

BHARATA MATA COLLEGE, THRIKKAKARA

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PROJECT

DEPARTMENT OF PHYSICS

MOLYBDENUM AS A CARRIER SELECTIVE LAYER IN SOLAR CELL

PROJECT REPORT SUBMITTED TO,

MAHATMA GANDHI UNIVERSITY, KOTTAYAM

SUBMITTED BY,

CHRISTINA J. THATTIL

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CERTIFICATE

This is to certify that the project report entitled “Molybdenum as a carrier selective layer in solar cell” is an authentic study carried out by Christina J. Thattil, Reg. No. 200021039165, for the partial implementation of the requirement for the award of a degree BACHELOR OF SCIENCE IN PHYSICS through the Post Graduate Department of Physics, Bharata Mata College, Thrikkakara, affiliated to Mahatma Gandhi University, Kottayam, Kerala.

Head of the Department

Dr. Lini Devassy

Class in Charge

Ms Ginu V.G.

Supervising guide

DECLARATION

This dissertation "MOLYBDENUM AS A CARRIER SELECTIVE LAYER IN SOLAR CELL" is a bonafied work done by me at Bharata Mata College, Thrikkakara under the guidance of Ginu V G Department of physics.

The comparative study published in the report is completely known to me and true.

Christina J. Thattil

Place: Thrikkakara

Date:23/4/23

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Apart from my efforts, the success of my project largely depends on the encouragement and guidance of others.

Firstly I thank God for all the blessings bestowed upon till the completion of this project. I take this opportunity to express my gratitude to people who has been instrumental in successful completion of this project.

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INTRODUCTION

A solar cell is a type of electronic device that turns sunlight directly into electricity. A current and voltage are produced by light striking the solar cell which results in electric power generation. First, a substance in which light is absorbed moves an electron to a higher energy state and then the electron in the higher energy state is transferred from the solar cell to an external circuit, thereafter losing its energy in the external circuit, the electron returns to the solar cell. The requirements for photovoltaic energy conversion can be met by a variety of materials and methods, but in reality, almost all photovoltaic energy conversion uses semiconductor materials in the form of a p-n junction.

THE PHOTOVOLTAIC EFFECT

Power generation is not a result of the collection of light-generated carriers alone. Both a voltage and a current must be produced in order to produce power. The "photovoltaic effect" is a process that creates voltage in a solar cell. The motion of electrons to the n-type side of the junction and holes to the p-type side is a result of the p-n junction's collection of light-generated carriers. Since the carriers leave the device as light-generated current in short circuit conditions, there is no charge build up. The difference between I_L and the forward bias current is the current generated in the solar cell.

When the circuit is open, the junction's forward bias rises to the point where the forward bias diffusion current completely balances the light-generated current, arising zero net current. The "open-circuit voltage" is the voltage needed to bring these two currents into equilibrium. At the metal-absorber contact, there are numerous defect states for diffused homojunction silicon solar cells. These defect states cause charge carrier recombination, which lowers fill factor and I^*V_n and lowers cell efficiency. The main barrier to silicon solar cells operating at their theoretical maximum efficiency is this recombination loss [10]. The method that is most frequently employed to suppress these recombination losses is heavy doping in the region beneath the metal contact. While blocking holes, the strongly doped n + area promotes the movement of electrons. Similar to the p + zone, which permits electrons to have high resistivity while also allowing holes to pass, the p + region lowers recombination losses. However, diffusion is a high-temperature (>800°C) and energy-intensive process. Other drawbacks of the diffusion process used to fabricate conventional diffused homojunction c-Si solar cells include the toxicity of doping materials like boron and phosphorus and the complexity of the doping technology. However, by combining the most effective heterojunctions (HJ) with interdigitated back contacts, crystalline silicon (c-Si) solar cells (SCs) have recently demonstrated a record efficiency of 26.6%. However, due to parasitic

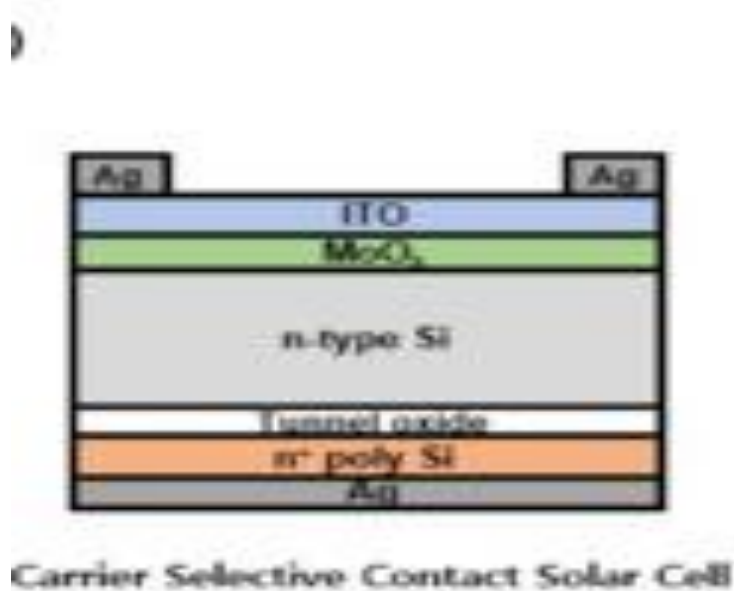
absorption/Auger recombination intrinsic to the doped films and the challenging process of integrating discrete p+- and n+-HJ connections, such SCs still cause optical/electrical losses and technological problems. These problems have spurred research into new functional materials and streamlined deposition techniques that enable the formation of carrier-selective connections (CSCs) directly on c-Si substrates.

An essential component of solar cells is carrier- selective connections. Realising that electrons and holes are captured by two different terminals, they work to separate carriers produced in absorbers. Therefore, the carrier- selective contacts' performance has a direct impact on how well solar cells operate. Carrier- selective contacts are of great interest and play a significant role in raising the power conversion efficiency of solar cells, whether they are used in crystalline silicon (c-Si), perovskite, or organic solar cells.

By externally covering the c-Si substrate with a thin p* or n* polysilicon film and sandwiching an ultrathin silicon oxide between them, carrier-selective connections can also be achieved. A high level of surface passivation and exceptional carrier selectivity (particularly for electron-selective contact) are demonstrated for such a structure. Additionally, extensively used as carrier- selective layers in c-Si solar cells, strongly doped and hydrogenated amorphous silicon films combine with intrinsic a-Si:H films and have proven to be highly effective in realising excellent cell performance. Other materials, such as different metal oxides, nitrides, fluorides, and organic compounds, are being investigated in recent years in addition to severely doped silicon. Using carrier-selective films, solar cells can be made more easily, more affordably, with less parasitic absorption, and with more carrier selectivity.

MOLYBDENUM AS A CARRIER SELECTIVE LAYER

Due to its better conductivities and suitable work functions, molybdenum oxide (MoO_x) was thought to be an excellent choice for carrier-selective contacts (CSCs) for crystalline silicon (c-Si) solar cells. The c-Si/ MoO_x interface's weak passivation and non-Ohmic contact, however, result in a decrease in the degree of hole selectivity. Carrier-selective characteristics are revealed by systematically examining the surface, interface, and bulk structures of MoO_x films using X-ray scattering, surface spectroscopy, and electron microscopy analysis. When exposed to air, surface layers with the chemical composition $\text{MoO}_{2.51}\text{N}_{0.21}$ develop, leading to an inflated work function and the origin of inferior hole selectivity. It has been demonstrated that the c-Si/ MoO_x interface exhibits long-term stability, offering suggestions for creating stable CSCs. To explain the better conductivity of the solar cell, a thorough evolution of the scattering length density, domain sizes, and crystallinity in the bulk phase is described. These multiscale structural studies provide a precise structure-function relationship for MoO_x films, which is a crucial source of inspiration for creating top-notch CSCs for c-Si solar cells.



PROPERTIES AND CHARACTERISTICS OF MOLYBDENUM AS A CSL

Due to its appealing oxide semiconductor properties and its high electron affinity (6.7 eV) and huge band gap (3.6 eV at ambient temperature), MoO_3 is widely used in cutting-edge optoelectronic devices. Along with these, MoO_3 possesses a variety of fascinating properties, such as a high refractive index, electrochromic capabilities, and a high degree of chemical stability. Because of these benefits, MoO_3 is a strong contender for a number of possible uses,

including transparent conductive coatings, battery electrodes, gas sensors, and hole-blocking layers in photovoltaics (PVs). MoO_3 has received a lot of interest in organic photovoltaic systems due to its capacity to improve charge injection and its collection. Therefore, it is crucial to investigate the impact of barrier height on MoO_3/Si heterojunctions capacity to block holes for use in hole-blocking PV cells.

WORK FUNCTION OF MOLYBDENUM

There is a certain work function for each metal. A metal's work function is the bare minimum of energy required to remove an electron from its atom's orbital. The energy of an electron rotating around a nucleus determines the value of the work function. Electron volts (eV) are used to measure it.

A common refractory metal is molybdenum. Even at extremely high temperatures, it still has strong mechanical characteristics. It is used to make bearing parts, lift brakes, furnace parts and forging dies and has low thermal expansion and strong heat conductivity. Due to its strong electrical conductivity, molybdenum, which has a melting point of $4,753^\circ\text{F}$ ($2,623^\circ\text{C}$), is utilised to create solids that melt glass. Molybdenum has a high work function of 4.36.

The Fermi level moves closer to the E_v of the n-c-Si absorber as a result of the band bending at a front interface, which is caused by the greater Ψ_m of MoO_x . This band bending denotes the carrier inversion, in which the minority electrons are prevented from travelling towards the anode by a wide Schottky barrier, thus reducing the amount of electrons at the front interface. Moreover, the absence of an extensive barrier makes it simple to transmit holes to the anode terminal

STRATEGIES FOR OPTIMISING THE PROPERTIES OF MOLYBDENUM CSL'S

The conductivity of the device regions close to the external metal electrodes plays a significant role in determining the selective extraction of the excess holes and electrons from the absorber into the external circuit. These device areas create the solar cell's hole- and electron-selective contacts. Specifically, the conductivity of the carrier species that must be prevented in these device locations must be as low as possible. In the same way as for the other species, for which the contact is meant to be selective, the local conductivity needs to be high enough to ensure an efficient carrier transport into the exterior electrodes.

In experiments, a strong asymmetry of the local hole (p) and electron (n) densities—which comes from enough doping and/or an induced junction—is primarily responsible for the extreme asymmetry of the local conductivity. Doping and the induced junction must be created with the goal of producing local p+ or n+ areas for which $p \gg n$ and $n \gg p$ be preserved under all operating conditions, respectively. This criteria is equivalent to the need to maintain low-injection conditions in the contact region, meaning that when the device is operating, the

majority carrier density must be significantly higher than the minority carrier density. The key distinction between the traditional homojunction and the relatively new or unique homojunction is how low-injection conditions are ensured.

The experimental methods utilised in traditional homojunctions to achieve a preferential hole/electron transport are always accompanied by an increased minority carrier recombination. Major losses result from the fact that (i) the metallized regions contacting the doped c-Si regions are not passivated and therefore exhibit a high recombination activity and (ii) the doped p+ and n+ c-Si regions are heavily doped (increasing Auger recombination and narrowing the band gap). This class of passivating and carrier-selective contact systems makes it possible to greatly reduce inherent losses. Their fundamental characteristics are dependent on the contact arrangements used in conductor-insulator-semiconductor solar cells.

COMPARISON OF MOLYBDENUM CSL'S WITH OTHER MATERIALS

A wide bandgap material with a high work function is frequently employed as the hole extraction pathway to achieve high efficiency in silicon heterojunction (SHJ) solar cells. Due to its wide bandgap and excellent work function, we introduced a molybdenum oxide (MoO_x) film as a useful hole-transfer layer in carrier selective contact (CSC) solar cells.

MoO_x films' passivation characteristics, optical, and electrical features were examined using various thickness and work function combinations.

The combination of 7 nm thermally evaporated MoO_x passivation layers and 6 nm hydrogenated intrinsic amorphous silicon (aSi:H(i)) passivation layers offers outstanding passivation qualities, lowers carrier recombination, and enhances cell performance. The MoO_x /c-Si(n) interface's high work function and broad bandgap created a significant internal potential and inhibited the electron-hole pair recombination mechanism. The cSi/TiOx interface exhibits a greater ΔEV between the two materials due to TiOx's wide band gap. Minority holes cannot be transported from the EV of cSi towards the cathode due to the greater overall energy barrier from cSi to TiOx (ΔEV 14 2.0 eV). However, cSi and TiOx's conduction band minimums are closely correlated with one another.

The thermal stability of the perovskite films deposited on top of the low-temperature, solution-processed zinc oxide (ZnO) layer continues to be a significant problem despite the fact that ZnO has been widely used as the electron collection layer (ECL) in perovskite solar cells (PSCs) due to its straightforward synthesis and excellent electrical properties, such as high charge mobility. Here, we used aluminum-doped zinc oxide (AZO) as the ECL to solve this issue and produce incredibly thermally stable perovskite layers. The decrease in the chemical Lewis acid-base reaction between perovskite and ECL was attributed to the improvement in heat stability. Notably, the exceptional conductivity and transmittance of the AZO layer make it a prime choice for transparent conductive electrodes, enabling a cell configuration of glass/AZO/perovskite

/Spiro-OMeTAD/Au. The champion cell exhibits an open-circuit voltage (V_{oc}) of 0.94 V, a short-circuit current (J_{sc}) of 20.2 mA cm^{-2} , a fill factor (FF) of 0.67, and an overall power conversion efficiency (PCE) of 12.6% under standard 1 sun illumination thanks to the optimisation of the perovskite layer. Additionally, it was discovered that the AZO/perovskite interface resulted in less quenching than that between perovskite and hole transport material using steady-state and time-resolved photoluminescence.

FABRICATION AND INTEGRATION OF MOLYBDENUM CSLS

Overview of the different methods for fabricating molybdenum CSLs, including sputtering, chemical vapor deposition, and thermal evaporation

Many different applications, such as solar cells and other electronic devices, rely on molybdenum carrier selective layers. The fabrication of molybdenum carrier selective layers can be accomplished in a number of ways, each with a unique set of benefits and drawbacks.

Sputtering : With this technique, molybdenum atoms are ejected from a molybdenum target by high-energy ions, which then deposit on a substrate to create a thin film. Sputtering can create very high quality films with exact control over thickness and composition, and it can be done in a vacuum or a gas atmosphere. It might necessitate high temperatures or other specialised equipment, but it can also be costly and time-consuming.

Chemical vapor deposition : In this process, a vaporised precursor reacts chemically with a substrate to deposit molybdenum onto the substrate. Excellent homogeneity, reproducibility, and control over film parameters like composition and thickness are all possible with CVD. But it can also be challenging and call for specialised tools and expertise.

Thermal evaporation : This process includes vaporising a molybdenum source in a vacuum to produce a thin film, which condenses onto a substrate. Thermal evaporation can provide films with good adherence and uniformity that are also reasonably cheap and easy to use. However, it may also be less accurate than other techniques and call for extreme temperatures or other specialised circumstances.

Overall, according to the particular needs of the application, any of these techniques can be utilized to produce molybdenum carrier selective layers with a variety of traits and qualities. Based on aspects like cost, time, complexity, and performance requirements, researchers and engineers can choose the optimum method

Challenges and opportunities for integrating molybdenum CSLs into different solar cell architectures, such as p-n and p-i-n junctions

In order to increase the effectiveness of solar cells, molybdenum carrier selective layers have been found as a promising component. However, integrating them into other solar cell topologies, such as p-n and p-i-n junctions, brings both challenges and opportunities.

Challenges

Compatibility with other cell components : The molybdenum selective layers must be compatible with other solar cell elements like the semiconductor material and the metal connections in order to prevent deterioration over time.

Optimum thickness and doping level : To obtain the necessary electrical characteristics and reduce carrier recombination, the thickness and doping level of the molybdenum selective layer must be optimised for each unique solar cell architecture.

High temperature processing : The performance and stability of the molybdenum selective layer may be impacted by high-temperature manufacturing procedures needed for some solar cell layouts.

Cost- effective deposition techniques : For the purpose of producing solar cells on a wide scale, the deposition methods utilised to create molybdenum selective layers must be affordable and scalable.

Opportunities

Improved open-circuit voltage : Solar cell's open-circuit voltage (Voc) can be increased by using molybdenum selective layers because they prevent charge carriers from recombining at the metal contact interface.

Enhanced carrier collection : The molybdenum selective layer can improve carrier collection and thus raise the current density of the solar cell by choosing an appropriate doping amount and thickness.

Compatibility with various semiconductor materials : Molybdenum selective layers are a flexible choice for solar cell integration since they have demonstrated compatibility with a range of semiconductor materials, such as silicon, perovskites, and organic photovoltaic materials.

Low manufacture cost : Molybdenum is reasonably priced in comparison to other selective layer components like gold and silver, which can aid in reducing the overall cost of solar cell manufacture.

Overall, there are opportunities and challenges associated with integrating molybdenum selective layers into various solar cell topologies. Researchers and producers can take advantage of the special qualities of molybdenum to increase the efficiency and lower the cost of solar cells by maximising the doping amount, thickness, and deposition methods.

Discussion of the impact of molybdenum CSLs on device performance and efficiency

Due to their potential to improve the performance and efficiency of many thin-film solar cell technologies, molybdenum carrier selective layers have attracted a lot of attention. As a selective barrier to the transit of charge carriers, these carrier selective layers permit only the desired carriers to pass through while obstructing the opposing carriers.

An important advantage of molybdenum carrier selective layers is the enhancement of charge carrier separation and collection efficiency. By lowering the recombination losses at the interface between the active layer and electrode, they can raise the open circuit voltage (Voc) and fill factor (FF). The decrease in recombination losses enables an increase in the current density (Jsc), which raises the device efficiency as a whole.

Molybdenum carrier selective layers can increase the stability and endurance of the device in addition to increasing charge carrier transport. As a protective layer, they can stop the diffusion of undesirable species into the device (such moisture, oxygen, and contaminants), which can over time cause deterioration and lower efficiency.

However, the deposition technique and layer thickness can also have an impact on the effectiveness and performance of molybdenum carrier selective layers in devices. Carrier selectivity, as well as the layer's physical and optical properties, can be impacted by the layer's quality and thickness. Therefore, in order to get the greatest efficiency gains, the deposition technique and layer thickness must be optimised.

In general, molybdenum carrier selective layers have demonstrated tremendous promise for enhancing the efficiency and performance of many thin-film solar cell systems. To further improve the efficiency and stability of these devices, future research in this field will concentrate on creating new deposition procedures and bettering the overall device architecture.

APPLICATION

Molybdenum in silicon cell

MOO thin films' properties were examined by adjusting their thickness, temperature, and ambient annealing. The 10 nm thick MoO_x films displayed a large optical bandgap of 3.25 eV

and strong optical transmittance (89.81%) in the visible near infrared (NIR) wavelength region (380-1100 nm). Due to fewer extra flaws in the MoO_x films, an increased minority carrier lifetime of 2.24 ms was obtained for O₂ ambient at 130°C.

MoO_x film, which is 10 nm thick, was used to create carrier selective contact (CSC) solar cells, which had outstanding performance metrics such open circuit voltage (Voc) of 708 mV, current density (sc) of 37.80 mA/cm², fill factor (FF) of 74.95%, and efficiency (η) of 20.06%.

Molybdenum inperovskite

Monolithic perovskite-silicon tandem solar cells with silicon bottom cells that have MoO_x hole selective contacts have an 8% power conversion efficiency. To collect holes, a thin 15 nm-thick MoO_x contact to n-type Si was utilised instead of a conventional p+ emitter, and a SiO_x/n poly-Si structure was coated on the device's other side enabling direct tunnelling of electrons. This silicon bottom cell construction has a power conversion efficiency of about 15%.

COMPARISON OF THE PERFORMANCE AND STABILITY OF MOLYBDENUM CSL'S WITH OTHER CSL'S AND CONVENTIONAL SOLAR CELL MATERIALS

Selective contacts with molybdenum carriers have drawn a lot of attention due to their excellent performance and stability in solar cell applications. To ascertain their potential benefits and constraints, they are frequently contrasted with alternative carrier selective contacts and traditional solar cell materials.

The conventional n-type silicon layer is one of the most often utilised carrier selective contacts. However, because of their increased transparency and reduced contact resistance, molybdenum carrier selective contacts have been proven to offer improved efficiency. Additionally, they are more stable under prolonged exposure to heat and light, extending the lifespan of the gadget.

Although organic ETLs have a high efficiency in solar cells, they are frequently vulnerable to deterioration over time and may have poor thermal stability.

Thus, for long-term performance, molybdenum carrier selective contacts might be a more dependable and stable option.

Molybdenum carrier selective contacts are a relatively recent innovation when compared to traditional solar cell materials like copper indium gallium diselenide (CIGS) and thin-film photovoltaic technologies like cadmium telluride (CdTe).

The efficiency of devices using molybdenum carrier selective contacts has, however, been found in certain investigations to be comparable to or even greater than that of devices using CdTe and CIGS.

Furthermore, compared to these materials, molybdenum carrier selective connections might provide better stability.

In conclusion, molybdenum carrier selective contacts offer a competitive alternative to conventional carrier selective contacts and conventional solar cell materials and show

potential for enhancing the efficiency and stability of solar cells. However, more investigation is required to completely comprehend their potential benefits and restrictions as well as to enhance their functionality in solar cell applications.

Discussion of potential future directions for research and development of Molybdenum CSLs in solar cells.

It has been demonstrated that molybdenum carrier selective layers (MCSLs) enhance charge carrier separation while lowering recombination losses, increasing the efficiency of solar cells. To enhance solar cell performance and increase their commercial viability, further study and development are still required in this area.

One potential future direction for research is the optimization of the deposition technique for Molybdenum CSLs. This can entail investigating various deposition techniques (such as chemical vapour deposition or atomic layer deposition) and enhancing process variables like temperature, pressure, and layer thickness. The effectiveness of the Molybdenum CSLs in raising the performance of solar cells may be further increased by enhancing their quality and uniformity.

Research could concentrate on the integration of MCSLs with other technologies to enhance the overall performance of solar cells in addition to material development. For instance, MCSLs could improve the efficiency of tandem or multi-junction solar cells by enabling better absorption of a wider spectrum of solar radiation wavelengths. Furthermore, MCSLs might be used in conjunction with other technologies to produce organic photovoltaics or perovskite solar cells, which could result in even larger improvements in solar cell efficiency and scalability.

The long-term stability and dependability of MCSLs also require examination. It's critical to make sure that the MCSLs continue to be efficient and stable over time because solar cells are designed to function for many years under a variety of environmental circumstances. Long-term improvements to the reliability and durability of solar cells can be made by researching the mechanisms of MCSLs' degradation and creating mitigation measures.

In conclusion, there are many potential future directions for the study and creation of molybdenum carrier selective layers in solar cells. Researchers can continue to raise the efficiency and scalability of solar cells by experimenting with various deposition methods, creating new materials, combining them with other technologies, and researching long-term stability, which will help the transition to a more sustainable energy future.

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