

**INVESTIGATION OF INTRINSIC AMORPHOUS SILICON  
PASSIVATION LAYERS FOR SILICON HETEROJUNCTION  
SOLAR CELLS FABRICATION**

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**INDIAN INSTITUTE OF TECHNOLOGY DELHI**

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SOLAR CELLS FABRICATION**

by

**ASHUTOSH PANDEY**

**Department of Energy Science and Engineering**

Submitted

In fulfillment of the requirements of the degree of Doctor of Philosophy

to the



**INDIAN INSTITUTE OF TECHNOLOGY DELHI**

**JANUARY 2024**

**Dedicated to my family...**

## **CERTIFICATE**

This is to certify that the thesis entitled “**Investigation of Intrinsic Amorphous Silicon Passivation Layers for Silicon Heterojunction Solar Cells Fabrication**” being submitted by **Mr. Ashutosh Pandey** to Indian Institute of Technology Delhi is ethical of consideration for the award of the degree of Doctor of Philosophy and is a record of the original and bonafide research work carried out by him under my guidance and supervision. The results obtained in the thesis have not been submitted in part or full to any other University or Institute for award of any degree/diploma.

Date:

Place: New Delhi

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## **ABSTRACT**

A feasible way to tackle the growing energy demand is to harvest solar energy efficiently to produce electricity via photovoltaic devices (also known as solar cells). Crystalline silicon-based solar cells are the leading technology in fulfilling the demand in the photovoltaic industry due to stability and reliability in fabrication processes. Silicon heterojunction (SHJ) based solar cell technology is one of the options apart from other silicon solar cell technologies due to the relatively higher power conversion efficiency.

This thesis addresses the strategies to improve the SHJ solar cell power conversion efficiency by investigating the hydrogenated intrinsic amorphous (i-a-Si:H) buffer layer grown by the plasma-enhanced chemical vapor deposition technique. The primary purpose of the i-a-Si:H is to passivate the c-Si surface's dangling bonds, lowering the defect density at the a-Si:H/c-Si interface. As a result, it has now been widely acknowledged that optimizing the i-a-Si:H passivating layers is the key to producing high-performance SHJ solar cells. The microstructure of the i-a-Si:H layer is directly linked to its deposition conditions and is mainly responsible for the passivation quality of the c-Si wafer in the minimization of minority carrier recombination.

With this motivation, we have first explored the effect of the total flow rate variation (30–80 sccm) of precursor gases on the passivation of the i-a-Si:H/c-Si interface during the PECVD deposition of i-a-Si:H layer using SiH<sub>4</sub>/H<sub>2</sub> (equal ratio) plasma. However, a window of intermediate gas flow rates has been identified to achieve relatively good quality surface passivation. At an intermediate gas flow rate, a maximum effective minority carrier lifetime ( $\tau_{\text{eff}}$ ) above 1 ms, implied open-circuit voltage ( $iV_{\text{oc}}$ ) of 710 mV, and low interface defect density ( $D_{\text{it}}$ ) of  $3.5 \times 10^9 \text{ cm}^{-2} \text{ eV}^{-1}$  is achieved. Besides, the precursor gasses (SiH<sub>4</sub>:H<sub>2</sub>) discharge emission characteristics and the a-Si:H film characteristics (hydrogen concentration, film

density, optical band gap, and refractive index) are also investigated. The front-junction silicon heterojunction solar cells with flow rate variation are fabricated on n-type textured silicon wafers, and ~17% conversion efficiency and open-circuit voltage ( $V_{oc}$ ) close to 690 mV is achieved at an optimized gas flow rate. Thus, this work on a variation of gas flow rate provided insight regarding the correlation of the transient plasma instability,  $SiH_4$  depletion, secondary reactions in the plasma, and flux of radicals towards the substrate for the film growth for a good level of surface passivation.

Furthermore, the surface passivation recovery by post-deposition annealing of a-Si:H/c-Si/a-Si:H in a vacuum and at different pressure conditions of annealing have been investigated. It is noticed that there has been a gradual improvement in the effective minority carrier lifetimes (MCL) and lowering of interface defect density ( $D_{it}$ ) with an increase in the annealing pressure when compared to vacuum annealing. Ambient annealing at atmospheric pressure (760 Torr), the lifetime drastically enhances from 456  $\mu s$  to 1057  $\mu s$  with the lowest  $D_{it}$  of  $8.1 \times 10^9 \text{ eV}^{-1} \text{ cm}^{-2}$  compared to the as-deposited and vacuum annealed conditions of  $1.77 \times 10^{10} \text{ eV}^{-1} \text{ cm}^{-2}$  and  $2.50 \times 10^{10} \text{ eV}^{-1} \text{ cm}^{-2}$ , respectively. This MCL's value variation can be related to the inter-diffusion of atomic hydrogen within the a-Si matrix and reorganization of the strained bonds leading to the structural improvement, which is supported by the spectroscopic ellipsometry as well as Fourier Transfer Infrared Spectroscopy analysis. During the initial growth conditions of the film, as-deposited films seem to be dominated by non-equilibrium local network structure at the interface whereas the annealed films may be equilibrated by decreasing the built-in strain of bulk a-Si:H network and saturating the silicon atom orbitals.

To further improve the crystalline silicon surface passivation by minimizing the interface defect density at the a-Si/c-Si interface, a stack of i-a-Si:H passivation layers deposited at two different temperatures is investigated. The microstructure factor ( $R^*$ ) of the

PECVD-grown intrinsic amorphous silicon (i-a-Si:H) layer plays a crucial role in crystalline silicon (c-Si) surface passivation and charge carrier transport in silicon heterojunction solar cells have been studied. The initial  $i_1$ -a-Si:H layer at  $\sim 150$  °C with a high  $R^*$ , whereas the second  $i_2$ -a-Si:H layer at 230 °C with a low  $R^*$  is deposited on the c-Si as a stack. Ex-situ ellipsometry analysis of i-a-Si:H layers provided information about the thin a-Si:H film's void fraction as a result of changes in the Si-H<sub>2</sub> and Si-H bonding environment, which is crucial for atomic H migration towards the i-a-Si:H/c-Si interface. Later, the low- and high-temperature i-a-Si:H layer stack in combination improved the cell precursor passivation to  $\sim 2.1$  ms with an implied  $V_{oc}$  of  $\sim 714$  mV. The device's power conversion efficiency increased to about 19.06 % by implementing the optimized thickness (2 nm + 8 nm) of the i-a-Si:H stack (with 40 % void fraction in the  $i_1$ -a-Si:H layer).

## सार

बढ़ती ऊर्जा मांग से निपटने का एक व्यवहार्य तरीका फोटोवोल्टिक उपकरणों (जिन्हें सोलर सेल के रूप में भी जाना जाता है) के माध्यम से बिजली का उत्पादन करने के लिए सौर ऊर्जा का कुशलतापूर्वक उपयोग करना है। विनिर्माण प्रक्रियाओं की स्थिरता और विश्वसनीयता के कारण फोटोवोल्टिक उद्योग की मांग को पूरा करने में क्रिस्टलीन सिलिकॉन-आधारित सौर सेल अग्रणी तकनीक हैं। सिलिकॉन हेटरोजंक्शन (SHJ) आधारित सौर सेल प्रौद्योगिकी अपनी अपेक्षाकृत उच्च ऊर्जा रूपांतरण दक्षता के कारण अन्य सिलिकॉन सौर सेल प्रौद्योगिकियों से अलग विकल्पों में से एक है।

यह थीसिस प्लाज्मा एनहांसड केमिकल वेपर डिपोजिशन (PECVD) तकनीक द्वारा विकसित हाइड्रोजनेटेड इंट्रिन्सिक एमोरफॉस (i-a-Si:H) बफर परत की जांच करके SHJ सोलर सेल बिजली रूपांतरण एफिशिएंसी में सुधार करने की रणनीतियों को संबोधित करती है। i-a-Si:H का प्राथमिक उद्देश्य c-Si सतह के डॅगलिङ्ग बॉन्ड्स को निष्क्रिय करना है, जिससे इंटरफ़ेस पर दोष घनत्व कम हो जाता है। परिणामस्वरूप, अब यह व्यापक रूप से स्वीकार कर लिया गया है कि i-a-Si:H निष्क्रिय परतों का अनुकूलन उच्च-प्रदर्शन वाले SHJ सोलर सेल के उत्पादन की कुंजी है। i-a-Si:H परत की सूक्ष्म संरचना सीधे इसकी डिपोजिशन स्थितियों से संबंधित है और माइनोंरिटी कैर्रिएर रीकॉम्बिनेशन को कम करने में c-Si वेफर की निष्क्रियता गुणवत्ता के लिए मुख्य रूप से जिम्मेदार है।

इस प्रेरणा के साथ, हमने सबसे पहले i-a-Si:H के PECVD डिपोजिशन के दौरान i-a-Si:H/c-Si इंटरफ़ेस के निष्क्रिय होने पर प्रीकर्सर गैसों की कुल प्रवाह दर भिन्नता (30-80 sccm) के प्रभाव का SiH<sub>4</sub>/H<sub>2</sub> (समान अनुपात) प्लाज्मा का उपयोग करके पता लगाया है। हालाँकि, अपेक्षाकृत अच्छी गुणवत्ता वाली सरफेस पेसीवेशन प्राप्त करने के लिए मध्यवर्ती गैस प्रवाह दरों की एक खिड़की की पहचान की गई है। एक मध्यवर्ती गैस प्रवाह दर पर, 1 ms से ऊपर अधिकतम प्रभावी माइनोंरिटी कैर्रिएर

लाइफटाइम ( $\tau_{\text{eff}}$ ), 710 mV का एक इम्पलॉइड ओपन-सर्किट वोल्टेज ( $i$ - $V_{\text{oc}}$ ), और  $3.5 \times 10^9 \text{ cm}^{-2} \text{ eV}^{-1}$  का कम इंटरफ़ेस दोष घनत्व ( $D_{\text{it}}$ ) हासिल किया गया है। इसके अलावा, प्रीकर्सर गैसों ( $\text{SiH}_4:\text{H}_2$ ) डिस्चार्ज उत्सर्जन विशेषताओं और a-Si:H फिल्म विशेषताओं (हाइड्रोजन मात्रा, फिल्म घनत्व, ऑप्टिकल बैंड गैप और अपवर्तक सूचकांक) की भी जांच की गई है। प्रवाह दर भिन्नता के साथ फ्रंट-जंक्शन सिलिकॉन हेटरोजंक्शन सोलर सेल (n type टेक्सचर्ड) वाले सिलिकॉन वेफर्स पर निर्मित किये गए हैं, और  $\sim 17\%$  रूपांतरण एफिशिएंसी और 690 mV के करीब ओपन-सर्किट वोल्टेज ( $V_{\text{oc}}$ ), एक अनुकूलित गैस प्रवाह दर पर प्राप्त किया गया है। इस प्रकार, गैस प्रवाह दर की भिन्नता पर इस कार्य ने क्षणिक प्लाज्मा अस्थिरता,  $\text{SiH}_4$  डिप्लीशन, प्लाज्मा में सेकन्डरी रिएक्शन और सरफेस पेसीवेशन के अच्छे स्तर तक फिल्म वृद्धि के लिए सबस्ट्रेट की ओर कट्टरपंथी प्रवाह के सहसंबंध में अंतर्दृष्टि प्रदान की है।

इसके अलावा, निर्वात में और एनीलिंग की विभिन्न दबाव स्थितियों में a-Si:H/c-Si/a-Si:H के डिपोजिशन के बाद एनीलिंग द्वारा सरफेस पेसीवेशन पुनर्प्राप्ति की जांच की गई है। यह देखा गया है कि वैक्यूम एनीलिंग की तुलना में एनीलिंग दबाव में वृद्धि के साथ प्रभावी माइनॉरिटी कैर्रिएर लाइफटाइम (MCL) में धीरे-धीरे सुधार हुआ है और इंटरफ़ेस दोष घनत्व ( $D_{\text{it}}$ ) में कमी हुई है। वायुमंडलीय दबाव (760 torr) पर परिवेशीय एनीलिंग से, एज-डिपोजिटेड  $D_{\text{it}} 1.77 \times 10^{10} \text{ eV}^{-1} \text{ cm}^{-2}$  और वैक्यूम एनीलड  $D_{\text{it}} 2.50 \times 10^{10} \text{ eV}^{-1} \text{ cm}^{-2}$  स्थितियों की तुलना में  $8.1 \times 10^9 \text{ eV}^{-1} \text{ cm}^{-2}$  न्यूनतम  $D_{\text{it}}$  के साथ लाइफटाइम 456  $\mu\text{s}$  से 1057  $\mu\text{s}$  तक बढ़ जाता है। यह MCL का मूल्य भिन्नता a-Si मैट्रिक्स के भीतर परमाणु हाइड्रोजन के अंतर-प्रसार और संरचनात्मक सुधार के लिए तनावपूर्ण बॉडों के पुनर्गठन से संबंधित हो सकती है, जो स्पेक्ट्रोस्कोपिक इलिप्सोमेट्री के साथ-साथ फूरियर ट्रांसफर इन्फ्रारेड स्पेक्ट्रोस्कोपी विश्लेषण द्वारा समर्थित है। फिल्म की प्रारंभिक विकास स्थितियों के दौरान, डिपोजिशन की गई फिल्मों के इंटरफ़ेस पर गैर-संतुलन स्थानीय नेटवर्क संरचना का प्रभुत्व प्रतीत होता है, जबकि एनीलड फिल्मों

को बल्क a-Si:H नेटवर्क के अंतर्निहित तनाव को कम करके संतुलित किया जा सकता है और सिलिकॉन परमाणु ऑर्बिटल्स को संतृप्त करना है।

a-Si/c-Si इंटरफ़ेस पर इंटरफ़ेस दोष घनत्व को कम करके क्रिस्टलीय सिलिकॉन सरफेस पेसीवेशन को और बेहतर बनाने के लिए, दो अलग-अलग तापमानों पर जमा किए गए i-a-Si:H सरफेस पेसीवेशन के ढेर की जांच की गई है। PECVD-विकसित हाइड्रोजनेटेड इंट्रिन्सिक एमोरफ़ॉस (i-a-Si:H) परत का माइक्रोस्ट्रक्चर फैक्टर ( $R^*$ ) क्रिस्टलीय सिलिकॉन (c-Si) सरफेस पेसीवेशन और सिलिकॉन हेट्रोजंगशन सोलर सेल में चार्ज कैरियर ट्रांसपोर्ट में महत्वपूर्ण भूमिका निभाता है। उच्च  $R^*$  के साथ  $\sim 150$  °C पर प्रारंभिक  $i_1$ -a-Si:H परत, जबकि कम  $R^*$  के साथ  $230$  °C पर दूसरी  $i_2$ -a-Si:H परत को स्टैक के रूप में c-Si पर जमा किया गया है। i-a-Si:H परतों के एक्स-सीटू इलिप्सोमेट्री विश्लेषण ने Si-H<sub>2</sub> और Si-H बॉन्डिंग वातावरण में परिवर्तन के परिणामस्वरूप पतली a-Si:H फिल्म के वॉर्ड फ्रैक्शन के बारे में जानकारी प्रदान की, जो i-a-Si:H/c-Si इंटरफ़ेस की ओर परमाणु H प्रवास के लिए महत्वपूर्ण भूमिका निभाती है। बाद में, संयोजन में निम्न और उच्च तापमान i-a-Si:H परत स्टैक ने सेल प्रीकर्सर पेसीवेशन को  $\sim 714$  mV के इम्पलॉइड Voc के साथ  $\sim 2.1$  ms तक सुधार हुआ है। i-a-Si:H स्टैक ( $i_1$ -a-Si:H परत में 40% वॉर्ड फ्रैक्शन के साथ) की अनुकूलित मोटाई (2 nm + 8 nm) को लागू करने से डिवाइस की बिजली रूपांतरण एफिशिएंसी लगभग 19.06% तक बढ़ गई।

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## ABBREVIATIONS

SHJ	Silicon heterojunction
CO <sub>2</sub>	Carbon dioxide
RE	Renewable based electricity
PV	Photovoltaics
Al-BSF	Aluminum Back Surface Field
PERC	Passivated Emitter and Rare Contact
TOPCon	Tunnel oxide passivating contact
SHJ	Silicon heterojunction
Al-BSF	Aluminum diffused back surface field.
HJT	Heterojunction Technology
HIT	Heterojunction with intrinsic thin layer.
PECVD	Plasma Enhanced Chemical Vapour Deposition
BSF	Back surface field
TCO	Transparent conducting oxide
ITO	Tin doped indium oxide
LID	Light induced degradation
SRR	Surface Recombination Rate
SRV	Surface recombination velocity
D <sub>it</sub>	Interface defect states
V <sub>oc</sub>	Open circuit voltage
SRH	Shockley-Read-Hall recombination
VHF	Very high frequency
LT	Low temperature
HT	High temperature
FZ	Float Zone
SE	Spectroscopic Ellipsometry
FTIR	Fourier Transform Infrared Spectroscopy
DI	Deionized
RCA	Radio corporation of America

MFC	Mass flow controller
TMP	Turbomolecular pump
PCD	Photoconductance decay
SSP	Single side polished
VASE	Variable angle spectroscopy ellipsometry
BEMA	Bruggeman effective medium approximation
OES	Optical emission spectroscopy
FF	Fill Factor
$iV_{oc}$	Implied open circuit voltage.
FR	Flow rates
TL	Tauc-Lorentz
DB	Dangling bonds
MPP	Maximum power point
OC	Open-circuit points
pFF	Pseudo fill factor
MCL	Minority carrier lifetime
QSSPC	Quasi-steady state photoconductance
ASD	As deposited
DE	Degraded
LSM	Low frequency stretching mode.
HSM	High frequency stretching mode.
TAT	Trap assisted tunneling.