

Design Constraints of Silicon Heterojunction Photovoltaic Cells: A Study

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Abstract— With the use of proper selective contact, the efficiency of the photovoltaic cell can be increased. Usage of the diffused p-n homojunction photovoltaic cell leads to the degradation of material and increase in the overall fabrication budget. So heterojunction cells with proper metal oxide-selective contact are the best candidates in achieving high efficiency along with reduced cost. These metal oxides with proper band offset replaces the back surface field and the heavily doped emitter and leads to the enhanced cell performance. This paper provides the overview of the design issues of both electron selective oxides and hole selective oxides. In addition to this, a comparison of electrons and hole selective contacts on the basis of effects such as Fermi level pinning and surface passivation has been portrayed.

Index Terms— CuAlO_2 , Fermi level pinning, NiO, Selective contacts, Surface passivation, TiO_2 , ZnO.

1 INTRODUCTION

THERE are two main basic concerns of a photovoltaic cell. One is the increase in the solar cell efficiency and another is the reduction in the manufacturing cost. Crystalline and multi-crystalline solar cells has over-ruled the photovoltaic industry for many years due to their reliability and great efficiency of almost 25% [1]. But in order to achieve the Shockley-Queisser limit for Silicon solar cell which is almost 30% [2] there is a need of proper contact selectivity. Selectivity of contacts allows the transportation of one type of carrier while blocking the other one. This gives rise to the two types of selective contacts: one is for electrons whose function is to block holes and another is for holes whose function is to block electrons. Selective contacts plays a major role by separating the carriers from absorber. Initially in p-n junction solar cell, diffusion is used for carrier selective contact. In this type of structure, n or p absorber is used along with heavily doped n++ and p++ with metal contacts. So, due to carrier concentration asymmetry, the carrier selectivity is obtained. But the drawback of this structure is that it does not provide high barrier to dark current which is highly undesirable. While on the other hand, fabricating a p-n Silicon homojunction cell [3] with dopant diffusion is a costly process and provides a low efficiency of approximately 23% even lower than the achieved limiting efficiency (29.13%) [4]. New researches have shown that the appropriate contact selectivity provided by heterojunctions is better than the homojunctions [5]. Heterojunction solar cells having a concept of smaller band offset for one type of carrier and larger band offset for another type of carrier is highly suitable for good contact selectivity. Heterojunction solar cells comprising of amorphous-Silicon/crystalline-Silicon are also known as HIT (Heterojunction with Intrinsic Thin films) cells.

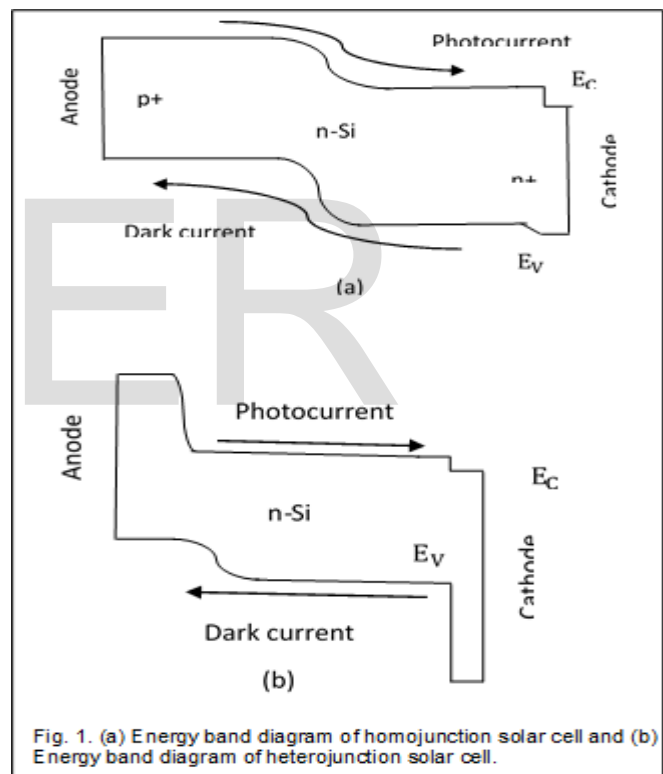


Fig. 1(a) shows the band diagram of the Silicon homojunction photovoltaic cell. This structure uses dissimilarity for the extraction of the carrier but this results in the increase in the dark current. Fig. 1(b) shows the energy band diagram of the Silicon photovoltaic cell having electron blocking layer and hole blocking layer. These cells have shown a great efficiency of more than 25%. Amorphous-Silicon have high valence band offset but low conduction band offset with crystalline-Silicon. The bandgap of Amorphous-Silicon is 1.72eV which absorb photons of light in the visible range of the spectrum which result in the loss of the short circuit current [6]. In a similar way a p-type doped amorphous-silicon also suffers from degradation of light [7]. Hence, band engineered semiconducting oxides having an asymmetric band offsets with silicon are the

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promising candidates for selective contacts in heterojunctions. The use of these oxides replaces the heavily doped emitter layer as well as the back surface field (BSF) thus resulting in the low temperature fabrication process. Transparent conducting films are the thin films that are optically transparent and electrically conductive. The properties of being heavily doped and having a wide bandgap make these oxides highly suitable as transparent conductive oxides (TCO) as well. TiO_2 (Titanium dioxide) and ZnO (Zinc Oxide) have a very low almost near to zero conduction band offset with Silicon which makes them well suited for electron selective oxides. These oxides are n-type semiconductors in which intrinsic as well as extrinsic doping can be done through oxygen vacancy [8]. On the same note, CuAlO_2 (Copper Aluminium Oxide) and NiO (nickel oxide) have very low valence band offset which makes them highly desirable for hole selective oxides. These oxides are p-type semiconductors in which intrinsic as well as extrinsic doping is possible through cation vacancy [8]. The bandgaps of NiO and TiO_2 is greater than 3eV hence these oxides are transparent to the radiance of the solar spectrum. Therefore TiO_2 and NiO are the perfect carrier oxides for electron selective contact and hole selective contact respectively [9]. Various non-ideal effects becomes the major hurdle in designing the heterojunction photovoltaic cells. In case of homojunction cells, the difference in the Fermi levels of the back surface field and highly doped emitter gives the built-in potential. But for heterojunction photovoltaic cells, Fermi level pinning and doping level plays a major role in deciding the barrier of majority and minority carriers. Besides this, surface passivation is also the necessary factor for carrier selectivity otherwise the minority carriers will recombine near contacts giving rise to the dark current.

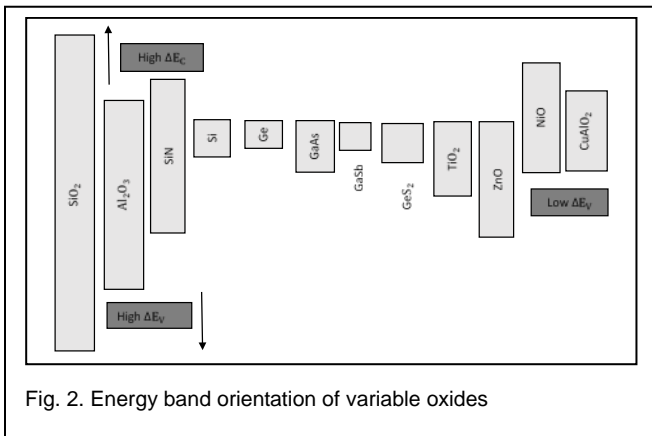


Fig. 2. Energy band orientation of variable oxides

Fig. 2 shows that the ZnO and TiO_2 have low conduction band offset and high valence band offset hence are completely reliable as hole blocking layer. While on the other hand, NiO and CuAlO_2 have low valence band offset and high conduction band offset hence these are well suitable as electron blocking layer.

2 SELECTIVE CONTACTS OF METAL OXIDES

2.1 Electron Selective Oxides

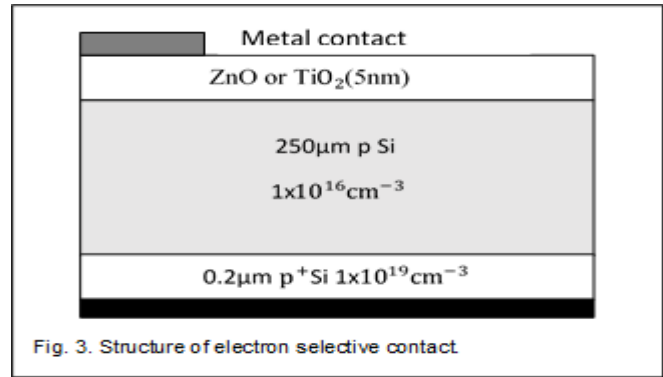


Fig. 3. Structure of electron selective contact

TiO_2 and ZnO have high ΔE_v i.e. valence band offset and low ΔE_c i.e. conduction band offset. Hence these oxides are well suitable for electron selective contacts and are also referred as hole blocking layer.

2.2 Hole Selective Oxides

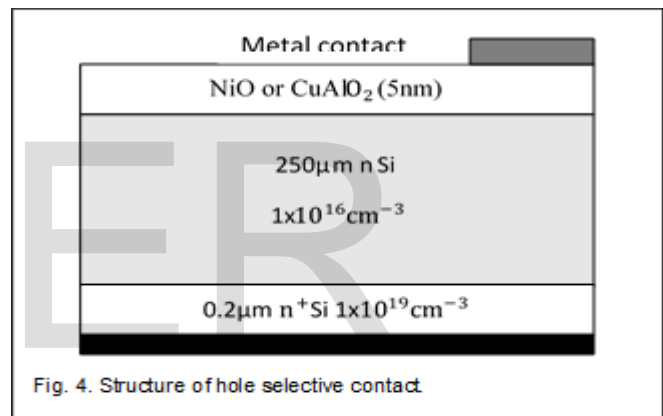


Fig. 4. Structure of hole selective contact

CuAlO_2 and NiO have high ΔE_c i.e. conduction band offset and low ΔE_v i.e. valence band offset. Hence these oxides are well suitable for hole selective contacts and are also referred as electron blocking layer.

3 FERMI LEVEL PINNING

Fermi level pinning is the effect that takes place at the semiconductor-metal interfaces. This creates a barrier of energy for holes as well as for electrons by band bending at the interface. At the metal-semiconductor interface the barrier height for the carriers whether for holes or for electrons from the band bending can be obtained by the workfunction of semiconductor ϕ_s and the workfunction of metals ϕ_m as well as by the semiconductor doping. In metals, the wave function of electrons creates the MIGS (Metal Induced Gap States) thus piercing within the band gap of semiconductor [10]. Due to this at interface a dipole charge is being created. In order to reduce the total dipole charge within the condition of equilibrium, the Fermi level of metal represented by E_{FM} is shifted towards the semiconductor's charge neutrality level i.e. E_{CNL} . This is the point where the characteristics of the MIGS transfers from donor like to acceptor like. As a result of this, at the metal-

semiconductor interface the barrier height becomes less reactive to the work function of the metal. This phenomenon is referred as the Fermi level pinning. Hence, a term called pinning factor [11] is used to obtain the pinning level of E_{FM} towards E_{CNL} . The pinning factor can be estimated by the equation:

$$S = \frac{\partial \phi_B}{\partial \phi_M} = \frac{1}{1 + 0.1(\epsilon_{\infty} - 1)} \quad (1)$$

Where,

ϵ_{∞} is the semiconductor dielectric constant at high frequency

ϕ_B is the barrier height at metal semiconductor junction

by $\phi_{M,eff}$ is the effective workfunction of metal and is given

$$\phi_{M,eff} = S\phi_M + (1 - S)\phi_{CNL} \quad (2)$$

Where, ϕ_{CNL} is referred as the charge neutrality level with vacuum.

4 EFFECT OF FERMI LEVEL PINNING ON OXIDES

4.1 Electron Selective Oxides

The effective metal wavefunction $\phi_{M,eff}$ depends upon the metal in contact with oxide not the oxide alone. Fermi level pinning helps in defining this wavefunction. When an amorphous Silicon is doped an extremely high concentration of dopant is obtained. But the surface near the effective metal wavefunction, the performance of the cell degrades because high barrier for electrons is created. Zinc Oxide (ZnO) shows a much less $\phi_{M,eff}$ of ~4.1eV due to which the performance of the cell is enhanced. The high barrier height leads to the increase in the total series resistance for the cell due to which the fill factor of the device degrades. In case of ZnO, the charge neutrality exists near to the conduction band so the barrier height of ZnO for electrons is much lower than the TiO_2 . Hence, the pinning of ZnO (0.58) is higher than the TiO_2 (0.24) [12] because of this ϕ_M can be varied by varying the height of barrier. The cells with less doping of oxides leads to more degradation. The Schottky barrier thickness has an inverse relationship with the doping. So when the doping is increased, the Schottky barrier thickness is decreased. The increased doping leads charge carriers in oxide to penetrate the effect of Fermi level pinning. This concludes that the effect of Fermi level pinning is minimised by the increase in the doping level of oxides where the built-in potential is determined by the Fermi level. When the doping of the oxides is high, the thickness of the barrier is low.

4.2 Hole Selective Oxides

The valence band offset (VBO) of NiO is negative with Silicon while the valence band offset of $CuAlO_2$ is positive. Negative valence band offset means that the valence band [13] lies below to the Silicon and positive valence band offset means that the valence band offset exists above to that of Silicon. In NiO, having a positive valence band offset build up another barrier for holes. While in case of $CuAlO_2$ an additional barrier is not

being created but this does not even help because E_{CNL} exists at a distance from the valence band which leads to the very high effective metal workfunction $\phi_{M,eff}$ (~4.7eV). This effect degrades the device performance. But in case of NiO, the pinning condition is much better.

5 SURFACE PASSIVATION

Surface passivation creates the band bending at the junction or the interface. Surface passivation is the major factor in realizing the performance of silicon heterojunction solar cells. High doping is necessary to compensate the interface passivation. The term called Interface trap states denoted as D_{it} act as an important factor in determining the effective selective contacts [14]. The inserted dark current can be reduced by high band offset. Hence with the help of high density of interface trap states within the mid side region, the minority carriers get recombined at the interface instead of reflecting back at the barrier of high band offset. However, an ideal solar cell must have high short-circuit current J_{SC} and high open circuit voltage V_{OC} . The open circuit voltage can be improved by improving the efficiency. The direction of flow of recombination current is reverse to the photocurrent which results in the increased dark current. As a result, the open circuit voltage reduces as it rely upon the fraction of photocurrent and dark current. The effect of having a proper band-engineered selective contact can be reduced by the bad interface passivation as this will give another path to the dark current to flow. The Interface trap density i.e. D_{it} transfers from donor like to acceptor like on moving from valence band to conduction band.

6 EFFECT OF SURFACE PASSIVATION ON OXIDES

6.1 Electron Selective Oxides

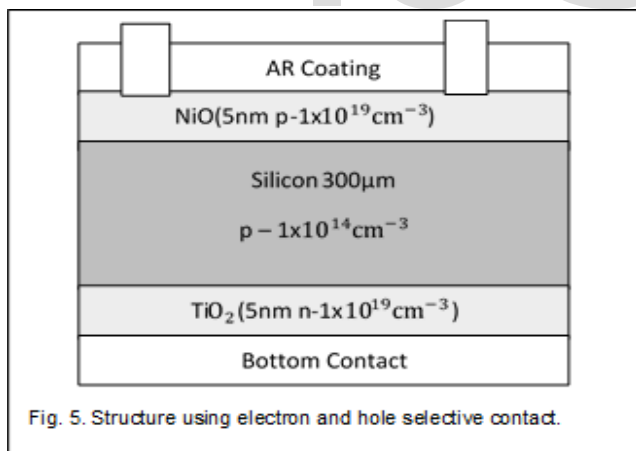
One of the important factor in determining the effects of heterojunction cell is doping. High doping leads to compensate the effects of deficient surface passivation. When no external biasing is applied, the condition of the device is determined by the thermodynamic equilibrium after the junction is formed. This scenario leads to the total band bending of the interface because of dissimilar carrier concentration within the heterojunction photovoltaic cells. The open circuit voltage (V_{OC}) symbolises a point on the surface where band bending occurs in such a way that photocurrent is equal to the induced forward current. At thermodynamic equilibrium, the increased band bending leads to the increased V_{OC} . The difference of conductivity of electrons and holes near the interface coordinates the open circuit voltage V_{OC} . Hence, the conductivity aside to the interface region is determined by the band bending at thermodynamic equilibrium. Therefore, the thermodynamic equilibrium calculates the total device performance. The thermodynamic equilibrium is increased by increased doping of oxide hence in ZnO $\phi_{M,eff}$ becomes less sensitive. But in TiO_2 the thermodynamic equilibrium reduces with the reduction in the effective metal workfunction. This is due to the reason that in TiO_2 there is high dielectric constant (approx. 86) in comparison to ZnO (approx. 7). Hence the increased doping leads to the dependence of band bending over the workfunction of

metal without disturbing the electric field. This concludes that ϕ_M of TiO_2 is more sensitive to open circuit voltage than of ZnO. In case of good surface passivation, the workfunction of metal is needed to be kept low. Hence, the oxide doping as well as the low dielectric constant are necessary. While in case of poor surface passivation, the addition of oxide doping, workfunction of metal and dielectric constant help in compensating the interface passivation.

6.2 Hole Selective Oxides

Copper Aluminium Oxide ($CuAlO_2$) has a negative band offset with silicon as compared to NiO [15]. This is the reason that withdrawal of carriers from silicon is easier in $CuAlO_2$ than NiO. Oxide doping is one of the important parameters in determining the workfunction of metals. Hence, the charge neutrality of $CuAlO_2$ exists at a distance from valence band which makes it difficult to lower the existing barrier between the oxide and the metal. In order to have a selective contact, the band offset is not the only factor responsible because Fermi level pinning and the oxide doping also plays a major role. The alarming point is that the open circuit voltage reduces in $CuAlO_2$ and silicon junction even after the application of high doping. It is always necessary to have a positive band offset so that the doping level and the Fermi level pinning is perfect in deciding the barrier height. Hence, the adequate band engineering is necessary. The addition of dopants within the oxides creates the trap level which help in proper contact selectivity.

7 RESULTS



From the comparison of the different selective contacts, the structure with the proposed oxides is used as shown in figure 5. The p-type Silicon absorber is used along with the interfacial layers of the TiO_2 and NiO. These insulating type materials provides a perfect bandgap line up with silicon that they are able to block one of the carriers (electron or hole) and let go the other one. TiO_2 is referred as the electron blocking layer of n-type whereas the NiO is referred as the hole blocking layer of p-type. NiO and TiO_2 both have bandgap higher than 3eV. Because of this, they are sensitive to the maximum of the

sunlight of the visible range of the spectrum. This structure does not require any p-n junction hence, this helps in reducing the fabrication cost. NiO (Nickel Oxide) is an inorganic material so it does not undergo lifetime degradation of the material. This structure provides the best selectivity contact of the oxides along with the very low manufacturing budget.

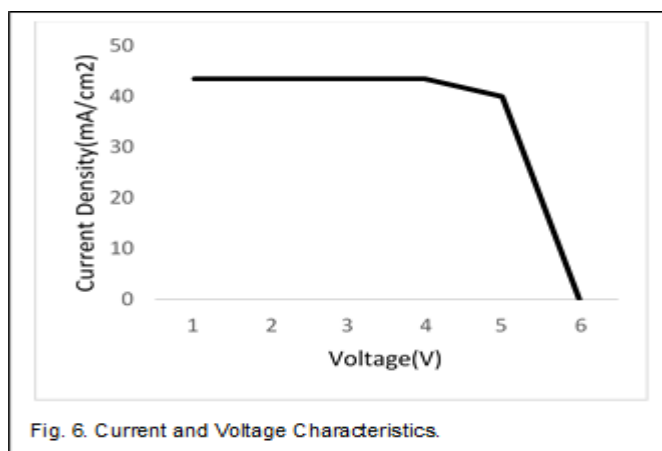
TABLE 1
PARAMETERS OF DIFFERENT OXIDES

Metal Oxide	ZnO	TiO_2	NiO	$CuAlO_2$
Bandgap (eV)	3.4	3.2	3.6	3.0
ϕ_{CNL} (eV)	4.12	4.6	4.85	4.2
Effective Density of States(Conduction band) (cm^{-3})	3.92×10^{18}	7.93×10^{20}	8.87×10^{18}	8.87×10^{18}
Effective Density of States(Valence band) (cm^{-3})	3.34×10^{18}	1.79×10^{19}	7.57×10^{18}	7.57×10^{18}
Pinning factor (S)	0.58	0.24	0.26	0.37

TABLE 2
PARAMETERS OF STRUCTURE WITH ELECTRON AND HOLE CONTACTS

V_{OC} (mV)	772.7
J_{SC} (mA/ cm^2)	43.63
FF(%)	82.99
Efficiency(%)	27.98

Table 2 represents the important and the valuable parameters of the structure given in figure 5. The photons of the light which are having energy above the 1.1 eV can easily be absorbed. The light that enters the structure passes many times the absorber. The open circuit voltage V_{OC} is attained by the proper selective contact and the direct recombination.



The graph in Fig. 6 represents the I-V characteristics of the structure having the use of TiO_2 and NiO as the selective contacts along with the Silicon absorber.

8 CONCLUSION

The paper gives the detailed overview of the various design constraints and the non-idealities related to the selective contacts which are being used in the Silicon heterojunction solar cell. The effects namely surface passivation and the Fermi level pinning plays a major role in determining the solar cells' performance while the high barrier height impose a negative effect on the cell performance. So the proper selection of selective contacts for heterojunction cells replaces the heavily doped emitter and the back surface field of the conventional p-n homojunction photovoltaic cell. In case of Fermi level pinning, the semiconductor charge neutrality must exist near to any of the band edge and must have a very high S i.e. pinning factor. High dielectric constant oxides are greatly influenced by the workfunction of the metal at the oxide-silicon junction as compared to the low dielectric constant oxides. Surface passivation is an important parameter and the role of poor interface passivation can be cancelled by using the high level of doping in the oxides. In ideal case, the band offset is assumed to be zero for majority charge carriers but in case if this is negative, it imposes an adverse effect on open circuit voltage as it will create a comparatively low barrier to the extraction of the charge carriers. So the adequate value of the band offset can be estimated with the help of doping of the oxide and the workfunction of the metal.

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