flows due to drift and diffusion by current-density equations. Designing and optimizing photovoltaic devices requires an understanding of these equations [61, 85].

Continuity Equations

Studying charge carriers within semiconductor materials requires continuity equations. Electric charge is conserved by these equations, which describe electron generation, recombination, and transport. These are the electron continuity equation and the hole continuity equation, respectively. Changes in electron or hole values within a semiconductor volume are balanced by differences in currents flowing into and out of the volume and carrier generation and recombination rates. The continuity equations are mathematically expressed as follows:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + G_n - R_n \quad (2.19)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + G_p - R_p \quad (2.20)$$

where (n) and (p) represent the electron and hole densities, J_n and J_p are the current densities, (G_n) and (G_p) are the generation rates, and (R_n) and (R_p) are the recombination rates.

Poisson's Equation

In semiconductor devices, Poisson's equation describes the electrostatic potential, which is related to the charge density within the device. This fundamental equation is crucial for understanding and modeling the behavior of electric fields and potentials in semiconductor materials. According to Gauss's law for electricity, this equation is expressed as:

$$\nabla^2 \psi = -\frac{\rho}{\epsilon} \quad (2.21)$$

(ψ) , is the electrostatic potential, (ρ) is the charge density, and (ϵ) is the permittivity of the material. The charge density (ρ) in a semiconductor includes contributions from electrons, holes, and ionized dopants. Ionized dopants, electrons, and holes all contribute to the charge density in semiconductors. For understanding charge carrier behavior, Poisson's equation and continuity equations can be solved within the device to determine the electrostatic potential and electric field.

Current-Density Equations

In the current density equations, charge carriers drift and diffuse, resulting in the flow of electric current. J_n and J_p are the current densities of electrons and holes, respectively:

2.4. PN Junction

$$\mathbf{J}_n = qn\mu_n\mathbf{E} + qD_n\nabla n \quad (2.22)$$

$$\mathbf{J}_p = qp\mu_p\mathbf{E} - qD_p\nabla p \quad (2.23)$$

where q is the electronic charge, electrons and holes have n and p concentrations, electrons and holes have mobilities μ_n and μ_p , and electric fields have E . D_n and D_p coefficients for electrons and holes, respectively. A drift current is represented by the first term in each equation, while a diffusion current is represented by the second term.

2.4 PN Junction

Solar cells convert solar energy to electricity (light-current conversion). The mechanism of the solar cell is based on three main processes: first, the photoelectric effect (photon absorption and charge generation), which is caused by the absorption material in the solar cell. Second, the P-N Junction Figure 2.1 separates charges, and finally, contacts collect electrons and holes [86, 87].

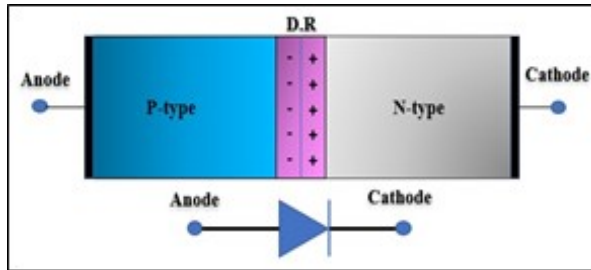


Figure 2.1: P-N junction at equilibrium with zero-bias voltage applied.

Due to differences in their impurities, n-type materials have slightly lower valence and conduction bands than p-type materials. As shown in Figure 2.2, the bands in the n region are lower than those in the p region and overlap. A free electron in the n region can quickly diffuse into the conduction band of the p region, losing energy and filling holes in its valence band. A depletion region forms with continued diffusion, lowering the energy level of the conduction band in the n-region. As shown in 2.3, when all electrons in the n-region conduction band

have exhausted their energy, they reach equilibrium and complete the depletion region. Electrons in the n-region benefit from an energy gradient across the depletion region. The energy gap between valence and conduction bands is constant regardless of band-level shifts so that valence electrons can become free electrons with the same amount of energy [86].

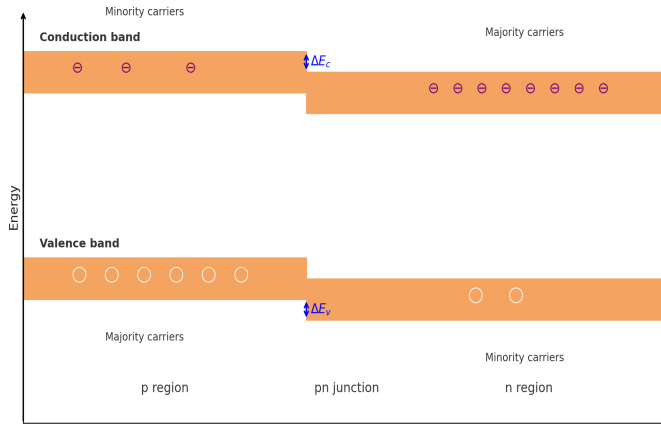


Figure 2.2: At the instant of the formation of the PN junction, the depletion region, and the energy diagram.

Doped semiconductors act as semiconductor devices on their own. Upon applying a voltage to contacts, charge carriers move in response to the electric field, causing current to flow. Nevertheless, the current flow is not as efficient as in a conductor, indicating that the charge carriers are fewer, resulting in a resistor-like behavior. A PN junction or diode is formed by joining p-doped (positive) and n-doped (negative) semiconductors. At the junction, a concentration gradient of charge carriers is formed. A diffusion current is generated by electrons diffusing from the n-doped region to the p-doped region and holes diffusing in the opposite direction. As a result of this diffusion, the space charge neutrality is disrupted, where protons and electrons are equal in any given region. Since the dopant atoms cannot move from their lattice positions, they contribute to a local electric field. Space charge neutrality is related to:

$$N_D + p = N_A + n \quad (2.24)$$

where the concentration of donor dopants is N_D , the concentration of acceptor dopants is N_A , the concentration of electrons is n , and the concentration of holes is p . In the depletion

2.4. PN Junction

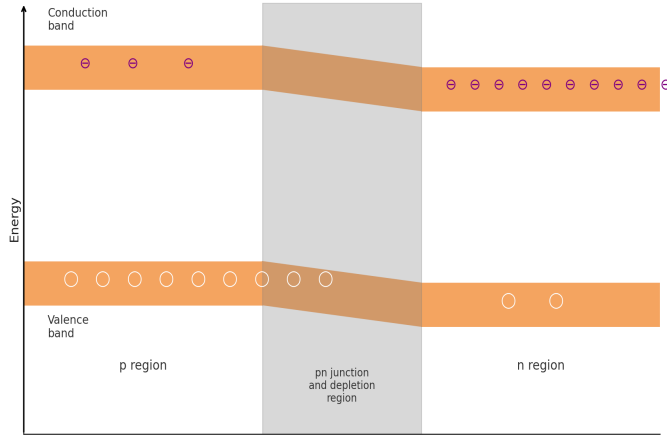


Figure 2.3: An energy diagram illustrating PN junction formation and depletion regions in equilibrium.

region, electrons fill the p-doped and n-doped sides, leaving no mobile charge carriers behind. When diffusion occurs across a junction, the electric field generates an opposing drift current. Charge carriers cannot move further across the junction until the drift and diffusion currents reach equilibrium. An important parameter is the built-in voltage V_b across the depletion region, which is defined as follows:

$$V_b = \frac{k_B T}{q} \ln \left(\frac{N_D N_A}{n_i^2} \right) \quad (2.25)$$

k_B is Boltzmann's constant, T is the temperature, q is the electronic charge, and n_i is the intrinsic carrier concentration. Applying an external voltage across the junction modifies minority carrier concentration exponentially, as described by:

$$p_n = p_n^0 \exp \left(\frac{qV_a}{k_B T} \right) \quad (2.26)$$

and

$$n_p = n_p^0 \exp \left(\frac{qV_a}{k_B T} \right) \quad (2.27)$$

A minority carrier concentration in an n-type region is p_n , while in p-type is n_p . The voltage applied is V_a . Applied voltage affects the current flowing through the device, which follows the Shockley diode equation:

$$I = I_0 \left(\exp \left(\frac{qV_a}{k_B T} \right) - 1 \right) \quad (2.28)$$

I_0 represents reverse-bias saturation current. PN junctions are fundamental components in modern electronics, e.g., solar cells, LEDs, and diodes.

2.5 Solar Cells

2.5.1 Solar Spectrum

Various wavelengths of electromagnetic radiation are emitted by the sun throughout the day and according to geographical location. Standards reference spectra have been established to ensure consistency and accuracy in evaluating the performance of photovoltaic devices produced by different companies and research laboratories. As a result of these standards, solar devices can be assessed under consistent conditions and compared [78, 88].

AM0 and ASTM E-490

ASTM E-490 defines the AM0 (Air Mass Zero) spectrum for space applications. An integrated power of 1366.1 W/m^2 is available in this spectrum. It is applicable outside Earth's atmosphere. Despite being constant in shape, the AM0 spectrum varies in magnitude as a function of the distance from the sun. Describes the solar spectrum without interference from the atmosphere in space see Figure 2.4 [89].

AM1.5 and ASTM G-173-03

ASTM G-173-03 defines two terrestrial standards spectrums at the surface of the Earth, taking into account atmospheric effects (see Figure 2.4) [7, 90] :

- **AM1.5 Global Spectrum:** This spectrum is designed for flat-plate photovoltaic modules with an integrated power of 1000 W/m^2 (100 mW/cm^2).
- **AM1.5 Direct Spectrum:** An integrated power density of 900 W/m^2 is combined with both direct and circumsolar components within a 2.5-degree disk around the sun to work as solar concentrators .

2.5. Solar Cells

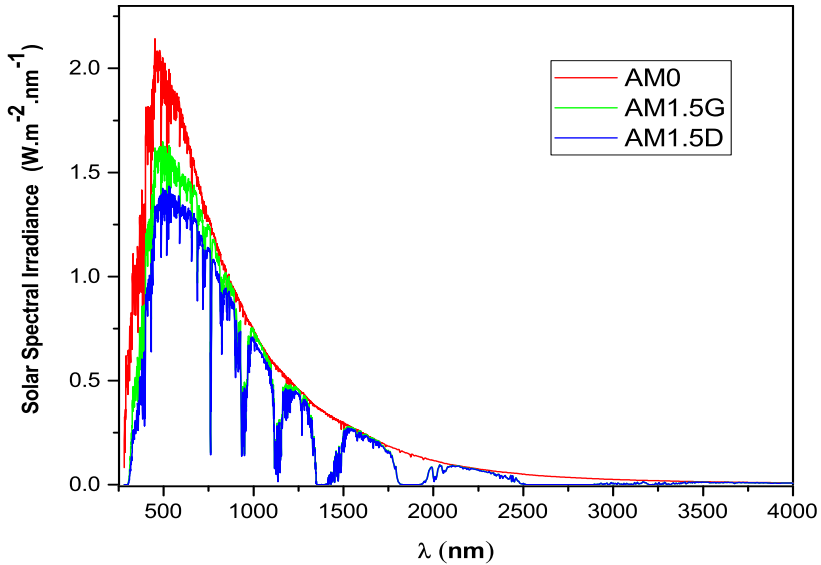


Figure 2.4: Standard Solar Spectra for space and terrestrial Applications.

2.5.2 The Structure Photovoltaic Cell

Solar cells are complex interplays of materials and engineering designed to maximize solar energy conversion. Each layer serves a specific purpose, such as reducing reflection and collecting charge carriers, to improve sunlight to electricity-conversion. A photovoltaic cell can be divided into the following categories based on its structure and efficiency [12,91,92]:

Anti-Reflective Coating

Photovoltaic cells utilize anti-reflective coatings to reduce light reflection and increase semiconductor light absorption. Typically, silicon nitride or titanium dioxide is used as this coating, which minimizes reflections and improves cell efficiency.

Front Contact

In photovoltaic cells, light generates electrons through thin metal lines on the front contact. Designing the cell to capture as much light as possible while ensuring sufficient conductivity for the collected charge carriers is essential. The engineering of the front contact must balance transparency and electrical conductivity to optimize performance [36].

P-N Junction

A photovoltaic cell consists of semiconductor layers that form a p-n junction. This junction includes a thin n-type semiconductor layer doped with donors to supply extra electrons and a thicker p-type layer doped with acceptors to create positive charge carriers. The interaction between these layers converts light into electricity.

Back Contact

Back contacts are metal layers on the rear side of the cell that collect holes and complete the electrical circuit. Typically, aluminum or other conductive metals are used in this layer, ensuring efficient extraction of electrical current from the cell and its delivery to the external load.

Encapsulation and Protection

Photovoltaic cells must be encapsulated and protected to ensure longevity and durability. The encapsulant layer, usually made of ethylene-vinyl acetate (EVA), cushions and insulates the cell. The front cover is tempered glass to protect the cell from physical damage, while the back sheet is made of durable plastic for additional protection and insulation.

2.5.3 Efficiency of Photovoltaic Cells

The efficiency of a semiconductor is influenced by its band gap, recombination losses, temperature, and light absorption. Materials science and technology advances are making photovoltaic (PV) cells more efficient and cost-effective, enhancing the viability and sustainability of solar energy [93, 94].

2.5. Solar Cells

Band Gap Optimization

In semiconductor materials, the ideal band gap is approximately 1.4 eV, which aligns well with the spectrum of sunlight. A semiconductor with this optimal band gap can effectively absorb and convert a wide range of photon energies into electricity.

Minimizing Recombination Losses

During electron-hole recombination, the number of charge carriers available for generating power is reduced as electrons and holes recombine before contributing to the electrical current. Minimizing these losses on the surface and within the semiconductor material is essential for improving cell efficiency.

Temperature Management

It is also important to note that temperature affects photovoltaic cell efficiency. The recombination rate increases at higher temperatures, and the open-circuit voltage decreases, reducing the cell's efficiency. Temperature management and cooling are crucial for mitigating these thermal losses and maintaining high performance.

Reflection and Absorption Enhancement

Higher efficiency can be achieved by minimizing reflections and maximizing sunlight absorption. Anti-reflective coatings are designed to reduce reflections, while semiconductor layers are designed to increase light absorption. Photovoltaic cells are significantly more efficient if they capture and convert all the available sunlight into electrical energy.

2.5.4 Solar Cell Operation

Solar cells are fundamentally PN junctions exposed to light. As excess carriers pass through the intersection, an electric field is generated along the edges, generating a photocurrent current that can power external circuits. The built-in voltage is present whenever no current flows through a cell. Voltage decreases exponentially with increasing current. The current-voltage (IV) curve shows this, where V_{OC} (open circuit voltage) represents the maximum voltage, and I_{SC} (short circuit current) represents the maximum current. During the "knee" of the IV curve, the maximum power point of a solar cell occurs. Depending on the recombination process,

fewer carriers may be available, resulting in reduced efficiency. Two processes are required for a current generation: photon absorption to create electron-hole pairs and p-n junctions to separate these carriers. The distance carriers need to travel relative to diffusion length determines the probability of collection [89,95,96]. Short-circuit current (I_{sc}), open-circuit voltage (V_{oc}), and fill factor (FF) are all important parameters when estimating a solar cell's performance. A short-circuit current density (J_{sc}) describes the maximum current density generated at zero voltage from a solar cell, where I_L is the light-generated current:

$$I_{sc} = I_0 \left(e^{\frac{qV}{nkT}} - 1 \right) - I_L \quad (2.29)$$

In a zero-current open-circuit, the voltage (V_{oc}) is the maximum voltage:

$$V_{oc} = \frac{nkT}{q} \times \ln \left(\frac{I_L}{I_0} + 1 \right) \quad (2.30)$$

Solar cells' performance is measured by their fill factor (FF), the ratio between the maximum power and the theoretical power they would produce at both open and short circuit voltages and currents combined:

$$FF = \frac{I_{mp} \times V_{mp}}{I_{sc} \times V_{oc}} \quad (2.31)$$

All previous parameters yield the calculation of the maximum power:

$$P_{max} = J_{sc} \times V_{oc} \times FF \quad (2.32)$$

Silvaco uses simulations and analyses to calculate solar cells' FF under specific conditions. At the beginning of the development process, the user defines solar cell materials, dopings, and layer profiles. Simulations simulate real-world operating scenarios by applying boundary conditions such as illumination and electrical parameters. Solving complex semiconductor equations determines solar cells' current-voltage (I-V) characteristics.

Key circuit parameters such as open-circuit voltage and short-circuit current can be determined using this I-V curve. I-V curves have a maximum power point (P_{max}) at the point where the product of current and voltage reaches its maximum. Solar cells are measured by their fill factor according to the formula below.

$$FF = P_{max} / (V_{oc} \times J_{sc}) \quad (2.33)$$

2.6. Advances in Photovoltaic Semiconductor Materials

Finally, the efficiency (η) of the solar cell can be calculated by comparing the output power (P_{out}) to the input power (P_{in}):

$$\eta = \frac{P_{out}}{P_{in}} \quad (2.34)$$

Substituting P_{out} :

$$\eta = \frac{J_{sc} \times V_{oc} \times FF}{P_{in}} \quad (2.35)$$

2.5.5 Factors Influencing the Performance of Solar Cells

Solar cell performance depends on many parameters, and we will present some of the most important ones.

Factors Reducing Solar Cell Performance

Several factors reduce the performance of solar cells. The cells' efficiency is considerably reduced due to the natural reflection of light from their surfaces; on untreated surfaces, 36%

Factors Improving Solar Cell Performance

On the other hand, several conditions could improve the solar cells' performance. A p+ layer under the cell is known as a back surface field (BSF), and it boosts the V_{OC} and I_{SC} , giving it a higher FF and hence increasing the efficiency of the cells. For example, anti-reflection coatings, like Silicon Oxide (SiO_2), and surface texturing decrease reflected light to a level of 36% to as low as 5% [97]. Surface texturing alone can raise the efficiency of the solar cell by around 8%. Placing a reflector on the back surface of a solar cell such that the back surface acts like a mirror and reflects the incident light through the cell increases efficiency by 3%. A last technique to improve the efficiency of the solar cells is using multi-layers on the finished product [48, 98]

2.6 Advances in Photovoltaic Semiconductor Materials

In the coming decades, researchers will continue to develop new materials and technologies to improve solar cells' efficiency and versatility, making solar power a more competitive and sustainable option for powering the world's electrical needs. A sustainable energy future requires continued investment in semiconductor research and development. Semiconductor

materials have recently been developed to overcome the limitations of silicon-based cells [10, 21, 99, 100]. There are several of the most promising technologies:

Multijunction Solar Cells

In multijunction solar cells, multiple layers of different semiconductors are used for different band gaps, capturing a broader range of the solar spectrum and achieving higher efficiencies. The layering of these semiconductors allows these cells to convert more sunlight into electricity than single-junction cells. Each layer absorbs a specific portion of the solar spectrum, reducing thermal losses and enhancing efficiency. For example, the top layer of a multijunction solar cell might capture high-energy blue and ultraviolet light, while the middle and bottom layers capture green and yellow light, respectively. This stratified approach enables multijunction cells to achieve efficiencies over 40% [101, 102].

Perovskite Solar Cells

Perovskite solar cells represent an emerging technology characterized by low production costs and high efficiency. These cells have an active layer composed of a perovskite-structured compound. The attractiveness of perovskites lies in their low cost and simple manufacturing processes, such as solution processing. However, long-term stability and performance challenges remain as perovskite materials deteriorate under high temperatures and moisture conditions. Through materials engineering and encapsulation techniques, efforts are underway to enhance their durability. If these issues are resolved, perovskite cells' high efficiency and affordability could revolutionize the solar industry [103, 104].

Thin-Film Technologies

Thin-film technology allows for creating flexible and lightweight solar panels by utilizing thin layers of semiconductor materials, significantly reducing material costs. Common materials used in thin-film solar cells include cadmium telluride (CdTe), copper indium gallium selenide (CIGS), and amorphous silicon (a-Si). These technologies offer several advantages over traditional silicon cells, including lower material consumption, lighter weight, and the ability to be manufactured on flexible substrates. This makes thin-film solar cells suitable for various applications, such as portable solar chargers and building-integrated photovoltaic sys-

2.6. Advances in Photovoltaic Semiconductor Materials

tems (BIPV). Today, the research aims to improve the efficiency of thin-film cells compared to crystalline silicon cells [105, 106].

CHAPTER 3

LITERATURE REVIEW

3.1 Multi-junction solar cells

The multi-junction solar cell (MJSC) is a leading technology in photovoltaics, offering efficiencies far better than traditional single-junction solar cells. Under standard test conditions, single-junction cells have an efficiency limit of approximately 33.7% due to the Shockley-Queisser limit. The MJSC, on the other hand, consists of layers (junctions) of different semiconductor materials, each with its bandgap [107, 108]. The design of these cells allows them to capture a broader spectrum of sunlight and convert it into electricity more effectively. Consequently, thermalizing and transmitting losses are minimized. MJSCs began to develop in the 1950s, with significant advancements occurring over the next several decades [72]. Due to its superior efficiency to silicon, Gallium Arsenide (GaAs) was initially used in MJSCs. Dual-junction (DJ) cells were the first significant milestone, followed by triple-junction (TJ) cells. The efficiency of the MJSC has been further improved by recent advancements at the National Renewable Energy Laboratory (NREL). NREL has developed III-V multijunction cells based on inverted metamorphic multijunction (IMM) architecture [89, 109]. Due to their high performance and radiation tolerance, these cells achieve efficiencies over 45% under concentrated sunlight [89]. A graded buffer layer is added to the top and middle cells before transitioning to the bottom cell. A specific portion of the solar spectrum is absorbed by each cell see Figure 3.1 [107]. This reduces defects in the structures. A typical MJSC structure consists of multiple P-N junctions connected in series by tunnel diodes. High efficiency has been achieved through improvements in doping concentrations, layer thicknesses, and surface passivation. Quantum efficiency can be enhanced by reducing recombination losses and enhancing quan-

3.1. Multi-junction solar cells

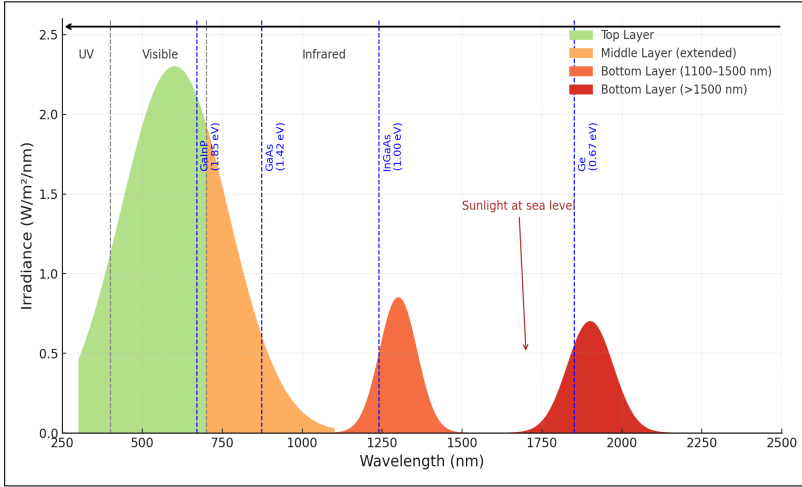


Figure 3.1: The absorption of solar radiation by multijunction solar cells.

tum efficiency. The main application for MJSCs is high-performance applications such as space missions, which require efficiency and durability. Concentrated photovoltaic (CPV) systems for terrestrial applications are becoming increasingly popular. Future development of MJSC technology will focus on increasing the number of junctions, including four-, five-, and six-junction cells. Concentrated sunlight can achieve efficiencies of over 45% with these configurations. To make these advancements, it is expected that new materials such as GaInNAs and InGaAsSb, as well as antireflective coatings and thermal management systems, will be vital [101, 110].

In recent years, modeling and simulation have emerged as critical tools in advancing multijunction solar cells (MJSCs), offering a cost-effective means to evaluate device performance before physical fabrication. In solar cell efficiency studies, researchers have been able to predict the effects of structural, thermal, and spectral changes using numerical simulation platforms such as Silvaco ATLAS, COMSOL Multiphysics, and detailed-balance models. The work of Hu et al. [111] shows how variations in doping profiles, layer thicknesses, and defect positions directly affect the performance of GaInP/InGaAs/Ge triple-junction cells. In a paper published in 2024, Nieto et al. [112] demonstrated that III-V MJ cells, even at ultra-high concentrations (up to 2200 suns), are thermally and spectrally dependent, underlining the importance of accounting for temperature-induced efficiency losses in simulations. Testa et al. [113]

also examined radiative cooling strategies for MJ cells using detailed-balance modeling, finding that passive cooling can yield notable efficiency gains in low- to moderate-concentration settings. In addition to mathematical modeling, analytical methods have gained support. For example, Nouri et al. [114] presented a simplified five-parameter estimation model tailored for multijunction cells, improving the accuracy of simulations of equivalent circuits based on diodes. Further, Beepat et al. [115] and Raisa et al. [116] demonstrated that interface optimization, spectral current matching, and tandem integration (e.g., III-V/Si combinations and perovskites/Ge combinations) increase conversion efficiency, based primarily on simulations. Not only have simulations proved valuable for designing and refining MJSCs, but they have also proven helpful in guiding experimental efforts, enabling new configurations, and guiding experimental refinement.

3.2 Homo and Hetero-multijunction solar cell

Homojunction solar cells are those in which the same semiconductor material is used throughout the device. In these cells, p-type and n-type regions are formed within the same semiconductor material using different dopants [117]. The most common example of a homojunction solar cell is a conventional silicon solar cell. These cells have been proven reliable, and as such, they have been widely produced over the years since their manufacturing processes were established. The benefits of homojunction solar cells include their simplicity and cost-effectiveness. Homojunction solar cells are relatively simple and, therefore, inexpensive to produce. This simplicity arises because these cells do not require the complex structures and processes needed for more advanced designs, often demanding significant materials and expertise. The homojunction cells have been developing and researching for years and have built a strong performance track record with a market presence. Furthermore, these cells are reputed to be stable and highly reliable long-term with different environmental conditions [118]. **Heterojunction** solar cells are built using two semiconductor materials of the p-type and n-type layers. The betterment of heterojunction solar cells provides enhanced efficiencies, minimizing recombination losses at the interface of the two materials. The difference in material band gaps can be exploited to make them optimal for light absorption and carrier collection. Besides, the different materials systems may provide a better band alignment and flow of charge carriers through them for improved cell performance [119, 120].

The study on homojunction GaAs solar cells is fascinating because of the fantastic prop-

3.3. Concentrated Photovoltaics

erties of Gallium Arsenide (GaAs), a III-V semiconductor known for excellent photovoltaic properties. The GaAs solar cells have presented high conversion efficiency compared with silicon-based cells. This results from the direct bandgap of GaAs, which would enable very efficient light absorption and effective conversion of photons into electrical energy. In addition, GaAs-based solar cells have shown excellent radiation hardness, for example, compared to silicon cells, even in space applications where cosmic radiation levels are exceptionally high, which would probably bring most other solar cell types out of commission. The cells can maintain their efficiency at high temperatures, making them suitable for terrestrial applications in hot climates and space missions [121]. Gallium arsenide (GaAs) solar cells are particularly advantageous because they can be lightweight and generate high power with a small surface area. This makes them ideal for CubeSats and other miniaturized satellites, where space and weight constraints are critical.

3.3 Concentrated Photovoltaics

Concentrated Photovoltaics (CPV) are designed to focus sunlight on small, high-performance solar cells. These systems can achieve efficiencies up to 47.6% under certain conditions [89]. This approach requires less expensive semiconductor material, significantly reducing the overall system cost. CPV systems are categorized based on their concentration ratios [122–124]:

1. Low Concentration: less than 10 suns.
2. Medium Concentration: More than 10 - 100 suns.
3. High Concentration: More than 100 - 1000 suns.
4. Ultra-High Concentration (UH): More than 1000 suns.

By concentrating sunlight, CPV systems maximize the efficiency of solar cells and make solar energy more cost-effective. UHCPV systems appear to be a valuable option for the effective and economically viable utilization of solar energy, returning efficiencies above 30%. Still, their wide application is hampered by losses of series resistance. However, thermal management has always been a concern with CPV systems, where elevated sunlight concentration raises solar cell temperatures, potentially resulting in lower efficiency and degraded lifetimes [125]. Concentrators and CPV systems are relatively new technologies, with a lot of current research activity in most areas. Recent research is concentrated on improving the optical

designs of concentrators, developing advanced cooling techniques, and integrating CPV systems with other energy technologies—innovations in material science and optical engineering aim at performance improvements and cost reductions. Continued research into CPV is focused on developing new materials for multi-junction solar cells capable of capturing a more extended section of sunlight, improvement in concentrator designs to maximize light capture and minimize losses, and innovation in cooling techniques to handle high-concentration systems with maximum efficiency. Other major trends in research are pointing toward coupling the CPV systems with other energy technologies to increase performance and reliability at the system level [102]. HCPV is one of the most promising technologies for improving efficiency and reducing the cost of solar energy. Further developments in materials science, optical engineering, and system design are crucial to achieving the full potential of CPVs for use on a large scale on the ground.

3.3.1 The Role of Ultra-High Concentrator Photovoltaics

Solar cells are becoming increasingly popular due to their widespread use on the ground and in space. In this application, the highest efficiency in converting solar radiation to electric power is one of the most critical objectives. Photovoltaics with high concentrations are designed to increase sunlight conversion efficiency and reduce electricity costs. The term UHCPV refers to CPV systems that have a power rating greater than 1000 suns. This type of technology is considered to be one of the most promising avenues for achieving low-cost and high-efficiency CPVs. By reducing the cell area, these extreme concentrations can dramatically increase theoretical efficiency while reducing the economic costs of the whole system [126, 127]. Despite the potential of UHCPVs, they are still in the early stages of development. Further analysis of different solar cell architectures with the most excellent efficiency for UHCPVs is required. Developing high-efficiency and low-cost new-generation technology is essential to achieve CPV systems with a concentration factor (Cratio) of over 1000 suns. As concentration ratios increase, solar cells become more efficient, and semiconductor materials become cheaper. The performance of photovoltaic cells is also improved by using ultra-high concentrations of concentrated light. Nowadays, CPV systems often consist of multijunction structures using multiple III-V semiconductors [128]. Multijunction fabrications can lead to a greater efficiency of solar energy, with a higher absorption coefficient. It has been proven that direct bandgap materials are highly effective in multijunction solar cells both on land and in space, producing highly efficient devices. Furthermore, multijunction solar cells are extremely ef-

3.3. Concentrated Photovoltaics

ficient, utilizing the vast majority of the solar spectrum, leading to very little power loss compared to monojunction solar cells. There are only two electrical connections on these cells: a top terminal and a back terminal [52, 129]. There are inevitable trade-offs between metal grid shadowing and series resistances (R_s). There seems to be a limitation in the ability of top-metal cell patterns or cells with a smaller area to reach UH levels. In contrast to current architecture, VMJ architecture reduces the R_s limitations. Each of these cells consists of several sub-cells connected by metallic contacts.

Researchers are exploring UHCPV, or solar cells exposed to 1000 sun concentrations. By using lenses or mirrors, concentrator photovoltaics (CPV) achieve high concentrations. The method improves efficiency significantly, especially for multijunction solar cells, which are high-cost but have superior efficiencies. Reducing material costs requires increasing efficiency. Secondly, concentrating sunlight could reduce the need for expensive photovoltaic material, which would improve solar energy's competitiveness. As a third reason, highly efficient, tiny solar cells are easier to deploy in space applications due to their low weight and space requirements [126, 127]. Further, this high-concentration approach enhances research in photovoltaic material science, enabling the development of new materials that are durable and efficient while pushing existing technologies to their limits. The soaring global energy demand and limited land are two reasons high-concentration solar systems become increasingly attractive for large-scale installations. Consequently, testing solar cells exposed to up to 10,000 rays of sunlight involves improving efficiency and assessing economic viability, material innovation, and space application possibilities.

3.3.2 GaAs Multi-Junction Solar Cells for Space and Terrestrial Applications

Multi-junction solar cells represent a class of very efficient photovoltaic devices wherein several semiconductor layers are applied to capture more sunlight in the spectrum. Such solar cells are essential for space applications, as they have high efficiency and are radiation resistant. Further, they have just recently started to get explored in terrestrial applications, mainly in concentrator photovoltaic (CPV) applications. For this reason, MJSCs are essential in space applications because of their significant efficiency and resilience against high radiation doses. These cells, typically based on III-V compound semiconductors, can have efficiencies of over 30% [130]. Such high efficiencies are actualized by engineering the MJSCs to operate under one-sun AM0 spectral conditions equivalent to the solar spectrum observed in space. For

instance, AZUR SPACE has fabricated MJSCs, demonstrating a beginning of life (BOL) performance of 30.6%. Furthermore, they exhibit exceptional radiation hardness. End-of-life (EOL) efficiencies of up to 25.8% have been achieved after irradiation with 1×10^{15} 1 MeV electrons/cm² [131, 132].

Space-qualified MJSC development began in the late 1990s, with key players being companies based in the US and European Union through Fraunhofer ISE and AZUR SPACE. This fact changes MJSCs into the most valuable cells in satellites and space vehicles, where their high efficiency and low weight are essential to compensate for the high cost of launching materials into space [133]. The primary material used in MJSCs that have gained much use for their space application is gallium arsenide (GaAs), having high resistance to radiation and heat, a direct bandgap, and allowing electrons to move six times faster than silicon. These properties make GaAs a good candidate for high-frequency applications and environments with high radiation exposures. GaAs is widely used in CubeSats, miniaturized satellites designed for many kinds of interplanetary missions [134, 135]. PhoneSat 2.5 was launched in 2013 as a CubeSat built by NASA Ames Research Center with GaAs technology, has dimensions of 10 cm by 10 cm by 11.35 cm, and weighs 1.5 kg. The Japan Aerospace Exploration Agency (JAXA) proposes using CubeSat technology to launch a solar power satellite (CS-SPS). CubeSats can serve various purposes and be placed in multiple locations depending on their mission. CubeSats are used for various missions in low earth orbit (LEO), including Earth observation and remote sensing. There are many applications for CubeSats, including navigation and communication. A CubeSat that is launched into medium earth orbit (MEO) is located between 2,000 and 35,786 kilometers above the surface of the earth. The geostationary earth orbit (GEO) CubeSat is a satellite that transmits and receives data from an altitude of 35,786 km. Scientists use CubeSats in lunar orbit to conduct scientific research and to explore the Moon's surface. CubeSats have been used in several interplanetary missions, such as Mars Cube One (MarCO).

Thanks to their material properties and resilience to low temperatures, multijunction solar cells made of Gallium Arsenide (GaAs) are excellent for space and terrestrial applications. Due to their high energy conversion efficiency, lightweight design, and robustness against space radiation and temperature fluctuations, GaAs solar cells are highly recommended in space, especially for miniaturized satellites. Despite the limited surface area of solar panels on nano-satellites, these cells provide reliable power generation even when weight constraints are critical.

3.4. Vertical Multijunction Solar Cell (VMJ)

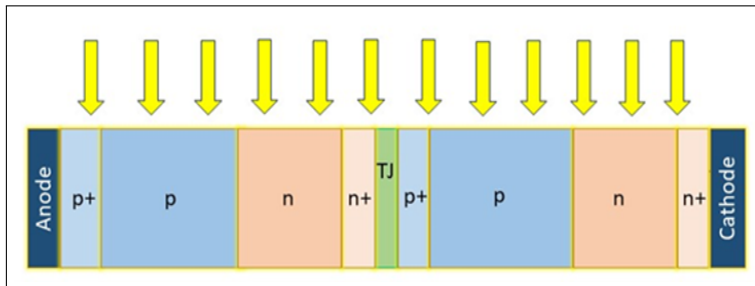


Figure 3.2: Schematic diagram of the VMJ structure.

3.4 Vertical Multijunction Solar Cell (VMJ)

Photovoltaic technology has advanced significantly with the advent of VMJ solar cells. Unlike traditional planar solar cells, VMJ cells are designed with PN junctions oriented vertically to the incident light [78]. This unique configuration reduces shading and series resistance issues, making them highly efficient under high-concentration conditions. The concept of VMJ solar cells is proposed as a solution to the limitations of planar solar cells under high-concentration solar illumination [52, 129]. Early VMJ designs aimed to mitigate the significant efficiency losses caused by series resistance and shading in conventional solar cells. By vertically orienting the junctions, VMJ cells allowed for a larger effective area for light absorption without the drawbacks of front and back contact contact.

3.4.1 Design and Advantages of VMJ

VMJ solar cells typically consist of multiple PN junctions connected in series or parallel, each receiving light vertically see Figure 3.2. This structure is advantageous because it eliminates the shading effect caused by metal grids in traditional cells and reduces series resistance significantly. Additionally, VMJ cells operate at high voltage and low current, which enhances their compatibility with various power processing loads and improves their performance under non-uniform illumination conditions.

3.4.2 Recent Advancements of VMJ

Recent advancements in VMJ technology have focused on optimizing these cells' materials and structural properties to maximize their efficiency. For example, gallium arsenide (GaAs)

has been extensively studied for its high conversion efficiency. A novel vertical tunnel-junction (VTJ) structure has been developed, featuring laterally positioned anode and cathode sub-cells connected by tunnel junctions. This design allows for efficient usage of direct bandgap semiconductor materials, significantly enhancing performance under UHCPVs.

3.4.3 The Applications of VMJ

Vertical multijunction (VMJ) solar cells are particularly suitable for applications requiring high efficiency and compact form factors, such as CubeSats and other space missions. Their ability to maintain high efficiency under ultra-high light concentrations makes them ideal for terrestrial and space-based applications. Their high voltage and low current operation also reduces heat generation and improves overall system reliability. VMJ solar cells represent a promising technology in the field of photovoltaics. Their unique vertical configuration addresses many efficiency limitations of traditional planar solar cells, making them suitable for high-concentration solar applications. Continued research and optimization of materials and cell structures are expected to enhance the performance and applicability of VMJ solar cells.

CHAPTER 4

METHODOLOGY : ATLAS SILVACO SIMULATION

4.1 Atlas Silvaco

Atlas Silvaco is a powerful and comprehensive simulation software platform extensively used in photovoltaics (PV). Developed by Silvaco, Inc., a global leader in electronic design automation (EDA) software, Atlas provides robust tools for modeling and simulating semiconductor devices [54, 136]. In photovoltaics, it is instrumental in optimizing the design and performance of solar cells, allowing researchers and engineers to simulate and analyze complex physical phenomena within PV devices. Silvaco, Inc. was founded in 1984 by Dr. Ivan Petic to deliver innovative and high-performance EDA tools for semiconductor design and manufacturing. The Atlas software suite, a flagship product of Silvaco, was developed to provide detailed simulation capabilities across various semiconductor devices, including those used in photovoltaics [137]. The adoption of Atlas in photovoltaics began as the demand for renewable energy sources grew, and the efficiency of solar cells became a critical focus. Solar cells can be simulated electrically, optically, and thermally, making the software an essential tool for researchers seeking to improve the efficiency of PV systems. In the early 2000s, with the increasing global emphasis on sustainable energy solutions, Atlas Silvaco gained prominence in academic and industrial PV application research. It enabled detailed analysis and optimization of novel materials and cell structures, significantly contributing to advancements in the field. Silvaco's continuous updates and enhancements to Atlas have kept it at the fore-

front of PV simulation technology [138, 139]. The integration of Silvaco with other tools, such as Victory Device and Victory Process, has further extended its capabilities, providing a comprehensive environment for developing next-generation photovoltaic devices. Today, Atlas Silvaco is widely used by researchers, engineers, and designers to simulate and optimize various PV technologies, including silicon-based, thin-film, and organic solar cells. Its detailed modeling capabilities help understand and improve device performance, pushing the solar energy industry's boundaries of efficiency and innovation. Atlas Silvaco's contribution to photovoltaics continues to be pivotal as it aids in the development of more efficient and reliable solar cells, aligning with the global drive towards sustainable energy solutions [139, 140].

4.2 ATLAS SILVACO Features for Photovoltaics

Atlas Silvaco provides state-of-the-art device simulation tools tailored for photovoltaic research. It offers a comprehensive set of tools for analyzing and optimizing solar cells, enhancing their efficiency and performance [141, 142]. There are several key features see Figure 4.1, including:

- **Detailed Optical Simulation:** Atlas has comprehensive optical simulation capabilities, allowing precise modeling of light absorption and generation within solar cells. This functionality is crucial for maximizing the light-harvesting efficiency of photovoltaic devices.
- **Advanced Material Models:** Atlas supports various material models, including silicon, III-V compounds, organic materials, and perovskites. This flexibility allows for the simulation of multiple types of solar cells, from traditional silicon-based to cutting-edge thin-film technologies.
- **Multiphysics Capabilities:** The software's ability to simultaneously simulate electrical, thermal, and optical phenomena is particularly beneficial for solar cell analysis. It helps understand the interplay between these factors and their influence on overall device performance.
- **Carrier Transport Models:** Atlas includes sophisticated carrier transport models considering drift-diffusion, recombination, and generation processes. These models are essential for accurately predicting solar cells' current-voltage characteristics and efficiency.

4.3. Essential Steps for ATLAS Photovoltaic Simulations

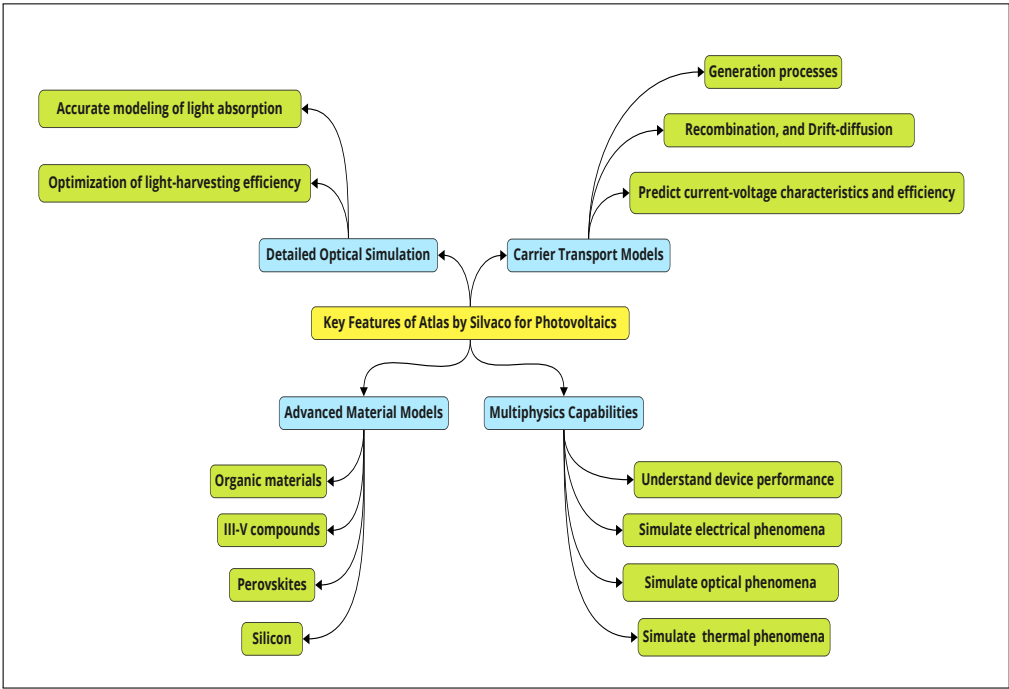


Figure 4.1: Photovoltaic Features of Atlas Silvaco.

4.3 Essential Steps for ATLAS Photovoltaic Simulations

Setting up ATLAS simulations for photovoltaic devices involves several crucial steps to ensure accurate and reliable outcomes. These include defining the simulation structure, specifying material models, and determining the numerical methods for solving device equations [53,54]. The following section details these essential steps, helping to ensure simulations accurately represent the behavior of photovoltaic devices. As illustrated in Figure 4.2, researchers can optimize and analyze the performance of solar cells using ATLAS if these steps are followed carefully.

To ensure accuracy in your ATLAS Silvaco simulations for photovoltaic devices, you must define constants and create a mesh, specify device regions and electrodes, set up doping profiles and material models, define the light source, select numerical methods, and capture and visualize the output. Adhering to these guidelines ensures that your simulations will be

precise and dependable.

4.3.1 Define Constants and Mesh Creation

Begin by setting up the simulation environment. This involves defining all necessary constants and creating a detailed mesh that accurately represents the physical structure of the photovoltaic device. The precision of this mesh is crucial for ensuring that the simulation accurately mirrors the device's real-world behavior.

4.3.2 Defining Regions and Electrode Specification

Next, specify the different regions of the device by assigning appropriate materials to each region and defining the electrodes. This step is essential for establishing the boundaries and functional areas of the device within the simulation.

4.3.3 Doping Profiles and Material Models

Set up the doping profiles and material models. This involves defining the distribution of dopants within the device and selecting the appropriate material properties. Accurate doping profiles and material models are essential for simulating the electrical characteristics of the photovoltaic device.

4.3.4 Light Source Specification

Defining the light source is necessary for photovoltaic simulations. This step includes modeling how solar radiation interacts with the device, which is critical for evaluating its performance under various lighting conditions.

4.3.5 Numerical Methods and Solution Specifications

Selecting the appropriate numerical methods for solving device equations is essential. Specifying the solution parameters meticulously is imperative to ensure that the simulation operates efficiently and accurately. The choice of numerical methods profoundly influences the precision and convergence behavior of the simulation.

4.4. ATLAS SILVACO Device Simulation Process

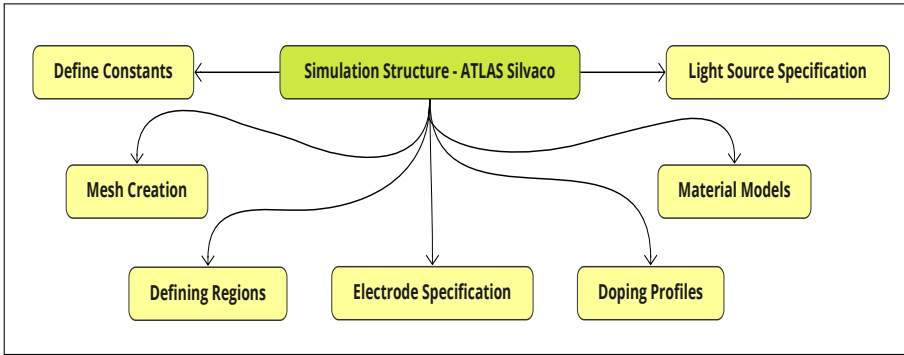


Figure 4.2: Key Steps in Setting Up ATLAS Simulations.

4.3.6 Output and Visualization

After executing the simulation, capturing the results and employing visualization tools such as TonyPlot for data analysis and interpretation is necessary. This step facilitates examining the photovoltaic device's performance and behavior, providing critical insights into potential enhancements and optimizations.

4.4 ATLAS SILVACO Device Simulation Process

The simulation of semiconductor devices is a multi-step process involving several specialized tools and detailed data analysis, as illustrated in Figure 4.3. This process begins with creating structure and command files using DevEdit, ATHENA, and DeckBuild, culminating in the simulation performed by the ATLAS Device Simulator. The resulting data, visualized through tools like TonyPlot, provides invaluable insights into the device's performance, aiding in the optimization and validation of semiconductor devices prior to physical fabrication [53, 54, 142]. This systematic approach enhances the accuracy and reliability of device development and significantly reduces the time and cost associated with physical prototyping.

4.4.1 Input Tools and Files

Simulating a device begins with preparing several input files that describe its structure and the conditions for simulation.

- **DevEdit:** DevEdit generates structure files that detail the physical layout and dimensions of semiconductor devices. Simulated devices are described by their output files, which serve as their physical blueprint.
- **ATHENA:** The ATHENA software creates command files explaining how the device structure is fabricated. The output contains a command file detailing the process steps for the subsequent simulation stages.
- **DeckBuild:** DeckBuild creates command files that specify the simulation parameters and conditions. DeckBuild is used as a primary interface for setting up and controlling simulations in ATLAS. The outputs are command files with defined simulation parameters critical for accurate simulation control and execution.

4.4.2 ATLAS Device Simulator

The ATLAS Device Simulator is the central part of the simulation process, and it does all the actual calculations to model a semiconductor device's behavior. Structures and command files are inputs, and advanced algorithms are used to solve nonlinear differential equations iteratively. Modeling devices involves using techniques like Newton's method to describe their electrical properties. As a result of this simulation process, it is possible to gain a thorough understanding of how a device performs electrically under a variety of conditions. The insights gleaned from these analyses are crucial for the next steps, such as device optimization and validation, which ensure that the device meets specifications and works as intended in practice.

4.4.3 Output Data

During and after performing the simulation, there are lots of types of output data that are produced, and each serves different purposes.

- **Runtime Output:** during the simulation process, immediate results allow for real-time monitoring of the progress of the simulation and spotting any immediate problems.
- **Log Files:** These logs for every step-by-step progress of the simulation, including any errors or warnings encountered, are very important for debugging purposes and in the simulation flow—one has to ensure that issues raised can be traced and resolved.

4.5. ATLAS Silvaco Code for Vertical Multijunction Solar Cell

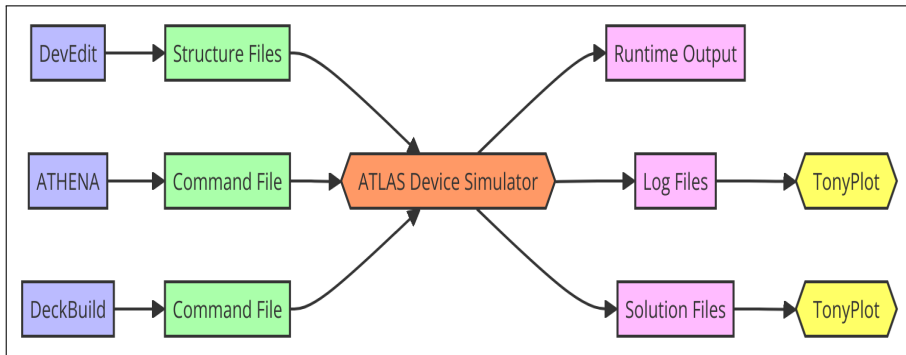


Figure 4.3: ATLAS Simulation Process, Data Flow, and Tools.

- **Solution Files:** Final simulation results, including electrical characteristics, carrier distributions, and other relevant data. The detailed data describe the performance of the device, which is very critical for analysis and validation.

4.4.4 Visualization Tools

Visualization tools, such as TONYPLOT, a graphical post-processor tool, visualize data from log and solution files to interpret the simulation results effectively. It can create various plots, including I-V curves, doping profiles, and other graphical representations, enabling a clear and detailed understanding of the simulation outcomes.

4.5 ATLAS Silvaco Code for Vertical Multijunction Solar Cell

The provided ATLAS Silvaco code simulates a vertical multijunction solar cell made of Gallium Arsenide (GaAs) with two cells and four layers. The code sets up the structure, materials, and simulation parameters, and it runs simulations to analyze the performance of the solar cell. [40, 143–145]

4.5.1 Parallel Processing

```
go atlas simflags="-p 3"
```

Runs the simulation using three processors in parallel for faster computation.

4.5.2 Thickness and Doping Parameters

Thickness: Sets the thickness of the layers in the solar cell.

```
set y_layer_P1=0.07 # Fixed thickness
set y_layer_P2=2.6  # Adjustable thickness
set y_layer_N1=2.1  # Adjustable thickness
set y_layer_N2=0.07 # Fixed thickness
```

Doping: Sets the doping concentration of the layers.

```
set P1_doping=5e19 # Fixed doping
set P2_doping=2e16 # Adjustable doping
set N1_doping=9e15 # Adjustable doping
set N2_doping=5e19 # Fixed doping
```

Tunnel Junction Parameters

Defines the properties of the tunnel junction, which connects the two cells.

```
set y_layer_tunnel_N=0.025 # Fixed thickness
set y_layer_tunnel_P=0.025 # Fixed thickness
set N_tunnel_doping=7e19   # Fixed doping
set P_tunnel_doping=7e19   # Fixed doping
set resistance=1.25e16     # Fixed resistance
```

4.5.3 Device Dimensions and Sun Concentration

Device Width: Fixed width of the solar cell.

```
set width=15.0 # Fixed width
```

Sun Concentration: Adjustable sun concentration.

```
set sun_concen=4000 # Adjustable
```

Tunnel Junction or Electrode Configuration

Determines whether the simulation uses a tunnel junction or an electrode.

```
set flag_tunnel=0 # Set to use an electrode
```

4.5. ATLAS Silvaco Code for Vertical Multijunction Solar Cell

4.5.4 Calculation of Illumination and Contact Areas

Calculates the total height, illumination area, and contact area of the solar cell.

```
set altura_SC=($y_layer_P1+$y_layer_P2+$y_layer_N1+$y_layer_N2)
set altura_tun=($y_layer_tunel_N+$y_layer_tunel_P)
set area_ilum=($altura_SC*2+$altura_tun)*1.0e-8
set area_cont=$width*1.0e-8
set altura_ilu=(( $altura_SC)*2+($altura_tun))/2.0
```

4.5.5 Mesh and Region Definitions

Defines the mesh for the simulation and specifies the regions for the first and second solar cells.

```
mesh auto
x.m loc=0.0 s=0.25
x.m loc=$width s=0.25
# First solar cell
region material=GaAs bot thick=$y_layer_P1 accept=$P1_doping ny=5
region material=GaAs bot thick=$y_layer_P2 accept=$P2_doping ny=20
region material=GaAs bot thick=$y_layer_N1 donors=$N1_doping ny=20
region material=GaAs bot thick=$y_layer_N2 donors=$N2_doping ny=5

# Region that connects both solar cells
region material=GaAs bot thick=$y_layer_tunel_N donors=$N_tunnel_doping ny=4
region material=GaAs bot thick=$y_layer_tunel_P accept=$P_tunnel_doping ny=4

# Second solar cell
region material=GaAs bot thick=$y_layer_P1 accept=$P1_doping ny=5
region material=GaAs bot thick=$y_layer_P2 accept=$P2_doping ny=20
region material=GaAs bot thick=$y_layer_N1 donors=$N1_doping ny=20
region material=GaAs bot thick=$y_layer_N2 donors=$N2_doping ny=5
```

4.5.6 Electrode and Contact Definitions

Defines the electrodes and contacts based on whether the tunnel junction is used.

```
if cond =($flag_tunnel=1)
  # Define tunnel area and mesh
  ...
```

```

electrode name=anode top
electrode name=cathode bottom
else
  electrode name=anode top
  electrode name=cathode bottom
  electrode name=tuncontact x.min=0.0 x.max=$width \
  y.min=$altura_SC y.max=$altura_SC+$altura_tun material=GaAs
  contact name=tuncontact resist=$resistance
if.end

```

4.5.7 Material Definitions and Physical Models

Defines the materials used and sets up the physical models for the simulation.

```

material mat=GaAs sopra=Gaas.nk taun0=4.4e-4 \
taup0=2.2e-4 nsrhn=2.7e13 nsrhp=2.7e13
material mat=InAlGaP sopra=Againp7.nk
material mat=AlGaAs sopra=Algaas7.nk
material material=InGaP index.file=solarex03.nk
material material=InGaP affinity=4.08
material material=AlGaAs affinity=3.54
models consrh fermi conmob optr auger bgn

```

4.5.8 Optical Source Definition

Specifies the properties of the light source used in the simulation.

```

beam num=1 x.o=-0.1 y.o=$altura_ilu angle=0 \
  wavel.start=0.305 wavel.end=3.455 wavel.num=300 \
  power.file=solarex03_15.spec out.power=solarex03_15.log

```

4.5.9 Simulation and Output

Step 1: Ramp the Bias

The first step is to ramp the bias voltage from 0.0V to 2.5V in steps of 0.05V. This is done in the dark, i.e., without any illumination.

```

log outf=vertical_qt_IV_dark.log
solve name=anode vanode=0.0 vstep=0.05 vfinal=2.5

```

4.5. ATLAS Silvaco Code for Vertical Multijunction Solar Cell

Step 2: Set Models Based on Tunnel Flag

The physical models are set based on whether the tunnel junction is used.

```
('flag_tunnel=1') or not ('flag_tunnel=0')
if cond =($flag_tunnel=1)
  models consrh fermi ni.fermi conmob optr auger bgn \
  bbt.nonlocal bbt.nlderivs
else
  models consrh fermi ni.fermi conmob optr auger bgn
if.end
```

Step 3: Ramp the Beam

Ramping the beam ensures convergence. The beam intensity is gradually increased from 0.01 suns to 1 sun.

```
solve b1=1.0e-2
solve b1=1.0e-1
```

Step 4: Adjust Sun Concentration in Steps

Adjust the sun concentration in steps until the desired concentration is reached. The number of steps and the increment value depend on the target concentration.

```
set v_b1=0
# General case
set add=100
set num_pasos=$sun_concen/$add
if cond =($sun_concen<100)
  set add=10
  set num_pasos=$sun_concen/$add
if.end
if cond =($sun_concen<10)
  set add=1
  set num_pasos=$sun_concen
if.end
loop steps = $num_pasos
  set v_b1=$v_b1+$add
  set ilu=($v_b1/10)
  solve b1=($v_b1/10)
```

```
1.end
```

Step 5: Ramp the Bias Back

Ramp the bias voltage back from 2.5V to -0.05V in steps. This step simulates the response of the solar cell under illumination.

```
log outf=vertical_qt_IV_sun.log
solve name=anode vanode=2.5 vstep=-0.01 vfinal=1.5
solve name=anode vanode=1.5 vstep=-0.05 vfinal=0.2
solve name=anode vanode=0.2 vstep=-0.01 vfinal=-0.05
```

Step 6: Extract Important Figures of Merit

Extract key performance metrics such as short-circuit current (Isc), open-circuit voltage (Voc), fill factor (FF), and efficiency (Eff) from the simulation results.

```
extract init infile="vertical_qt_IV_sun.log"
extract name="Isc" y.val from curve(v."anode", i."cathode") where x.val=0.0
extract name="JscmAcmm2" $Isc*1e03/$area_cont
extract name="Voc" x.val from curve(v."anode", i."cathode") where y.val=0.0
extract name="Pm" max(curve(v."anode", (v."anode" * i."cathode")))
extract name="Vm" x.val from curve(v."anode", (v."anode"*i."cathode") ) \
  where y.val=$"Pm"
extract name="Im" $"Pm"/$"Vm"
extract name="FF" ($"Pm"/($"Isc"*$"Voc"))*100
extract name="Opt_int" max(beam."1")
extract name="Eff" ($Pm/($Opt_int*$area_illum))*100
```

Step 7: Plot the Results (Optional)

Optionally, plot the results using TonyPlot.

```
# tonyplot vertical_IV.log -set solarex03_1.set
```

Step 8: Output Simulation Data

Specify the output variables to be included in the final structure file based on whether the tunnel junction is used.

4.6. Ultra-High Concentration Homo-Multijunction Solar Cells: Innovations for CubeSats and Ground-Based Systems

```
if cond =($flag_tunnel=1)
  OUTPUT J.CONDUC QFN QFP J.ELECTRON J.HOLE J.TOTAL \
    BAND.PARAM CHARGE CON.BAND DEVDEG E.MOBILITY \
    E.TEMP E.VELOCITY FLOWLINES H.MOBILITY H.TEMP \
    H.VELOCITY HCTE.JOULE J.DISP J.DRIFT \
    J.DIFFUSION L.TEMPER PERMITTIVITY NLAT.GAMMA PHOTOGEN \
    QTUNN.BBT QTUNN.EL QTUNN.HO RECOMB T.QUANTUM TAURN TAURP \
    TRAPS TRAPS.FT U.AUGER U.BBT U.LANGEVIN U.RADIATIVE U.SRH \
    U.TRANTRAP U.TRAP VAL.BAND
else
  OUTPUT J.CONDUC QFN QFP J.ELECTRON J.HOLE J.TOTAL \
    BAND.PARAM CHARGE CON.BAND DEVDEG E.MOBILITY \
    E.TEMP E.VELOCITY FLOWLINES H.MOBILITY H.TEMP \
    H.VELOCITY HCTE.JOULE J.DISP J.DRIFT \
    J.DIFFUSION L.TEMPER PERMITTIVITY PHOTOGEN \
    RECOMB TAURN TAURP \
    TRAPS TRAPS.FT U.AUGER U.LANGEVIN U.RADIATIVE U.SRH \
    U.TRAP VAL.BAND
if.end

save outf=vertical_qt_sun.str
```

Step 9: Quit the Simulation

Terminate the simulation.

```
quit
```

4.6 Ultra-High Concentration Homo-Multijunction Solar Cells: Innovations for CubeSats and Ground-Based Systems

This study focuses on optimizing and evaluating a novel vertical solar cell structure inspired by the work of Fernández, E. F. et al., utilizing lattice-matched configurations under UHCPV [128]. These semiconductor structures are analyzed using physical-based numerical modeling by analyzing their performance between 1 and 10,000 suns. Figure 4.4 illustrates the careful optimization of structural properties, including thickness and doping. By selecting materials based on their bandgap, the design allows for both direct-gap and indirect-gap semiconduc-

tors to be used. Thus, it is possible to tailor the energy gap to meet the needs of a particular application. This study models a single-band structure and implements an optimization procedure to estimate the structure's maximum efficiency. Findings from this study indicate that this device can be utilized effectively in CPV systems under high concentration factors. In addition to guiding future improvements in solar cell manufacturing and characterization, this work represents an initial step toward the design of ultra-high-efficiency concentrator solar cells.

4.6.1 Device Structure and Simulation Technique

In this study, we have optimized and assessed an innovative vertical solar cell design. This optimization allows for selecting an appropriate energy gap tailored to specific applications. Our objective is to determine the highest possible efficiency of a single-band structure by fine-tuning its electrical parameters. Additionally, we examine how varying the concentration ratio influences the device's performance. The outcomes of this research are expected to contribute to developing a new generation of competitive concentrated photovoltaic (CPV) systems. We aim to design an ultra-efficient concentrator solar cell, with its manufacturing and characterization processes informed by our findings.

We investigate an edge-illumination multijunction solar cell composed of vertically aligned, non-monolithic junctions. The PN junction is exposed to incident light vertically, and each sub-cell features metal contacts on its sides. These sub-cells are narrow but tall, effectively eliminating shading issues and minimizing series resistance. The VMJ configuration is compatible with many power supplies and functions as a high-voltage, low-current cell.

In this work, we optimize a gallium arsenide (GaAs) vertical tunnel-junction (VTJ) cell. This cell consists of laterally arranged anodes and cathodes connected by tunnel junctions (TJs), as illustrated in Figure 4.4. Each VTJ cell includes two identical sub-cells, each containing four layers linked by a tunnel junction. At this stage, only GaAs is used for the TJs to ensure lattice matching, allowing for monolithic growth without mismatching issues. Each sub-cell within the VTJ cell comprises four layers connected by a tunnel junction. The anode (A) and cathode (C) are positioned on the sides. We have varied the thickness (width) and doping levels of the p^+ and n^+ layers across concentration levels ranging from one sun to ten thousand suns. The n^+/p^+ GaAs tunnel junction is 25 nm wide and doped to $7 \times 10^{19} \text{ cm}^{-3}$. Our simulations incorporate both direct tunneling and trap-assisted tunneling models. The p^+ and n^+ layers each have a width of $0.07 \mu\text{m}$ and a constant doping concentration of $5 \times 10^{19} \text{ cm}^{-3}$. Figure 4.4

4.6. Ultra-High Concentration Homo-Multijunction Solar Cells: Innovations for CubeSats and Ground-Based Systems

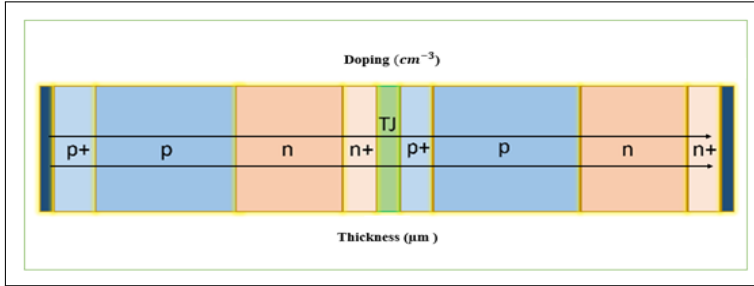


Figure 4.4: Primary schematic diagram of the VMJ structure.

depicts the fundamental structure and dimensions of a vertical tunnel-junction GaAs solar cell selected for its high conversion efficiency. The proposed design features two identical sub-cells connected via tunnel junctions. Each sub-cell consists of two successive P-layers, the first highly doped to $5 \times 10^{19} \text{ cm}^{-3}$ and the second to $2 \times 10^{17} \text{ cm}^{-3}$, followed by two N-layers doped to $4 \times 10^{16} \text{ cm}^{-3}$ and $5 \times 10^{19} \text{ cm}^{-3}$, respectively. Both tunnel junction layers are 25 nm wide and doped to $7 \times 10^{19} \text{ cm}^{-3}$. The entire structure measures $9.73 \mu\text{m}$ in width and $1.25 \mu\text{m}$ in height. The height (H) can be increased without compromising cell performance, allowing for taller structures that reduce front contact shading and lower series resistance (R_s) by extending the lateral metallic contacts. The VTJ solar cell requires only two electrical terminals to extract the generated current, as shown in dark gray in Figure 4.4, since it is oriented perpendicularly to incoming sunlight. The PN junction is illuminated vertically using an AM1.5D reference spectrum at 1000 W/m^2 and a cell temperature of 25°C , adhering to Standard Test Conditions (STC). Our simulations consider reflection, heat effects, and three-dimensional factors negligible. We utilized Silvaco ATLAS, a leading semiconductor simulator for photovoltaic devices, to design and enhance multi-bandgap concentrator solar cells. This software provides realistic and reliable results, enabling the simulation of the thermal, optical, and electrical behaviors of semiconductor devices in both two and three dimensions. ATLAS takes the physical structure from the Athena process simulator as input to predict all characteristics of the solar cell, all developed by SILVACO. We optimized the GaAs multijunction solar cell (MJSC) structure, achieving key parameters such as current density (J_{SC}), open-circuit voltage (V_{OC}), fill factor (FF), and conversion efficiency (η). Figure 4.5 outlines our methodology for determining the electrical characteristics of the GaAs MJSC.

4.6.2 Optimization Procedure

To ensure the accuracy of our model, we first compare it against established solar cells with well-documented characteristics and performance metrics. The primary objective of this study is to construct a solar cell and subsequently enhance its performance. The next section outlines the optimization process for the structure depicted in Figure 4.5, while Table 4.1 details the design and material properties. Our approach involves a dual-phase procedure: adjusting intrinsic parameters (such as thickness ranging from 3 to 8 μm and doping levels from 10^{12} to 10^{17} cm^{-3}) and modifying extrinsic parameters (concentration levels from 1 to 10,000 suns). We maintain a constant layer thickness of 15 μm throughout the simulation. In the initial phase, we focus on identifying optimal thickness and doping levels for the P- and N-layers by keeping concentration levels fixed and varying the intrinsic parameters. Once the optimal intrinsic values are determined, we move to the second phase, where we alter the concentration levels and reiterate the optimization steps.

The optimization process starts with adjusting the thickness of the P-layers to maximize efficiency, ensuring that the N-layer thickness and the doping levels of both P- and N-layers remain constant. After determining the optimal P-layer thickness, we adjust the N-layer thickness while keeping the doping levels unchanged to find the most effective value. Next, we refine the doping levels of the P-layer by first establishing the best doping values for both P- and N-layers. We then vary the P-layer doping while maintaining the N-layer doping at its optimal value. Subsequently, we adjust the N-layer doping to achieve the highest possible performance. Upon completing the concentration adjustments, we select a new concentration level within 1 to 10,000 suns to finalize the optimal structure for our solar cell design.

4.6. Ultra-High Concentration Homo-Multijunction Solar Cells: Innovations for CubeSats and Ground-Based Systems

Table 4.1: Design and material properties of GaAs VMJ solar cells.

Category	Parameter	Value
Thickness	Layer P+ (μm)	0.07
	Layer P (μm)	3–8
	Layer N (μm)	1–6
	Layer N+ (μm)	0.07
Doping	P+ doping (cm^{-3})	5×10^{19}
	P doping (cm^{-3})	2×10^{12} – 2×10^{17}
	N doping (cm^{-3})	9×10^{12} – 9×10^{17}
	N+ doping (cm^{-3})	5×10^{19}
Connection Region	Layer tunnel N (μm)	0.025
	Layer tunnel P (μm)	0.025
	N tunnel doping (cm^{-3})	7×10^{19}
	P tunnel doping (cm^{-3})	7×10^{19}
	Resistance ($\Omega \cdot \text{cm}^2$)	1.25×10^{16}
Device Settings	Width (μm)	15.0–20.33
	Sun concentration (sun)	1–10,000
Material Properties	Gap energy (eV)	1.42
	Dielectric Permittivity (E)	13.2
	Affinity χ (eV)	4.07
	Lattice constant ($\text{\AA}$)	5.65
	Auger coefficient (n) (cm^6/s)	1.9×10^{-31}
	Auger coefficient (p) (cm^6/s)	12×10^{-31}

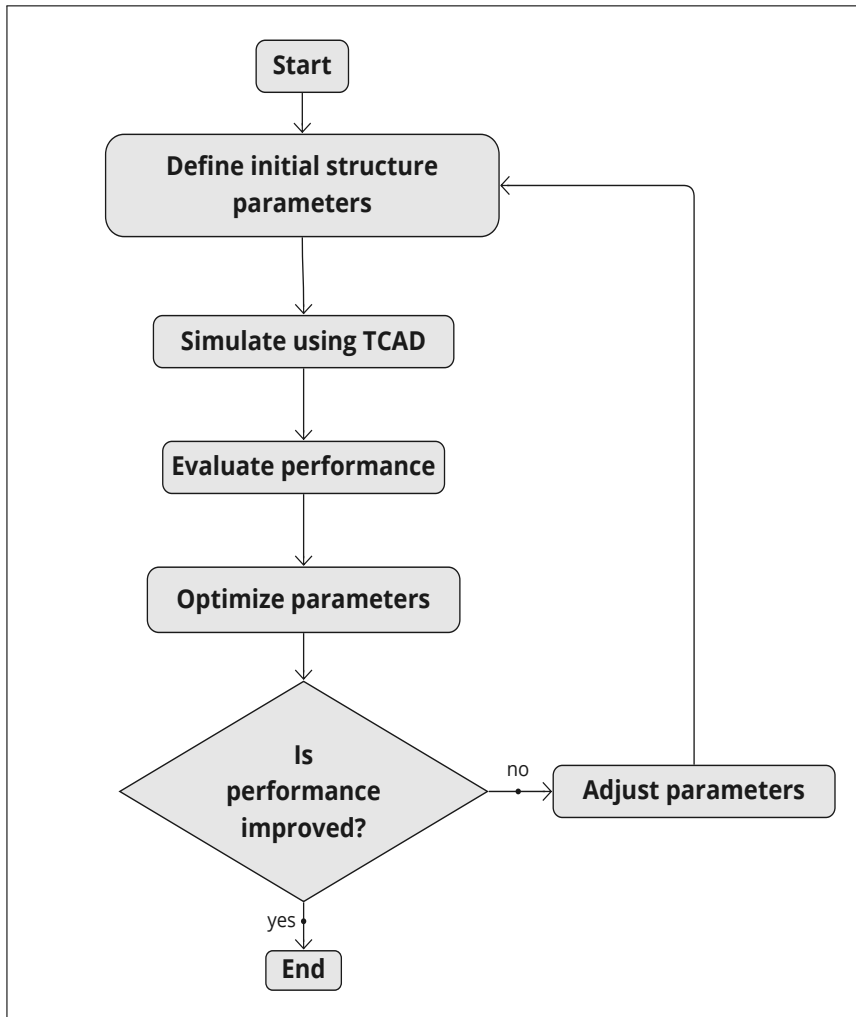


Figure 4.5: A flowchart depicting the methodology for determining the best VMJSC structure.

CHAPTER 5

RESULTS AND DISCUSSION

Our research on GaAs-based VMJ solar cells leverages high-concentration photovoltaic systems to address the escalating global need for renewable energy. This study is particularly relevant for applications on Earth and in space, where efficiency and reliability are crucial. The methodologies outlined here provide a detailed exploration of the simulation and optimization techniques used to enhance the performance of these solar cells. Simulation and optimization techniques that help improve the performance of such solar cells. The results presented in this chapter are based on two key publications, which offer an elaborate overview of VMJ solar cells. At the heart of our work is the ATLAS-SILVACO simulator, a state-of-the-art Technology Computer-Aided Design (TCAD) simulator, which we use to model and analyze different designs of solar cells accurately and numerically. With this simulator, we can study in detail and examine many design parameters, for instance, the doping concentrations and the layer thicknesses—to measure their effect on the efficiency of solar cells. The simulator provides detailed modeling of semiconductor devices, which the researchers will use to construct, characterize, and analyze the performance of the solar cells in this study.

5.1 Inclusion of Published Work and Co-author Details

This section provides full bibliographic and authorship information for the publications included in this thesis. The following details are provided for each work: the complete list of authors in the order of appearance, their institutional affiliations, the full reference of the publication, the publisher, and the ISSN or ISBN number.

1. **Publication Title:** Ultra-High Concentration Vertical Homo-Multijunction Solar Cells for CubeSats and Terrestrial Applications.

Authors and Affiliations:

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Nour El I. Boukortt, *Centro Singular de Investigación en Tecnoloxías de Información (CiTIUS), Universidad de Santiago de Compostela, Spain*

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2. **Publication Title:** Simulation-Enhanced Insights for High-Concentration Solar Cells for Nano-Satellites.

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Full Reference: Proceedings of the 2023 2nd International Engineering Conference on Electrical, Energy, and Artificial Intelligence (EICEEI), IEEE, pp. 1–7, 2023.

Publisher: Institute of Electrical and Electronics Engineers (IEEE)

DOI: <https://ieeexplore.ieee.org/abstract/document/10590254>

5.2 Simulation and Experimental Setup

This research aims to push the boundaries of solar cell technology by developing more efficient and cost-effective solutions. The findings presented here offer a robust framework for

5.3. Device Simulation and Numerical Analysis

understanding the optimization of GaAs-based VMJ solar cells, contributing to the broader adoption of renewable energy technologies. The detailed methodologies and results outlined in this section set the stage for further advancements in this critical area of research, promising significant impacts on global renewable energy strategies.

5.2.1 Specific Conditions of Simulations

Varying Doping Concentrations

The doping concentrations of the P and N regions were systematically varied to optimize the performance of the solar cells. The simulations explored a range of doping levels from 10^{12} to 10^{17} cm^{-3} , examining their impact on key performance metrics such as efficiency, fill factor, current density, and open-circuit voltage.

Thicknesses of P and N Regions

The thicknesses of the P and N regions were also varied in the simulations. Different thickness combinations were tested to determine the optimal structure that would maximize the efficiency of the solar cells. The thickness of the P region varied from $3 \mu\text{m}$ to $7 \mu\text{m}$, and the N region from $1 \mu\text{m}$ to $6 \mu\text{m}$, depending on the specific conditions of the simulations.

Sunlight Concentration (AM0 and AM1.5 Conditions)

The simulations were conducted under two different sunlight conditions: AM0 (space environment) and AM1.5 (terrestrial environment).

5.3 Device Simulation and Numerical Analysis

- **Construction of the Device Model:** The initial step involved constructing a detailed model of the VMJ solar cell within the ATLAS-SILVACO framework. This included defining the geometric dimensions, material properties, and doping profiles of the P and N regions.
- **Simulation of Electrical Characteristics:** In this research, simulation under different conditions has been performed for electrical characteristics of solar cells; for example, such as current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and efficiency

(η). These simulations enlighten the performance of solar cells under different doping concentrations and thicknesses.

- **Optimization and Analysis:** Extracted simulation results were analyzed to obtain the optimum doping levels and thicknesses to maximize efficiency. These performance metrics have been compared under both AM0 and AM1.5.
- **Numerical Results:** The numerical results from the simulations were compiled into tables and graphs, highlighting the key findings and allowing for a detailed analysis of the performance improvements achieved through optimization. The studies systematically varied the doping concentrations and thicknesses. They simulated the solar cells under different sunlight conditions, providing valuable insights into designing and optimizing high-efficiency VMJ solar cells for space and terrestrial applications.

5.4 Results: Simulation-Enhanced Insights for High-Concentration Solar Cells for Nano-Satellites

This section discusses the performance characteristics of vertical Gallium Arsenide (GaAs) homo-multijunction solar cells. We demonstrate their high efficiency and cost-effectiveness as a renewable energy source for space and terrestrial applications. This advanced solar cell technology was developed, characterized, simulated, and analyzed using the ATLAS-SILVACO simulator (TCAD) under various conditions to evaluate its suitability for UHCPV. An in-depth analysis of performance metrics, such as current density, voltage, power output, fill factor, and overall efficiency, is conducted in the study, which examines the influence of different doping levels and thicknesses in the P and N regions. The primary objective is to identify the optimal configuration for these solar cells under 4000 concentrated sunlight conditions.

The values produced for this structure for space environments (AM0) and terrestrial environments (AM1.5) are as follows. Tables 5.1 present Electrical Characteristics with Changing Doping for AM0, while Table 5.2 show Electrical Characteristics with Changing Doping for AM1.5. Table 5.3 Electrical Characteristics with Changing Thickness for AM0 Table 5.4 present Electrical Characteristics with Changing Thickness for AM0

5.4. Results: Simulation-Enhanced Insights for High-Concentration Solar Cells for Nano-Satellites

Table 5.1: Electrical Characteristics with Changing Doping for AM0.

P-doping (cm^{-3})	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)	N-doping (cm^{-3})	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)
12	9331.13	2.2853	88.1	25.3902	12	9369.87	2.2846	88.5	25.5841
13	9333.20	2.2851	88.1	25.3906	13	9369.87	2.2846	88.5	25.5826
14	9343.47	2.2846	88.0	25.3876	14	9369.27	2.2844	88.4	25.5621
15	9345.60	2.2830	88.1	25.4180	15	9345.60	2.2830	88.2	25.4180
16	9265.07	2.2776	88.9	25.3551	16	9044.00	2.2795	88.3	24.5807
17	8436.73	2.2733	89.0	23.0721	17	7702.33	2.3311	88.6	20.9972

Table 5.2: Electrical Characteristics with Changing Doping for AM1.5.

P-doping (cm^{-3})	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)	N-doping (cm^{-3})	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)
12	10954.4	2.2936	88.1	29.566	12	9912.87	2.2898	88.6	29.8019
13	10956.9	2.2934	88.1	29.6556	13	9912.93	2.2898	88.6	29.8001
14	10970.3	2.2929	88.0	29.5618	14	9912.13	2.2897	88.5	29.7759
15	10973.1	2.2914	88.1	29.5991	15	9884.33	2.2882	88.3	29.6064
16	10880.4	2.2860	88.9	29.5534	16	9530.33	2.2840	88.4	28.5200
17	9908.13	2.2818	89.1	26.8996	17	7954.60	2.2814	88.7	23.8566

Table 5.3: Electrical Characteristics with Changing Thickness for AM0.

P Thickness (μm)	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)	N-Thickness (μm)	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)
3	4714.53	2.2555	89.0	25.1766	1	7423.47	2.2701	89.1	25.2441
4	5630.15	2.2618	89.0	25.2583	2	8349.73	2.2740	89.0	25.3241
5	6541.41	2.2668	89.0	25.3060	3	9265.07	2.2776	88.9	25.3551
6	7448.00	2.2708	89.0	25.3238	4	10163.1	2.2807	88.8	25.3339
7	8349.73	2.2740	89.0	25.3241	5	11040.2	2.2832	88.8	25.2620
8	9246.4	2.2768	88.9	25.3100	6	11887.4	2.2855	88.7	25.1424

Table 5.4: Electrical Characteristics with Changing Thickness for AM1.5.

P-Thickness (μm)	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)	N Thickness (μm)	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)
3	5527.37	2.26479	89.0	29.2900	1	7659.33	2.2743	89.1	29.4212
4	7683.20	2.2759	88.9	29.4976	2	8754.93	2.2793	89.0	29.5223
5	8754.07	2.2802	88.9	29.5406	3	9819.87	2.2833	88.9	29.5557
6	9819.87	2.2833	88.9	29.5557	4	10873.7	2.28676	88.9	29.5278
7	10880.4	2.2860	88.9	29.5534	5	11903.1	2.2899	88.9	29.4379
8	11935.5	2.2885	88.9	29.5354	6	12897.5	2.2923	88.7	29.2891

These results allow us to figure out and describe the best structure. We can understand the relation between the doping efficiency for the P and N regions see Figs 5.1 and 5.2. Fur-

thermore, Figures 5.3 and 5.4 show the efficiency when we are changing the thickness of the structure. Results presented here demonstrate the performance characteristics of junction solar cells exposed to two distinct solar spectrums, AM0 and AM1.5. As well as varying levels of P and N doping, these results consider the thicknesses of the P and N layers. For both AM0 and AM1.5 spectra, increasing levels of P doping and N doping enhance device performance. The response of V_{oc} levels, however, is much more complex. V_{oc} increases with doping level for both spectra. Once doping concentrations are reached, they plateau or decrease slightly. Thicker P and N layers tend to yield higher values for J_{sc} and FF, although their effect on V_{oc} is more nuanced, with some fluctuations observed. These findings provide insights into trade-offs and optimization strategies that can enhance junction solar cell efficiency under different doping concentrations and layer thicknesses.

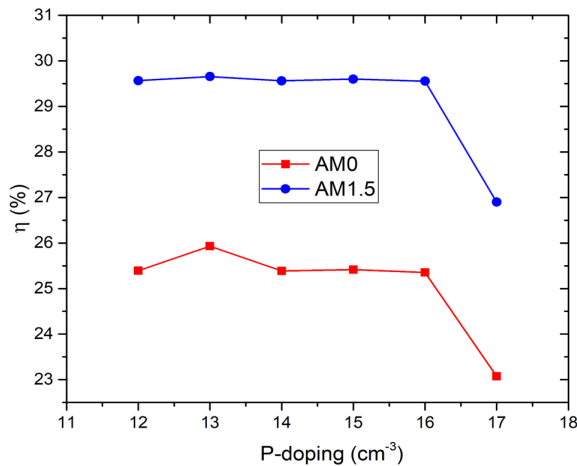


Figure 5.1: P-doping vs efficiency.

5.4. Results: Simulation-Enhanced Insights for High-Concentration Solar Cells for Nano-Satellites

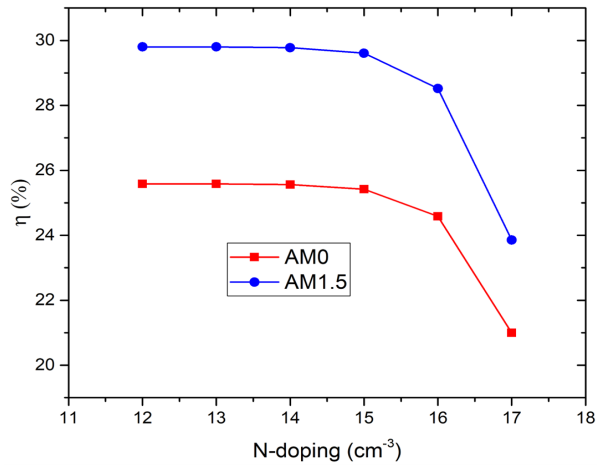


Figure 5.2: N-doping vs efficiency.

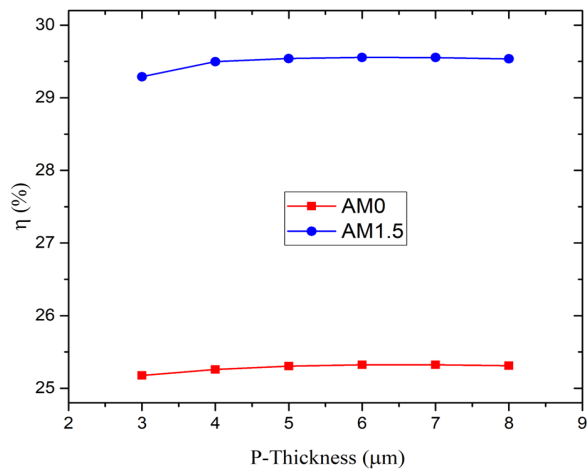


Figure 5.3: P-Thickness vs efficiency.

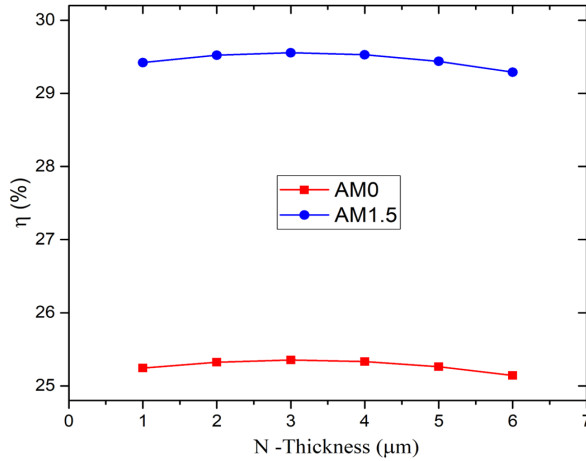


Figure 5.4: N-Thickness vs efficiency.

Under the air mass condition of AM0 and AM1.5, with the consecration of 4000 suns, Figure 5.1 shows the doping concentration versus the efficiency reaches the values of 25.42 % and 29.60 % when the doping is 10^{15} cm^{-3} . Under the previous conditions with the P-doping value, Figure 5.2 shows that the efficiency reaches the value of 25.57 % and 29.78 % when the N-doping is 10^{14} cm^{-3} . Figure 5.3 shows that in the previous conditions when P- thickness equals $7 \mu\text{m}$, the efficiencies are 25.32 % and 29.56 %. Then, with all previous values of the doping and P-thickness, Figure 5.4 shows the efficiencies of 25.35% and 29.56 % when the N-thickness equals $4 \mu\text{m}$.

We summarized the properties of the best structure in Table 5.5, showing The best thickness and doping results of HOMO GsAs– VMJ-UHCPV. Furthermore based on previous results, Table 5.6 represent the Electrical Characteristics of HOMO GaAs– VMJ-UHCPV. under AM0 has a thickness of $7 \mu\text{m}$ and $4 \mu\text{m}$ for P and N regions with concentrations of 10^{15} cm^{-3} and 10^{14} cm^{-3} . This structure has an efficiency of 25.56 %, a fill factor of 88.4 %, a current density of 9369.27 mA/cm^2 , and an open circuit voltage of 2.287 V. Also, the best structure under AM1.5 has a thickness of $6 \mu\text{m}$ and $3 \mu\text{m}$ for P and N regions with doping concentrations of 10^{15} cm^{-3} and 10^{15} cm^{-3} . This structure has an efficiency of 29.61 %, a fill factor of 88.3%, a current density of 9884.33 mA/cm^2 , and an open circuit voltage of 2.288 V. In scenarios involving extremely high concentration ratios, this characteristic contributes to the outstanding photovoltaic performance of VMJ solar cells. These unique characteristics

5.5. High-Efficiency Vertical Homo-Multijunction Solar Cells for CubeSats and Earth-Based Applications

of VMJ solar cells allow photons and currents to be decoupled. Therefore, wavelength and depth do not affect carrier collection probabilities. There is also lateral current flow in VMJ solar cells. Due to this, there is no resistance loss in the series of electrodes and emitters. As concentration levels rise, VMJ solar cells reduce the compensation challenges encountered in conventional solar cells caused by the interplay between frontal contact and series resistance.

Table 5.5: The best Thickness and Doping Results of HOMO GAAS– VMJ-UHCPV.

AM	P Thickness (μm)	P Thickness (μm)	P-doping (cm^{-3})	N-doping (cm^{-3})
AM0	7	4	10^{15}	10^{14}
AM1.5	6	3	10^{15}	10^{15}

Table 5.6: Electrical Characteristics of HOMO GAAS– VMJ-UHCPV.

AM	Jsc (mA/cm^2)	Voc (V)	FF (%)	η (%)
AM0	9369.27	2.284	88.4	25.56
AM1.5	9884.33	2.288	88.3	29.61

5.5 High-Efficiency Vertical Homo-Multijunction Solar Cells for CubeSats and Earth-Based Applications

5.5.1 Influence of P-Type Absorber Layer Thickness on Photovoltaic Performance

The thickness of the sensitizer or absorber layer plays a crucial role in determining the cell's efficiency, short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), and fill factor (FF). Specifically, J_{sc} increases as the front layer thickness decreases, enhancing the collection efficiency of the space charge region and thereby increasing the short-circuit current density. Additionally, considering surface recombination, the proximity of the depletion region to the surface can reduce collection efficiency. Thus, thickness significantly impacts overall performance. The performance of photovoltaic (PV) cells is directly influenced by the absorber layer's thickness, which affects the diffusion lengths of charge carriers. If the absorber layer is too thin, charge carriers may recombine before being collected, leading to incomplete absorption of incident radiation. Conversely, excessively thick absorber layers can result in charge carriers recombining before they reach the electrodes. The thickness of the P-type layer in a solar cell affects the cell's efficiency, open-circuit voltage, fill factor, and short-circuit cur-

rent. Increasing the P-type layer thickness can enhance V_{oc} by increasing the built-in potential across the P–N junction. However, a thicker P-type layer may reduce J_{sc} due to a lower number of generated carriers (electrons and holes). The fill factor, which measures the cell's ability to convert light into electricity, is defined as the ratio of the maximum power output to the product of V_{oc} and J_{sc} . Typically, a thinner P-type layer results in a higher fill factor, although the optimal thickness depends on the material system and cell design. Balancing increased V_{oc} with decreased J_{sc} is essential for maximizing overall cell efficiency, and determining the optimal P-type layer thickness usually requires experimentation and optimization. In our study, the thickness of the P-type region was varied from 3.0 μm to 8.0 μm in both N- and P-type regions, with optimized doping concentrations of $9 \times 10^{15} \text{ cm}^{-3}$ and $2 \times 10^{16} \text{ cm}^{-3}$, respectively. We achieved a maximum J_{sc} of 2.45 mA/cm² and V_{oc} of 1.86 V under a concentration of one sun, and J_{sc} of 24.5935 mA/cm² and V_{oc} of 2.33 V at a concentration of 10,000 suns with a 2.1 μm N-type region thickness (see Figure 5.5). However, the fill factor and efficiency initially increased to a peak value before declining as recombination accelerated with increased P-region thickness. Conversely, increasing the thickness of the N-type region led to higher short-circuit current density and open-circuit voltage, which is in line with the solar cell's characteristics.

5.5. High-Efficiency Vertical Homo-Multijunction Solar Cells for CubeSats and Earth-Based Applications

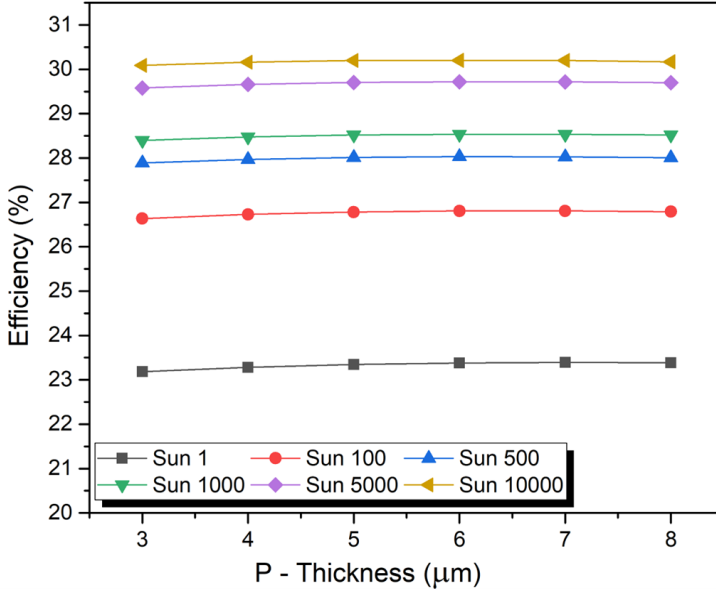


Figure 5.5: Influence of P-Type Absorber Layer Thickness.

5.5.2 Influence of N-Type Absorber Layer Thickness on Photovoltaic Performance

An effective absorber layer can significantly enhance photovoltaic (PV) performance, which largely depends on the quality and morphology of the absorber. Critical factors such as the absorber layer's thickness and defect density must be carefully managed to achieve optimal performance metrics. This section explores the impact of the N-type absorber layer thickness (N_t) on solar cell performance. Increasing the thickness of the N-type layer boosts the short-circuit current density (J_{sc}) by generating more charge carriers (electrons and holes) within the cell. However, thicker N-type layers may reduce the open-circuit voltage (V_{oc}) due to an expanded surface area that facilitates carrier recombination.

The fill factor (FF) is a key parameter that evaluates a cell's power output by relating the maximum power point to the product of V_{oc} and J_{sc} . The conversion efficiency of light to electricity is influenced by the material system employed and whether increased N-type layer thickness results in a higher fill factor. The overall efficiency of a solar cell hinges on the balance between J_{sc} and V_{oc} . Determining the optimal N-type layer thickness involves

experimental and optimization processes tailored to the specific material system and cell design. In our experiments, the N-type region thickness was varied from $1.0\mu\text{m}$ to $6.0\mu\text{m}$, with optimized doping concentrations of $9 \times 10^{15} \text{ cm}^{-3}$ for the N-type and $2 \times 10^{16} \text{ cm}^{-3}$ for the P-type regions. The highest observed values of J_{sc} reached 3.23 mA/cm^2 and V_{oc} reached 1.86 V under one sun concentration. Under a concentration of 10,000 suns, J_{sc} increased to 29.81 mA/cm^2 and V_{oc} to 2.34 V at an N-type thickness of $7.0\mu\text{m}$ (see Figure 5.6). While increasing the N-type layer thickness enhanced the rates of carrier recombination, it also led to higher J_{sc} and V_{oc} . Conversely, the fill factor and efficiency initially peaked before declining.

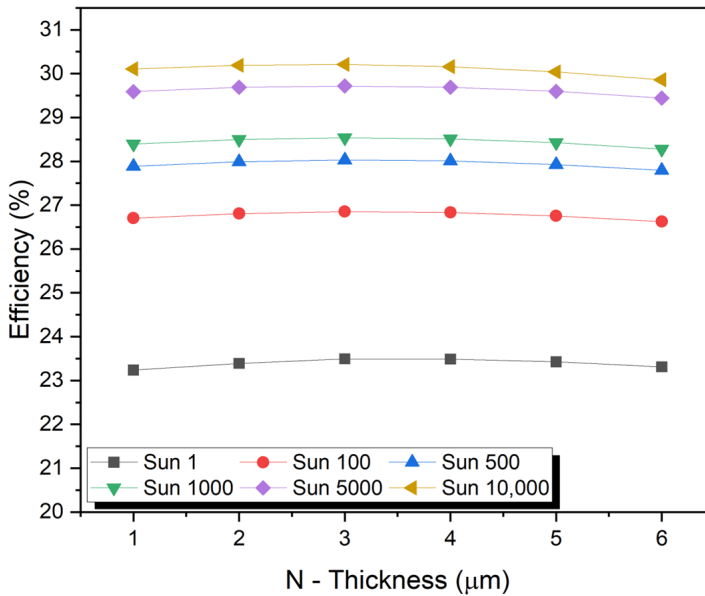


Figure 5.6: Influence of N-Type Layer Thickness.

5.5.3 Optimizing P-Type Doping to Enhance Solar Cell Performance

The doping level in P-type semiconductors plays a crucial role in determining the width of the depletion region and the built-in potential of the solar cell. A wider depletion region and a higher built-in potential facilitate the effective separation of electrons and holes generated by sunlight, thereby increasing the short-circuit current density (J_{sc}). P-doping is fundamental in designing more efficient solar cells as it forms the P-side of the P-N junction, which is

5.5. High-Efficiency Vertical Homo-Multijunction Solar Cells for CubeSats and Earth-Based Applications

essential for separating charge carriers during light absorption. Enhancing the concentration of free electrons in P-type material can boost J_{sc} , but it may also lead to a reduction in the built-in potential of the P–N junction, negatively impacting the fill factor (FF) by lowering the open-circuit voltage (V_{oc}). A high fill factor indicates that a solar cell can sustain a high power output across various operating conditions. Applying a higher dopant concentration to the P-type material increases current flow, improving the fill factor. However, excessive doping may reduce the fill factor due to increased recombination of electrons and holes. The efficiency of a photovoltaic cell depends on the balance between J_{sc} , V_{oc} , and FF , all of which are influenced by the doping levels of the P-type material. Therefore, the effect of P-type doping on efficiency is contingent upon the solar cell's design and the interplay between these parameters. Optimal doping levels are determined through careful experimentation and optimization, tailored to the specific material system and cell architecture. Overdoping can lead to enhanced recombination rates, resulting in decreased overall efficiency. In our experiments, the doping concentration in the P-type region was varied from $9 \times 10^{12} \text{ cm}^{-3}$ to $9 \times 10^{17} \text{ cm}^{-3}$, as illustrated in Figure 5.7. The P-type region maintained a thickness of $7.0\mu\text{m}$, while the N-type region was set to $5.0\mu\text{m}$ with an optimized doping concentration of $2 \times 10^{16} \text{ cm}^{-3}$. Under one sun concentration, the maximum observed values were $J_{sc} = 2.74 \text{ mA/cm}^2$ and $V_{oc} = 2.1 \text{ V}$. When subjected to a concentration of 10,000 suns, J_{sc} increased to 27.43 mA/cm^2 and V_{oc} to 2.34 V at an N-type thickness of $7.0\mu\text{m}$ (see Figure 5.7). While increasing the N-type layer thickness enhanced the rates of carrier recombination, it also resulted in higher J_{sc} and V_{oc} . Conversely, the fill factor and overall efficiency initially rose to peak values before experiencing a decline.

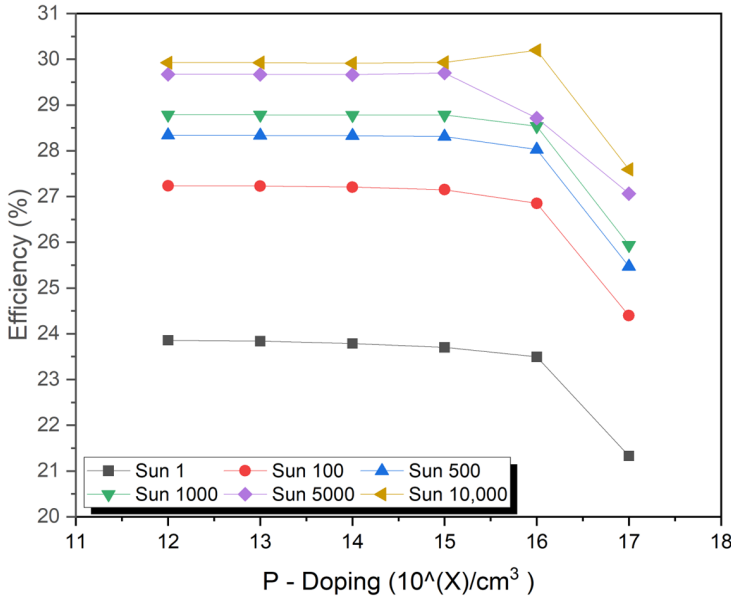


Figure 5.7: Optimizing P-Type Doping and Solar Cell Performance.

5.5.4 Optimizing N-Type Doping to Enhance Solar Cell Performance

Incorporating N-type materials into a solar cell enhances its conductivity and alters its electrical characteristics. As the material's conductivity increases, the short-circuit current density (J_{sc}) may rise. At the same time, the open-circuit voltage (V_{oc}) can decrease due to a diminished built-in potential across the P–N junction, which may, in turn, reduce the fill factor (FF). When both J_{sc} and V_{oc} decline, overall efficiency may drop, though the extent of this effect depends on the specific doping conditions and the inherent material properties. In this study, the N-type doping concentration ranged from $2 \times 10^{12} \text{ cm}^{-3}$ to $2 \times 10^{17} \text{ cm}^{-3}$, as illustrated in Figure 6. The P-type region had a thickness of $7.0 \mu\text{m}$ and was optimally doped at $9 \times 10^{12} \text{ cm}^{-3}$, while the N-type region was $5.0 \mu\text{m}$ thick. Under one-sun illumination, the solar cell achieved a maximum J_{sc} of 2.75 mA/cm^2 and a V_{oc} of 1.86 V . At a concentration of $10,000$ suns, J_{sc} rose to 24.7155 mA/cm^2 , while V_{oc} reached 2.33 V . Figure 5.8 depicts how varying the absorber N-layer doping influences these performance metrics.

5.5. High-Efficiency Vertical Homo-Multijunction Solar Cells for CubeSats and Earth-Based Applications

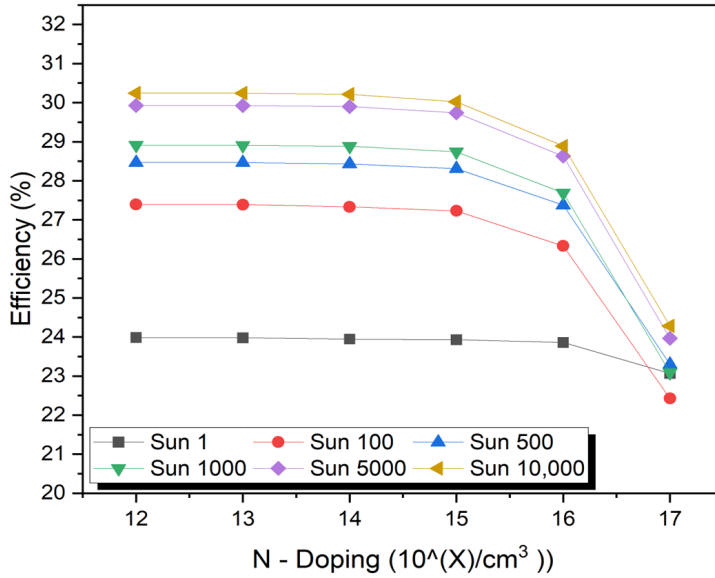


Figure 5.8: Optimizing N-Type Doping and Solar Cell Performance.

5.5.5 Influence of the Sun Concentrations

Silvaco ATLAS, an electronic device simulator recognized for its reliable results, was used to design multibandgap concentrator solar cells. The phrase “number of suns” refers to how incoming light intensity compares to the standard level of sunlight at Earth’s surface (1 sun). As the light concentration increases, the short-circuit current (J_{sc}) generally rises, providing higher output power. Because more electron-hole pairs are generated under intense illumination, the open-circuit voltage (V_{oc}) can also increase. However, as the concentration grows, the fill factor (FF) may decline—often due to higher resistance or a decrease in V_{oc} . Consequently, while overall efficiency can benefit from intensified light, it depends on the cell’s design and materials. Balancing the current gain with potential fill-factor losses is thus essential. Additional factors, including cell temperature, material selection, and interface quality, influence key performance parameters V_{oc} , FF , J_{sc} , and efficiency. Most solar cells are evaluated under standard test conditions (STC), which specify 1000 W/m^2 illumination and a cell temperature of 25°C . Efficiency values reported typically reference these STC conditions. In this work, the sunlight concentration was varied from 1 to 10,000 suns. The P-type doping level

was set at $2 \times 10^{16} \text{ cm}^{-3}$, while the N-type doping level was $2 \times 10^{15} \text{ cm}^{-3}$. The P-type layer had a thickness of $7.0 \mu\text{m}$, and the N-type layer measured $5.0 \mu\text{m}$. Under one-sun illumination, the cell achieved a maximum J_{sc} of 2.75 mA/cm^2 and a V_{oc} of 1.86 V . At 10,000 suns, J_{sc} rose to $24.715.5 \text{ mA/cm}^2$, and V_{oc} reached 2.33 V . Notably, efficiency increased from 23.93% at one sun to 30.2% at 10,000 suns, with intermediate values of 27.2% (100 suns), 28.3% (500 suns), 28.74% (1000 suns), and 29.74% (5000 suns). Figure 5.9 and Figure 5.10 illustrate the corresponding current-voltage (I - V) characteristics and voltages across this range.

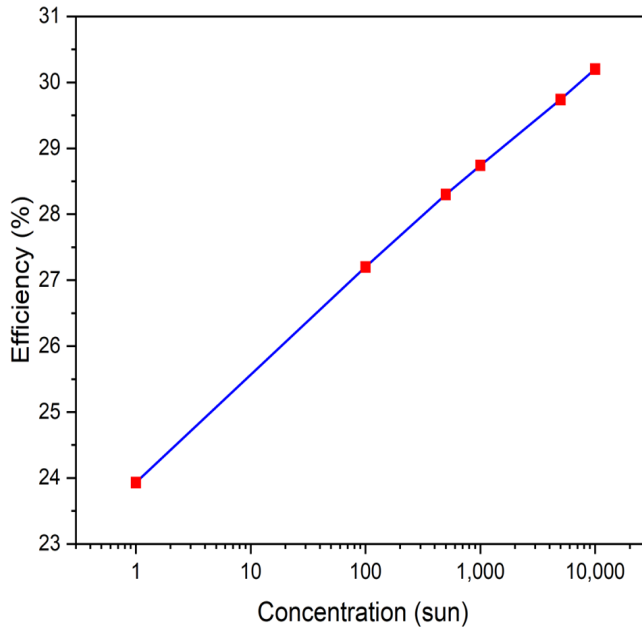


Figure 5.9: The efficiency and the concentration of 1 to 10,000 suns.

5.5. High-Efficiency Vertical Homo-Multijunction Solar Cells for CubeSats and Earth-Based Applications

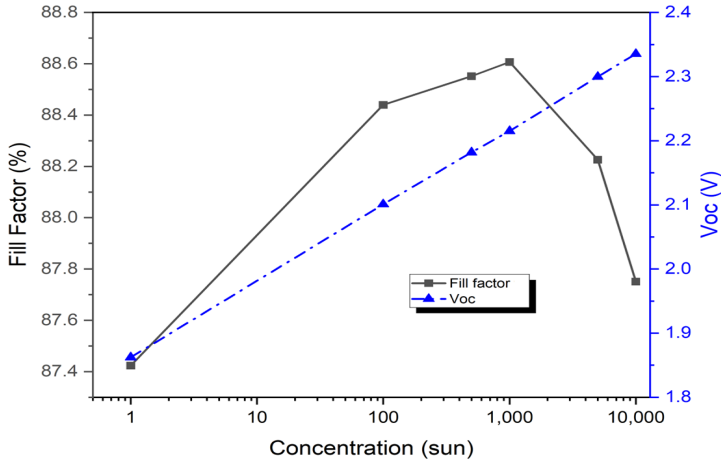


Figure 5.10: Influence of the Sun Concentrations.

5.5.6 The Combination Structure

This section focuses on optimizing the design parameters of ultra-high concentration vertical GaAs multijunction solar cells. The primary goals include refining layer thicknesses, doping concentrations, and solar radiation intensity to maximize overall device efficiency. By running simulations, researchers can identify the most promising structural designs and compare their performance to alternative configurations, ultimately selecting an approach that aligns with available materials and manufacturing methods. Figure 5.11 illustrates the optimized VTJ solar cell, which measures $20.33\ \mu\text{m}$ in width (W) and $1.25\ \mu\text{m}$ in height (H). Increasing H does not affect cell performance, so the structure can be extended laterally to reduce series resistance (R_s) without limit. The open-circuit voltage (V_{oc}) of the VTJ cell, shown as a function of concentration, reflects contributions from Auger, SRH, and radiative recombination. On a logarithmic scale, V_{oc} rises nearly linearly from 1.86 V at 1 sun to 2.4 V at 10,000 suns. Including all recombination mechanisms lowers V_{oc} by about 3.45% at 1 sun and 2.13% at 10,000 suns. Below 100 suns, SRH, and radiative recombination have some influence, but at higher concentrations, radiative effects dominate while SRH becomes less significant. Figure 5.12 presents VTJ cell efficiencies versus concentration for various recombination scenarios, while Figure 5.13 explores the combined impact of Auger, radiative, and SRH mechanisms on fill factor (FF). Auger recombination increases with concentration,

mirroring the logarithmic rise in both FF and efficiency. Although FF climbs up to around 1000 suns in all cases, it declines slightly at more intense irradiance levels. Including all recombination mechanisms places FF in the 87.5–88.5% range between 1 sun and 1000 suns, dipping marginally to 88.3% at 10,000 suns. This amounts to a difference of roughly 1% across all tested conditions. Present-day ultra-high concentration vertical homo-multijunction solar cells exhibit relatively low efficiency due to very small R_s values, approximately an order of magnitude below those of conventional concentrator cells. Designing and fine-tuning photovoltaic systems to optimize performance under varying sunlight intensities remains a key objective, as highlighted in Figure 5.14 shows the current-voltage (I – V) characteristics from 1 sun to 10,000 suns. As illumination increases, the short-circuit current and open-circuit voltage both rise, demonstrating the cell's capacity to produce more power under stronger light. The flat portion of each curve indicates the maximum current, whereas intersections with the axes represent peak voltage or current. The area under the curve is a critical metric for cell efficiency.

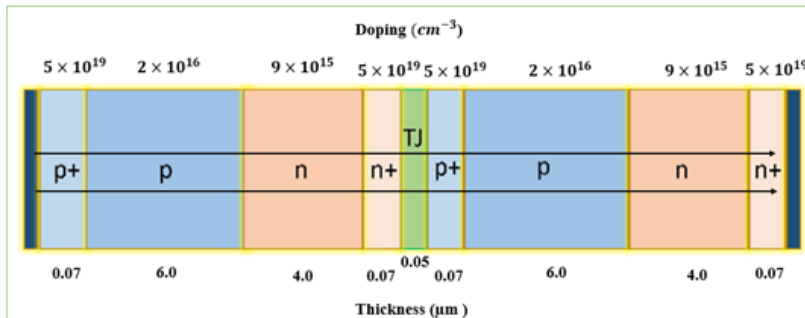


Figure 5.11: An illustration of the best structure of a HOMO GAAS–VMJ–UHCPV solar cell

5.5. High-Efficiency Vertical Homo-Multijunction Solar Cells for CubeSats and Earth-Based Applications

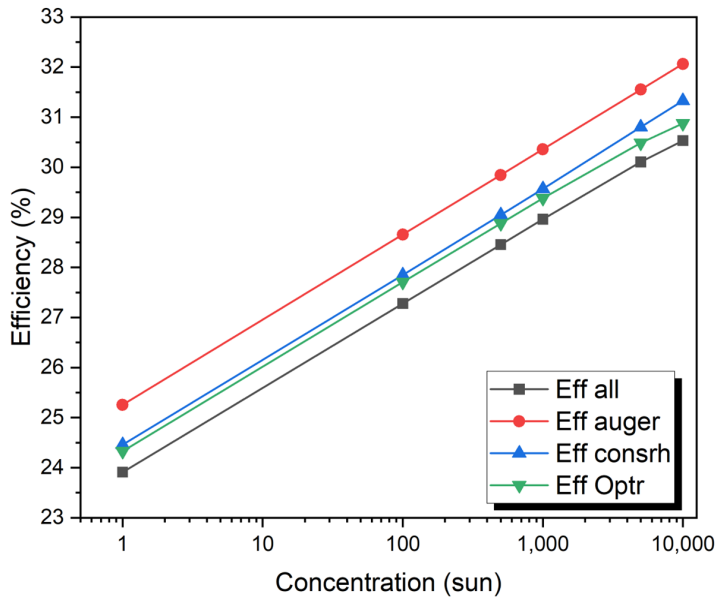


Figure 5.12: The efficiencies of HOMO GaAs- VMJ-UHCPV as a function of the concentrations with recombination mechanisms and with all recombination VTJ solar cells.

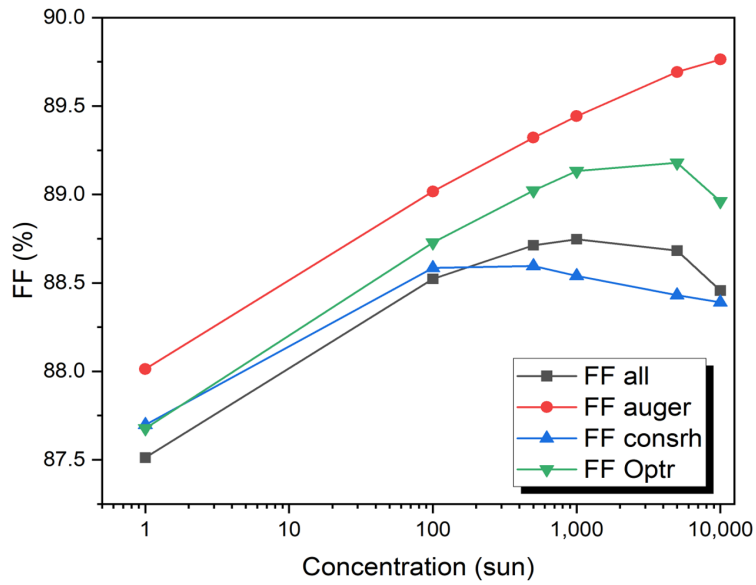


Figure 5.13: The fill factors of HOMO GaAs-VMJ-UHCPV for each recombination mechanism and all recombination.

5.6. Comparative Analysis of GaAs-Based VMJ and VTJ Solar Cells

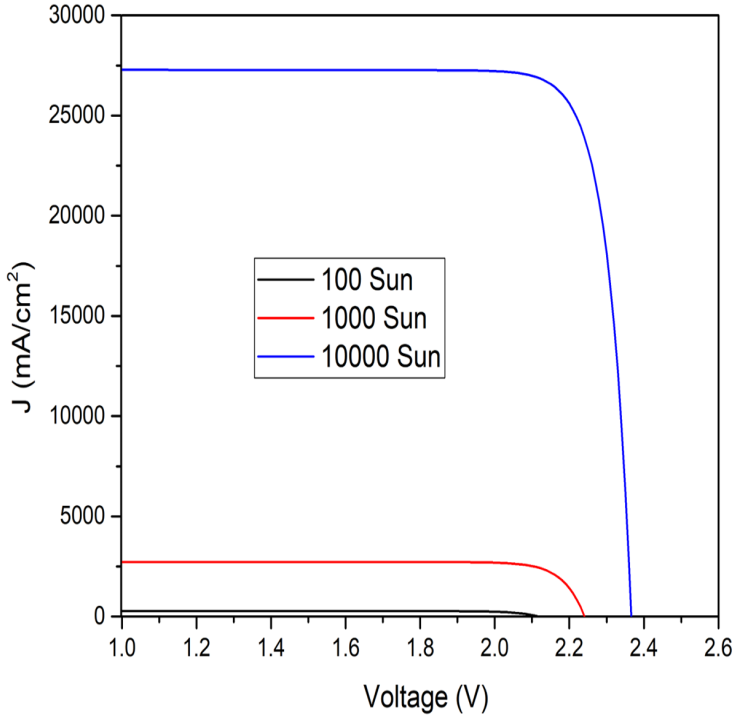


Figure 5.14: Solar cell J-V characteristics at different sun concentrations.

5.6 Comparative Analysis of GaAs-Based VMJ and VTJ Solar Cells

This section compares different vertical multijunction (VMJ) and vertical tunnel junction (VTJ) solar cell architectures under high and ultra-high solar concentrations. Segev and Kribus (2013) and Xing et al. (2013) focused on silicon-based VMJ structures and achieved efficiency levels of 30% for concentration ratios up to 1000 suns [146, 147]. These designs addressed series resistance and voltage optimization, offering high voltage operation but limited adaptability to scenarios involving very high concentrations (see Table 5.7). In contrast, GaAs-based VTJ cells, such as those studied by Outes et al. (2020), Fernández et al. (2019), and Seoane et al. (2021), demonstrated improved performance by reducing resistive losses [128, 129, 148]. According to Seoane et al. (2021), the VTJ model can achieve the-

oretical efficiencies exceeding 40% by incorporating intrinsic layers. However, such models are primarily theoretical. Across these studies, balancing series resistance, recombination losses, and manufacturability at ultra-high concentrations has remained a common challenge (refer to Table 5.9). As a result, the current work by Abushattal et al. [149, 150] demonstrates a significant advance. An optimized solar cell structure simulated using SILVACO TCAD (ATLAS) achieved a conversion efficiency of 29.61% in the IEEE study (2024a) under AM1.5 and 25.42% in the Micromachines study (2024b) under AM0, both at 4000 suns with a homo-multijunction GaAs VMJ architecture (see Table 5.7). These results confirm the device's adaptability to both terrestrial and space environments. Unlike many previous implementations, the design achieved an open-circuit voltage above 2.28 V while maintaining a high fill factor (86%) and outstanding voltage stability. In addition, this vertical configuration offers superior performance under non-uniform illumination, enhanced spectral response, and thermal stability—qualities that make it highly suitable for CubeSats and nanosatellites with limited surface area (as summarized in Table 5.8). In contrast to conventional horizontal designs, the proposed architecture minimizes series resistance by taking advantage of large carrier cross-sections and optimizing lateral contacts. This design enables decoupling between photon absorption depth and carrier collection efficiency. Compared to existing literature, this work stands out for its high efficiency, manufacturability, and application versatility. In addition to demonstrating the viability of GaAs-based VMJ structures at ultra-high concentration, it introduces an innovative method for integrating these devices into next-generation terrestrial and aerospace energy systems.

5.6. Comparative Analysis of GaAs-Based VMJ and VTJ Solar Cells

Table 5.7: Efficiency and concentration levels of VMJ and VTJ solar cells.

Study	Cell Type	Efficiency	Optimal Concentration (suns)
Segev & Kribus (2013)	Si VMJ	~30%	~1000
Xing et al. (2013)	Si VMJ	30.56%	1000
Outes et al. (2020)	GaAs VTJ	32.2%	10,000
Fernández et al. (2019)	GaAs VTJ	28.4%	15,000
Seoane et al. (2021)	GaAs i-VTJ	>40%	15,000
Khalis & Masrour (2021)	Si VMJ	26.2%	100
Zekry et al. (2018)	General PV	N/A	General
Outes et al. (2018)	GaAs VMJ	23.25%	10,000
Abushattal (2024 - Micromachines)	GaAs VMJ	30.2%	4000
Abushattal (2024 - IEEE)	GaAs VMJ	29.61% (AM1.5) / 25.42% (AM0)	4000

Table 5.8: Simulation tools, structure types, materials, and target applications.

Study	Simulation Tool	Structure	Material	Application
Segev & Kribus (2013)	Analytical	Vertical	Si	High CPV
Xing et al. (2013)	TCAD	Vertical	Si	High CPV
Outes et al. (2020)	TCAD	Vertical-Tunnel	GaAs	Ultra-high CPV
Fernández et al. (2019)	TCAD	Vertical-Tunnel	GaAs	Ultra-high CPV
Seoane et al. (2021)	TCAD	Intrinsic-VTJ	GaAs	Ultra-high CPV
Khalis & Masrour (2021)	Analytical/TCAD	Vertical	Si	Moderate CPV
Zekry et al. (2018)	Circuit/TCAD	General	General	General PV
Outes et al. (2018)	TCAD	Vertical	GaAs	High/Ultra-high CPV
Abushattal (2024 - Micromachines)	Silvaco TCAD	Vertical Multi-junction	GaAs	UHCPV, CubeSats
Abushattal (2024 - IEEE)	Silvaco TCAD	Vertical Multi-junction	GaAs	UHCPV, CubeSats

5.7. Economic Feasibility and Implementation Potential

Table 5.9: Performance insights: resistance, voltage, recombination, and advantages.

Study	Series Resistance	Voltage Characteristics	Recombination Management	Advantages
Segev & Kribus (2013)	Addressed	High	N/A	Good Efficiency
Xing et al. (2013)	Addressed	High	Detailed	Good Efficiency
Outes et al. (2020)	Minimized	Optimized	Extensive	High Efficiency
Fernández et al. (2019)	Minimized	Optimized	Optimized	High Efficiency
Seoane et al. (2021)	Minimized	Optimized	Highly Optimized	Ultra-high Efficiency
Khalis & Masrour (2021)	High at high suns	High	Critical at high suns	Moderate Efficiency
Zekry et al. (2018)	General	General	General	General Use
Outes et al. (2018)	Addressed	High	Addressed	Moderate Efficiency
Abushattal (2024 - Micromachines)	Highly Minimized	Optimized High Voltage	Highly Optimized	High efficiency, CubeSat ready, optimized structure
Abushattal (2024 - IEEE)	Highly Minimized	Optimized High Voltage	Highly Optimized	Efficient for space/terrestrial, compact and scalable

5.7 Economic Feasibility and Implementation Potential

VMJ solar cells based on GaAs exhibit not only excellent electrical performance. Furthermore, it can be implemented in CubeSat missions and terrestrial ultra-high concentration pho-

photovoltaic (UHCPV) systems with high economic reliability. Structure-wise, the design uses a simplified homo-junction architecture, minimizing material and fabrication complexity and reducing the need for lattice-matched tunnel junctions. Consequently, costs will be lower. According to an approximate cost analysis, a prototype-level device could cost between \$70 and \$100 per cell based on commercially available 2-inch GaAs wafers, Metal-Organic Chemical Vapor Deposition (MOCVD) growth, metal contacts, and encapsulation. The material costs \$10-\$15 (\$10 for GaAs substrates, \$15 for metallization, \$55 for anti-reflective coatings, and \$60 for processing, including cleanrooms and labor) [151–153]. CubeSat applications can benefit from the high efficiency of 29.61% (AM1.5) and 25.42 % (AM0) at 4000 suns, reducing power generation surface area and launch costs - key economic drivers. It provides superior heat dissipation and performance in non-uniform illumination conditions, making it more reliable when operating under variable space conditions. UHCPV installations requiring high concentration ratios are especially well-suited to this type of VMJ structure. Arrays designed with this technology can reduce balance-of-system (BoS) costs thanks to its robust efficiency, and its vertical geometry makes it possible to create them compactly. Using SILVACO TCAD, a simulation-optimized design can be implemented faster and at lower costs, reducing development time and prototyping cycles early. In addition to its technical performance and economic feasibility, the device offers a high-performance, scalable solution that can be used in both aerospace and renewable energy applications.

CHAPTER 6

CONCLUSIONS AND FUTURE WORK

6.1 Conclusions

The conclusion focuses on how vertical multijunction solar cells, especially those with GaAs substrates, are optimized for UHCPV applications. Significant improvements were achieved in doping concentration, layer thickness, and efficiency, attaining performance metrics exceeding 30% efficiency at 10,000 suns. Additionally, the potential of GaAs-based VMJ solar cells for CubeSats and terrestrial systems highlights their adaptability, reliability, and high energy conversion efficiency. Insights into recombination mechanisms such as Auger, SRH, and radiative recombination provide a deeper understanding of performance trade-offs under varying conditions. By utilizing the advanced simulation tool Silvaco ATLAS, the study demonstrates how predictive modeling can reduce prototyping costs and refine future experimental efforts.

Optimization of VMJ Solar Cells

- The study reveals that VMJ solar cells, particularly those based on GaAs, offer critical advantages for UHCPV applications.
- Optimized doping concentrations and layer thicknesses in P- and N-type regions improved metrics such as short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), and efficiency.

- Efficiencies exceeding 30% at 10,000 suns were achieved, showcasing the potential for VMJ cells in high-intensity scenarios.

Applications in CubeSats and Terrestrial Systems

- GaAs-based VMJ solar cells were identified as ideal for CubeSats due to their robustness against radiation and temperature extremes and their high energy conversion efficiency.
- This research bridges terrestrial and space applications, demonstrating their adaptability to diverse environments.

Recombination Mechanisms and Performance

- The study highlights the dominance of radiative recombination at higher sun concentrations and its effect on performance metrics such as V_{oc} and efficiency.
- Insights into recombination mechanisms (Auger, SRH, radiative) provided a clearer understanding of performance trade-offs under different conditions.

Advanced Simulation Techniques

- The use of Silvaco ATLAS for simulations demonstrated its efficacy in optimizing solar cell designs, predicting performance outcomes, and guiding experimental validations.
- These simulations minimized the reliance on expensive physical prototypes.

6.2 Future Research Directions

This section explores pathways to maximize the potential of VMJ solar cells while addressing the challenges highlighted in this study. Key recommendations include exploring alternative III-V materials and hybrid semiconductors for enhanced performance and cost efficiency, developing advanced thermal management techniques for UHCPV systems, and integrating energy storage solutions for continuous power supply. Scalable manufacturing methods and applications in wearable technology and disaster relief are also emphasized. Machine learning and AI are suggested to optimize design parameters and predict performance trends, paving the way for next-generation solar cells tailored to various applications and environments.

6.2. Future Research Directions

Exploration of Material Alternatives

- Investigate III-V semiconductor materials like InGaP or AlGaAs to enhance performance and reduce manufacturing costs.
- Study hybrid materials that combine the benefits of inorganic and organic semiconductors.

Thermal Management Strategies

- Develop advanced heat dissipation techniques for UHCPV systems to address thermal challenges at high sun concentrations.
- Incorporate both passive and active cooling systems into VMJ cell designs.

Integration with Energy Storage

- Explore the integration of VMJ cells with advanced energy storage systems such as batteries and hydrogen cells to enable continuous power supply in space and terrestrial applications.

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Appendix A: ATLAS Silvaco Code for Vertical Multijunction Solar Cell

```
# GaAs VTJ 2 cells with 4 layers (electrode or tunnel)

# parallel version with N processors
go atlas simflags="-P 3"

# thickness solar cell (CHANGE ONLY y_layer_P2, y_layer_N1)
set y_layer_P1=0.07 # Do NOT CHANGE
set y_layer_P2=2.6
set y_layer_N1=2.1
set y_layer_N2=0.07 # Do NOT CHANGE

# doping solar cell (CHANGE ONLY P2_doping, N1_doping)
set P1_doping=5e19 # Do NOT CHANGE
set P2_doping=2e16
set N1_doping=9e15
set N2_doping=5e19 # Do NOT CHANGE

# Connection region (widths, dopings, resistance)
set y_layer_tunnel_N=0.025 # Do NOT CHANGE
set y_layer_tunnel_P=0.025 # Do NOT CHANGE
set N_tunnel_doping=7e19 # Do NOT CHANGE
set P_tunnel_doping=7e19 # Do NOT CHANGE
set resistance=1.25e16 # Do NOT CHANGE
# set width of the device
set width=15.0 # Do NOT CHANGE
# set sun concentration
# WARNING: possible values must be divisible by 10 (1, 10, 20, 300, 500,
etc)
```

Appendix A: ATLAS Silvaco Code for Vertical Multijunction Solar Cell

```

set sun_concen=4000
# set tunnel (flag_tunnel=1) or electrode (flag_tunnel=0)
set flag_tunnel=0

# Set parameters: area illumination, contact area, illumination height
set altura_SC=($y_layer_P1+$y_layer_P2+$y_layer_N1+$y_layer_N2)
set altura_tun=($y_layer_tunel_N+$y_layer_tunel_P)
set area_ilum=($altura_SC*2+$altura_tun)*1.0e-8
set area_cont=$width*1.0e-8
set altura_ilu= (($altura_SC)*2+($altura_tun))/2.0

#####
# NO CHANGES BELOW THESE LINES
#####
mesh auto
#
x.m loc=0.0 s=0.25
x.m loc=$width s=0.25
# First solar cell
region material=GaAs bot thick=$y_layer_P1 accept=$P1_doping ny=5
region material=GaAs bot thick=$y_layer_P2 accept=$P2_doping ny=20
region material=GaAs bot thick=$y_layer_N1 donors=$N1_doping ny=20
region material=GaAs bot thick=$y_layer_N2 donors=$N2_doping ny=5

# Region that connects both solar cells
region material=GaAs bot thick=$y_layer_tunel_N donors=$N_tunnel_doping
ny=4
region material=GaAs bot thick=$y_layer_tunel_P accept=$P_tunnel_doping
ny=4

# Second solar cell
region material=GaAs bot thick=$y_layer_P1 accept=$P1_doping ny=5
region material=GaAs bot thick=$y_layer_P2 accept=$P2_doping ny=20
region material=GaAs bot thick=$y_layer_N1 donors=$N1_doping ny=20
region material=GaAs bot thick=$y_layer_N2 donors=$N2_doping ny=5

if cond =($flag_tunnel=1)
    set begin_tunnel_area=$altura_SC-($y_layer_N2/10.0)
    set vertical_tunnel=$altura_SC+$y_layer_tunel_N
    set end_tunnel_area=$vertical_tunnel+$y_layer_tunel_P+($y_layer_P1
        /10.0)
    qtx.m loc=0.0 s=0.10

```

Appendix A: ATLAS Silvaco Code for Vertical Multijunction Solar Cell

```
qtx.m loc=$width s=0.05
qty.m l=$begin_tunnel_area s=0.0002
qty.m l=$vertical_tunnel s=0.0001
qty.m l=$end_tunnel_area s=0.0002
electrode name=anode top
electrode name=cathode bottom
else
electrode name=anode top
electrode name=cathode bottom
electrode name=tuncontact x.min=0.0 x.max=$width \
y.min=$altura_SC y.max=$altura_SC+$altura_tun material=GaAs
contact name=tuncontact resist=$resistance
if.end

# The complex index data will mostly use the Sopra database.
# The index data for InGaP is supplied in a file.
material mat=GaAs sopra=Gaas.nk taun0=4.4e-4 \
taup0=2.2e-4 nsrhn=2.7e13 nsrhp=2.7e13
material mat=InAlGaP sopra=Againp7.nk
material mat=AlGaAs sopra=Algaas7.nk
material material=InGaP index.file=solarex03.nk

# Here we define the affinity for InGaP and AlGaAs to
# set up the band alignment
material material=InGaP affinity=4.08
material material=AlGaAs affinity=3.54

# Enable physical models
models consrh fermi conmob optr auger bgn

# Method parameters
method itlimit=40 maxtraps=10

# Here we specify the optical source. It propagates normal to the
# surface from above. We specify a multispectral source using
# the POWER.FILE parameter to identify the spectrum. We output
# the spectrum for Tonyplot using the OUT.POWER parameter.
# The spectrum is resampled via specification of the parameters
# WAVEL.START, WAVEL.END and WAVEL.NUM. This indicates that
# the optical propagation problem will be solved at 300 uniformly
# spaced samples of wavelength between 0.305 and 3.445 microns.
# In this case a ray trace will be performed at each of the 300
```

Appendix A: ATLAS Silvaco Code for Vertical Multijunction Solar Cell

```
# sample wavelengths. If we omit the WAVEL.START, WAVEL.END
# and WAVEL.NUM parameters the sampling will occur at each
# wavelength specified in the spectrum file (POWER.FILE).
beam num=1 x.o=-0.1 y.o=$altura_ilu angle=0 \
    wavel.start=0.305 wavel.end=3.455 wavel.num=300 \
    power.file=solarex03_15.spec out.power=solarex03_15.log

# Plot input solar spectrum
# tonyplot solarex03_15.log -set solatonyrex03_0.set

# Here is an alternate simplified am0 solar spectrum
# power.file=solarex03_0.spec out.power=solarex03_0.log

# You may also choose to use the public domain spectra available
# from NREL by simply specifying the AM1.5 or AM0 parameter on
# the beam statement and taking out the POWER.FILE assignment.
# If you use either of these it is strongly suggested that you
# also specify the sampling using WAVEL.START, WAVEL.END and WAVEL.NUM
# since these spectra have many samples.

# Output optical intensity.
output band.temp opt.int

# Save the initial structure
# tony
save outf=vertical_ini.str
# tonyplot vertical_ini.str

# Ramp the bias
# Note that this could be used for IV dark
log outf=vertical_qt_IV_dark.log
solve name=anode vanode=0.0 vstep=0.05 vfinal=2.5

# Set models
if cond =($flag_tunnel=1)
    models consrh fermi ni.fermi conmob optr auger bgn \
        bbt.nonlocal bbt.nlnderivs
else
    models consrh fermi ni.fermi conmob optr auger bgn
if.end

# Here we ramp the beam. This is not to simulate
```

Appendix A: ATLAS Silvaco Code for Vertical Multijunction Solar Cell

```
# sunrise but to insure convergence. Often setting
# an optical source directly to its final value
# can present difficulties in convergence for
# Newton's method so it may be advisable to
# ramp the optical source.

# sun_concentration=0.1 suns
solve b1=1.0e-2
# sun concentration=1 suns
solve b1=1.0e-1

set v_b1=0

# General case
set add=100
set num_pasos=$sun_concen/$add

if cond =($sun_concen<100)
  set add=10
  set num_pasos=$sun_concen/$add
if.end
if cond =($sun_concen<10)
  set add=1
  set num_pasos=$sun_concen
if.end

loop steps = $num_pasos
  set v_b1=$v_b1+$add
  set ilu=($v_b1/10)
  solve b1=($v_b1/10)
l.end

# Ramp the bias back.
log outf=vertical_qt_IV_sun.log
solve name=anode vanode=2.5 vstep=-0.01 vfinal=1.5
solve name=anode vanode=1.5 vstep=-0.05 vfinal=0.2
solve name=anode vanode=0.2 vstep=-0.01 vfinal=-0.05

# Extract important figures of merit.
extract init infile="vertical_qt_IV_sun.log"
extract name="Isc" y.val from curve(v."anode", i."cathode") where x.val
=0.0
```

Appendix A: ATLAS Silvaco Code for Vertical Multijunction Solar Cell

```

extract name="JscmAc2" $Isc*1e03/$area_cont
extract name="Voc" x.val from curve(v."anode", i."cathode") where y.val
    =0.0

extract name="Pm" max(curve(v."anode", (v."anode" * i."cathode")))
extract name="Vm" x.val from curve(v."anode", (v."anode"*i."cathode") )
    \
    where y.val="$Pm"
extract name="Im" "$Pm"/"$Vm"
extract name="FF" ($"Pm"/($"Isc"*$"Voc"))*100
extract name="Opt_int" max(beam."1")
extract name="Eff" ($Pm/($Opt_int*$area_illum))*100

# Plot the results
# tonyplot vertical_IV.log -set solarex03_1.set

## Variables to be included in the .str output

if cond =($flag_tunnel=1)
    OUTPUT J.CONDUC QFN QFP J.ELECTRON J.HOLE J.TOTAL \
        BAND.PARAM CHARGE CON.BAND DEVDEG E.MOBILITY \
        E.TEMP E.VELOCITY FLOWLINES H.MOBILITY H.TEMP \
        H.VELOCITY HCTE.JOULE J.DISP J.DRIFT \
        J.DIFFUSION L.TEMPER PERMITTIVITY NLAT.GAMMA PHOTOGEN \
        QTUNN.BBT QTUNN.EL QTUNN.HO RECOMB T.QUANTUM TAURN TAURP \
        TRAPS TRAPS.FT U.AUGER U.BBT U.LANGEVIN U.RADIATIVE U.SRH \
        U.TRANTRAP U.TRAP VAL.BAND
else
    OUTPUT J.CONDUC QFN QFP J.ELECTRON J.HOLE J.TOTAL \
        BAND.PARAM CHARGE CON.BAND DEVDEG E.MOBILITY \
        E.TEMP E.VELOCITY FLOWLINES H.MOBILITY H.TEMP \
        H.VELOCITY HCTE.JOULE J.DISP J.DRIFT \
        J.DIFFUSION L.TEMPER PERMITTIVITY PHOTOGEN \
        RECOMB TAURN TAURP \
        TRAPS TRAPS.FT U.AUGER U.LANGEVIN U.RADIATIVE U.SRH \
        U.TRAP VAL.BAND
if.end

save outf=vertical_qt_sun.str

quit

```



This research is the advancement of vertical multijunction (VMJ) gallium arsenide (GaAs) solar cells that are essential for ultra-high concentration photovoltaic (UHCPV) systems. The advantages of VMJ solar cells are their high energy conversion efficiency, robustness against space radiation, and suitability for CubeSats. Several key parameters, ranging from doping density to layer thickness and solar concentration, are addressed in this study using the ATLAS Silvaco simulation platform. An advanced modeling technique investigated the interaction between intrinsic parameters (e.g., doping and thickness of the P and N layers) and extrinsic conditions (e.g., sun concentration levels under AM0 and AM1.5 spectrums).