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TCAD Based Simulation and Performance Optimization of InxGa(1-X)N based Solar Cell

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Indium Gallium Nitride (InGa_N) solar cells might yield high benefits concerning efficiency and reliability, because its bandgap can be tuned through the Indium composition (from 0.7 eV to 3.42 eV) and its energy range covering approximately the total solar spectrum[1].

Keywords: indium gallium nitride (InGa_N), energy band gap (EG), efficiency, fill factor (FF), open-circuit voltage, short-circuit current density, iii-nitride.

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TCADBASEDSIMULATIONANDPERFORMANCEOPTIMIZATIONOFINXGAXNBASEDSOLARCELL

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TCAD Based Simulation and Performance Optimization of $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ based Solar Cell

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Abstract- Solar cells are a promising renewable and carbon-free electric energy resource to address the fossil-fuel shortage and global warming. Various studies on solar cells using III-nitrides semiconductors in the photovoltaic applications have been done. Among them the InGaN alloy is a promising candidate for the photovoltaic applications because it exhibits attractive photovoltaic properties such as high tolerance to radiation, high mobility, and large absorption coefficient allowing thinner layers of material to absorb most of the solar spectrum.

Indium Gallium Nitride (InGaN) solar cells might yield high benefits concerning efficiency and reliability, because its bandgap can be tuned through the Indium composition (from 0.7 eV to 3.42 eV) and its energy range covering approximately the total solar spectrum [1]. In this paper we report the TCAD simulation and performance optimization of $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ based solar cell. Evaluation of the performance of the device has been performed for various values of mole fraction x of In in InGaN. Dark and illuminated I-V characteristics of the device has been simulated and performance parameters of the device have been extracted. The extracted optimized performance parameters of the device are: open circuit voltage (V_{oc}) of 1.08 V, Short circuit current (I_{sc}) is 0.027A, Fill Factor (FF) is 88.58%, Maximum voltage (V_{max}) is 0.99 V, Maximum current (I_{max}) is 0.26A and overall efficiency is 19.36%.

Keywords: indium gallium nitride (InGaN), energy band gap (EG), efficiency, fill factor (FF), open-circuit voltage, short-circuit current density, iii-nitride.

I. INTRODUCTION

Group III-V nitride are now a widely studied class of semiconductor materials. $\text{In}_x\text{Ga}_{(1-x)}\text{N}$, with small x , are very efficient light emitters, even in samples with relatively high densities of structural defects are used as component layers in a wide range of optoelectronic devices. Its high light absorption and its Indium-composition-tuned band gap, the Indium Gallium Nitride (InGaN) ternary alloy is a good candidate for high-efficiency-high-reliability solar cells able to operate in harsh environments.

Moreover, the most important advantage of InGaN alloy might be the direct band gap energy which can be adjusted according to the indium composition.

Thus, the InGaN's energy band gap can be tuned from 0.7 eV to 3.42 eV, covering approximately the total solar spectrum [1]. In this paper, we present simulation of InGaN based p-n homo junction solar cell at different Indium composition. The layers of InGaN solar cell can be deposited using the cost-effective techniques, such as Metal Organic Chemical Vapor Deposition (MOCVD), Metal Organic Vapor Phase Epitaxy (MOVPE), and Molecular Beam Epitaxy (MBE) [2]. Whatever the deposition technique used, higher growth rates (~ 1.0 Angstrom/second) and lower temperature (~ 550 °C) characterize the InGaN growth [3].

II. MODELLING AND SIMULATION

a) Structure

As the numerical simulation is an important way to explore the possibility of a new solar cell structure the InGaN single p-n junction solar cell has been studied using commercial device simulator Atlas from Silvaco Inc [4].

All the simulations were performed under normalized conditions that are 1 sun, a temperature of 300 K, and AM0 illumination. The $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ single p-n junction solar cell structure studied consists of p-type emitter and n-type base as shown in Fig. 1.

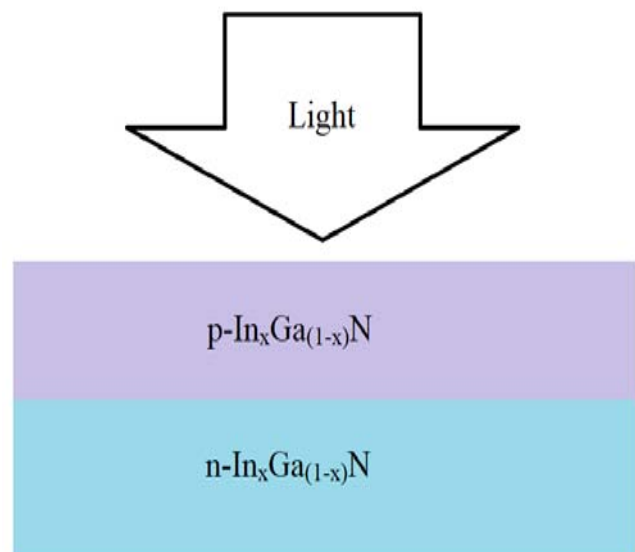


Fig. 1: $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ single p-n junction solar cell structure

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Table 1: Energy Band Gap of $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	Energy band gap (E_g)
GaN	3.42
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	2.6612
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	2.1672
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	1.7375
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	1.4401
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	1.1076
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	0.9063
InN	0.77

b) Physical & Optical Parameters

The energy band gap of $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ is depended on concentration of Indium (x) and energy band gap of $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ is given by following formula

$$E_g(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = x.E_g^{\text{InN}} + (1-x).E_g^{\text{GaN}} - b.x.(1-x) \quad (1)$$

where the band gap energy of InN denoted as E_g^{InN} and band gap energy of GaN denoted as E_g^{GaN} is 0.7eV and 3.42eV, respectively, x is the indium content and b is the bowing parameter ($b = 1.43$) [5-6].

The other modeling parameters of the $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ alloy were calculated using the following equations- Electron Affinity[7-9]: -

$$\chi(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 4.1 + 0.7(3.4 - E_g) \quad (2)$$

Relative permittivity[6]: -

$$\varepsilon(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 15.3x + 8.9(1-x) \quad (3)$$

Table 2: Value of electron affinity and relative permittivity of $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at different value of x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	Electron Affinity(X)	Relative permittivity(E)
GaN	4.092	8.9
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	4.3955	10.18
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	4.5931	11.14
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	4.765	12.1
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	4.884	12.868
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	5.017	13.892
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	5.0975	14.66
InN	5.152	15.3

Effective density of conduction band[8-9]: -

$$N_c(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = (0.9x + 2.3(1-x)).10^{18} \quad (4)$$

Effective density of valence band[8-9]: -

$$N_v(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = (5.3x + 1.8(1-x)).10^{19} \quad (5)$$

Table 3: Value of Effective density of conduction Band and valence band in $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at different value of x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	Effective density of Conduction band (N_c) (1×10^{18})	Effective density of Valence Band (N_v) (1×10^{20})
GaN	0	0
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	1.8	1.06
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	3.15	1.855
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	4.5	2.65
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	5.58	3.286
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	7.02	4.134
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	8.1	4.77
InN	9	5.3

Effective mass of electron[7]

$$m_n(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 0.12x + 0.2(1-x) \quad (6)$$

Effective mass of hole

$$m_h(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 0.17x + 1.0(1-x) \quad (7)$$

$$\eta(\%) = \frac{I_{SC} \cdot V_{OC} \cdot FF}{P_{in}} \quad (9)$$

Table 4: Value of effective masses of electron and hole in $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at different value of x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	Effective Mass of Electron (Mn)	Effective Mass of Hole (Mh)
GaN	0.2	1
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	0.184	0.834
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	0.172	0.7095
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	0.16	0.585
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	0.1504	0.4854
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	0.1376	0.3526
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	0.128	0.253
InN	0.12	0.17

Intrinsic carrier concentration: -

$$n_i^2 = N_C N_V e^{-E_g/K_B T} \quad (8)$$

Where K_B is Boltzmann constant and T is lattice temperature

Efficiency: -

$$U_0(N, T) = U_{\min, i} \left(\frac{T}{300} \right)^{B1} + \frac{(U_{\max, i} - U_{\min, i})(T/300)^{B2}}{1 + (N/N_{\text{ref}}(T/300)^{B3})^{(T/300)^{B4}}} \quad (10)$$

The following equation (11,12) is simplified equation for electron & hole mobility for InGaN alloy.

$$U_n(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = (524 * x) + U_{n(\text{GaN})} \quad (11)$$

$$U_h(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = (6.5 * x) + U_{h(\text{GaN})} \quad (12)$$

$$n(E) = \sqrt{A \left(\frac{E_{ph}}{E_g} \right)^{-2} \left\{ 2 - \sqrt{1 + \frac{E_{ph}}{E_g}} - \sqrt{1 - \frac{E_{ph}}{E_g}} \right\} + B} \quad (13)$$

Where E_{ph} is photon Energy A & B is coefficient dependent on material composition that equation giving by following equation.

$$A(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 13.55x + 9.31(1-x) \quad (14)$$

$$B(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 02.05x + 3.03(1-x) \quad (15)$$

$$\alpha(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 10^5 \sqrt{C(E_{ph} - E_g) + D(E_{ph} - E_g)^2} \quad (16)$$

Where C & D are fitting parameter that is given by following equation (17,18)

Where I_{SC} is short circuit current, V_{OC} is open circuit voltage, P_{in} is incident optical power and FF is fill factor of the solar cell.[10]

Table 5: Value of mobility of electron and hole $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at different value of x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	Mobility of Electron (MUN or Un)	Mobility of Hole (MUP or Uh)
GaN	1000	170
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	1104.8	171.3
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	1183.4	172.275
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	1262	173.25
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	1324.9	174.03
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	1408.7	175.07
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	1471.6	175.85
InN	1524	176.5

Mobility[11]: -

Where the $U_{n(\text{GaN})}$ is 1000 & $U_{h(\text{GaN})}$ is 170.

For the $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys, Adachi's wavelength-dependent refractive index model is given by the following equation [6, 12]:

This real part of refractive index is approximate same 2.32

Its slightly worry for InGaN alloy with different composition of x from 2.30 to 2.34.

The InGaN alloys absorption coefficient α is given by equation (16)[13]

$$C(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 3.525 - 18.29x + 40.22x^2 - 37.52x^3 + 12.77x^4 \dots\dots\dots(17)$$

$$D(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = -0.665 + 3.616x - 2.460x^2 \dots\dots\dots(18)$$

Following equation is simplified expression of absorption coefficient α (19)

$$\alpha(\text{In}_x\text{Ga}_{(1-x)}\text{N}) = 2.2 * 10^5 \sqrt{\frac{1.24}{\lambda} - E_g} \dots\dots\dots(19)$$

Where λ is photon wavelength

For the $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys, wavelength- dependent imaginary part of refractive index is given by the following equation

$$K = \frac{\lambda \alpha}{4\pi} \dots\dots\dots(20)$$

Where π is 3.14.

Following Fig. 2 is graph of wavelength vs imaginary part of refractive index at different value of x

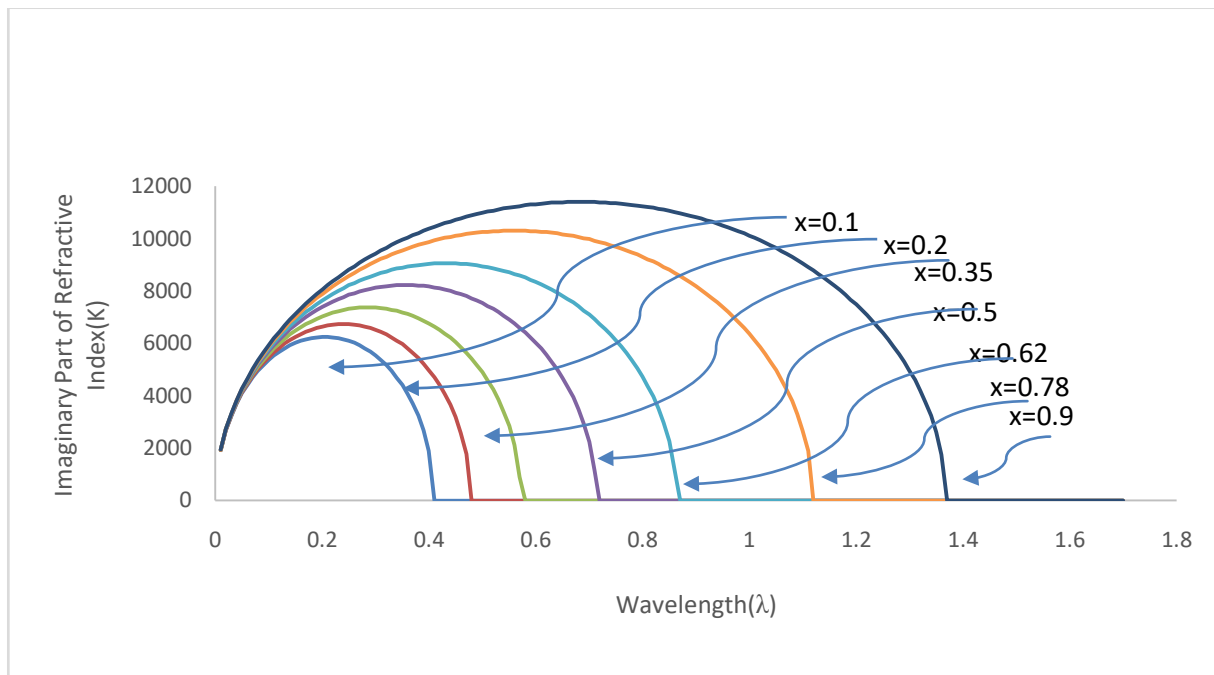


Fig. 2: Graph of wavelength vs imaginary part of refractive index at different value of x

Some initial parameter are given in the following table-6

Table 6: Initial optimized values for simulation

Parameter Used	Value
Thickness of n-InGa _N layer	0.015 micron
Thickness of p-InGa _N layer	0.63 micron
n-type doping [cm^{-3}]	2×10^{18}
p-type doing [cm^{-3}]	1×10^{17}
Velocity of electron & hole ($S_{n,h}$) [cm/s]	10^3
Recombination time of electron & hole ($\tau_{n,h}$) [sec.]	1ns

III. RESULT & DISCUSSION

For the case studied, the initial physical and geometrical parameter values used for $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ single p-n junction solar cell are presented in table 6. After

modeling & simulation get results with the help of above work following results are tabulates

Table 7: Simulation results of short circuit current and open circuit voltage $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at different value of x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	Isc (mA/cm^2)	Voc (V)
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	0.00813315	1.9963
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	0.0158621	1.51555
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	0.0274789	1.08184
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	0.0385468	0.781803
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	0.0539032	0.446001
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	0.0654447	0.242227

This above table 7 presents simulation results of short circuit current & open circuit voltage at different composition of x for single p-n junction solar cell.

Table 8: Simulation results of maximum current and maximum voltage $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at different value of x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	I_m (mA/cm ²)	V_m (V)
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	0.00798644	1.88
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	0.01556	1.41
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	0.0265989	0.99
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	0.0372977	0.69
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	0.0507992	0.369998
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	0.0563837	0.19

This above table 8 presents simulation results of maximum current and maximum voltage at different composition of x for single p-n junction solar cell.

Table 9: Simulation results of fill factor and efficiency $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ at different value of x

Material $\text{In}_x\text{Ga}_{(1-x)}\text{N}$	Fill Factor	Efficiency
$\text{In}_{0.20}\text{Ga}_{0.80}\text{N}$	92.4754	11.0401
$\text{In}_{0.35}\text{Ga}_{0.65}\text{N}$	91.2636	16.1321
$\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$	88.5801	19.3624
$\text{In}_{0.62}\text{Ga}_{0.38}\text{N}$	85.3975	18.9231
$\text{In}_{0.78}\text{Ga}_{0.22}\text{N}$	78.1818	13.8203
$\text{In}_{0.90}\text{Ga}_{0.10}\text{N}$	67.5787	7.87713

This above table 9 shows simulation results of fill factor and efficiency at different composition of x for single p-n junction solar cell.

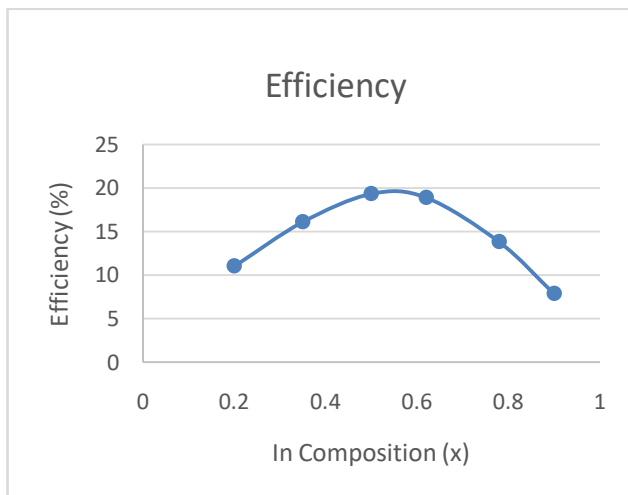


Fig. 3: Graph of In composition (x) efficiency at different value of x

After getting all results we get maximum efficiency is 19.36% at $\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$ single p-n junction solar cell.

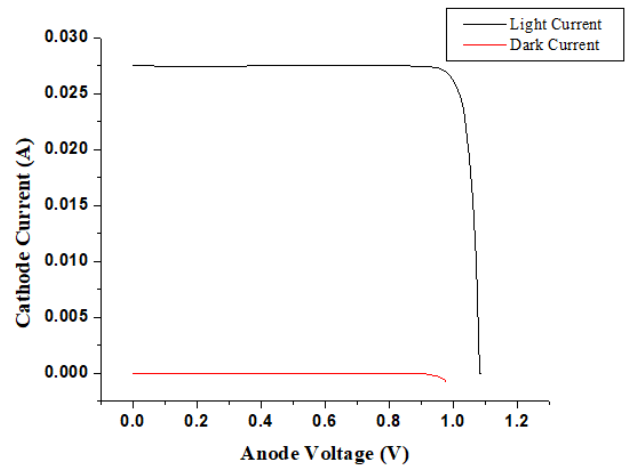


Fig. 4: Dark and Illuminated Characteristics for $\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$ Solar cell

Dark region characteristics and illumination region characteristics have been shown in Fig.4. In this figure the cathode current vs. anode voltage of dark region is shown by red color and of illuminated region is by black color.

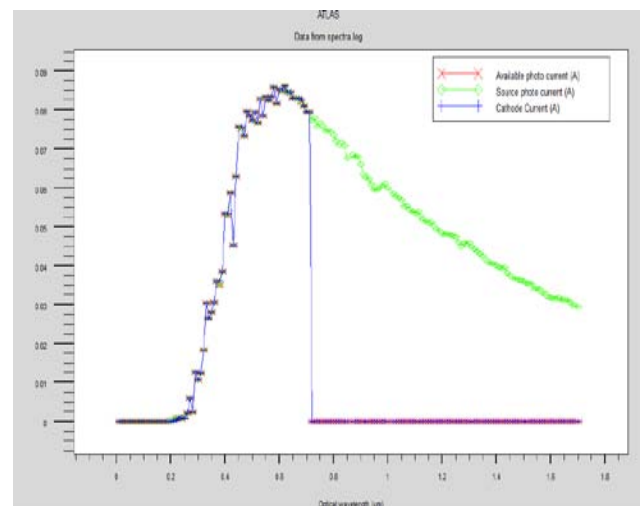


Fig. 5: Spectral Response for $\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$ Solar cell

Spectral response with respect to wavelength has been shown above in Fig.5. Source photo current is maximum possible total current due to incident photons, available photo current is current due to total generated electron-hole pair and cathode current is total current collected at terminals. Among these three, source current is always greater than other two. Total photons incident losses due to reflection, transmission, thermalization etc. Further there is loss of some of the generated electron-hole pairs due to recombination and hence collected cathode current is less than or equal available photo current.

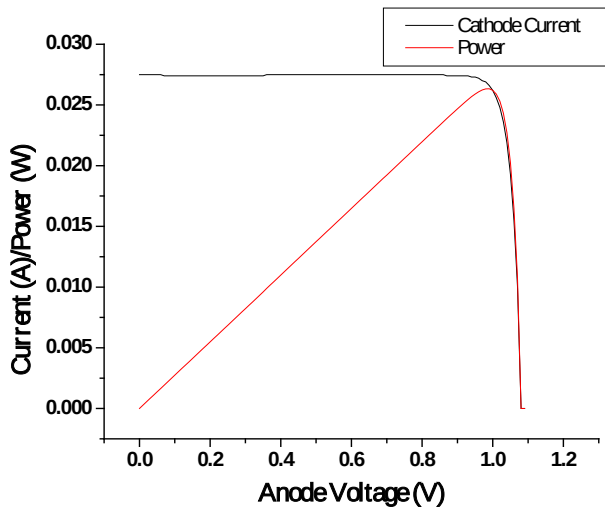


Fig. 6: VI & VP Characteristics for $\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$ Solar cell

VI characteristics and VP characteristics has been shown in Fig. 6. In this figure the IV characteristics is shown by black color and of VP is by red color.

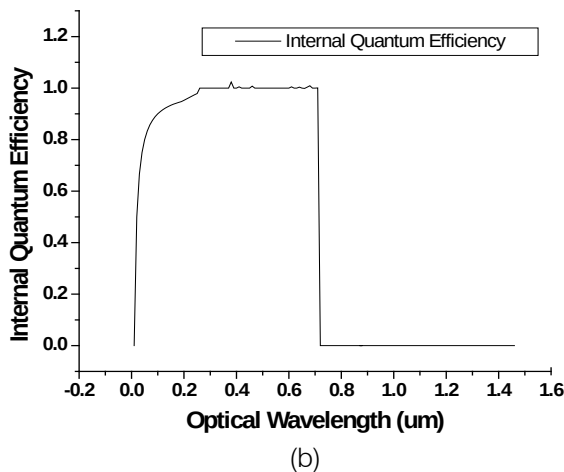
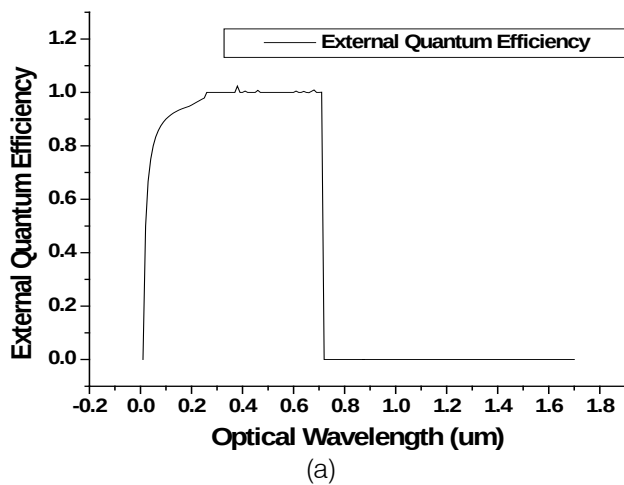


Fig. 7: Quantum efficiency Characteristics for $\text{In}_{0.50}\text{Ga}_{0.50}\text{N}$ Solar cell

Fig. 7(a) is shown for External Quantum Efficiency (EQE) that is defined as ratio of cathode current to source photo current and Fig. 7(b) shows the Internal Quantum Efficiency (IQE) that is defined as ratio of cathode current to available photo current. Theoretically IQE is always greater than EQE hence justify the above graph.

IV. CONCLUSION

In this paper we report the TCAD simulation and performance optimization of $\text{In}_x\text{Ga}_{(1-x)}\text{N}$ based solar cell. Evaluation of the performance of the device has been performed for various values of mole fraction x of In in InGaIn . Extracted performance parameters such as current, voltage, power, fill factor and efficiency from the proposed structure are: open circuit voltage (V_{oc}) of 1.08 V, Short circuit current (I_{sc}) is 0.027 A, Fill Factor (FF) is 88.58%, Maximum voltage (V_{max}) is 0.99 V, Maximum current (I_{max}) is 0.26 A and overall efficiency is 19.36%.

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