Materials Science in Semiconductor Processing 41 (2016) 219–225

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

Numerical simulation of InGaN Schottky solar cell

Sidi Ould Saad Hamady [a,b,*], Abdoulwahab Adaine [a,b], Nicolas Fressengeas [a,b]

[a] Université de Lorraine, Laboratoire Matériaux Optiques, Photonique et Systèmes, EA 4423, Metz F-57070, France
[b] CentraleSupélec, Laboratoire Matériaux Optiques, Photonique et Systèmes, EA 4423, Metz F-57070, France

ARTICLE INFO

Article history:
Received 3 July 2015
Received in revised form
24 August 2015
Accepted 1 September 2015

Keywords:
Simulation
Solar cell
InGaN
Schottky

ABSTRACT

The Indium Gallium Nitride (InGaN) III-Nitride ternary alloy has the potentiality to allow achieving high efficiency solar cells through the tuning of its band gap by changing the Indium composition. It also counts among its advantages a relatively low effective mass, high carriers' mobility, a high absorption coefficient along with good radiation tolerance. However, the main drawback of InGaN is linked to its p-type doping, which is difficult to grow in good quality and on which ohmic contacts are difficult to realize. The Schottky solar cell is a good alternative to avoid the p-type doping of InGaN. In this report, a comprehensive numerical simulation, using mathematically rigorous optimization approach based on state-of-the-art optimization algorithms, is used to find the optimum geometrical and physical parameters that yield the best efficiency of a Schottky solar cell within the achievable device fabrication range. A 18.2% efficiency is predicted for this new InGaN solar cell design.

1. Introduction

The Indium Gallium Nitride (InGaN) III-Nitride ternary alloy can lead to high efficiency solar cells. Indeed its band gap can cover the whole solar spectrum, including the visible region, solely by changing the Indium composition [1–3]. The InGaN alloy also counts among its advantages relatively low effective mass and high mobilities for electrons and holes [4], a high absorption coefficient [5–7] as well as a good radiation tolerance [8], allowing its operation in extreme conditions.

However, the main drawbacks are the poor InGaN crystal quality, the difficulty to grow InGaN with Indium content covering the interesting range for solar application [9], the difficulty of p-type doping mainly due to the high residual donors' concentration and the lack of *ad hoc* acceptors [10], and the difficulty to realize ohmic contacts on p-doped layers [11]. For these reasons the InGaN based solar cell is still in early development stages and the reported photovoltaic efficiency is still very low to be competitive with other well established III–V and silicon technologies [12]. It is then vital to leverage these drawbacks and to develop alternative technologies. One possible paths could be the Schottky technology. This technology is largely used elsewhere in the III-Nitride based power devices and photodetectors [13] but is very new to the InGaN photovoltaic technology. The first experimental work was published in 2009 by Jun-Jun [14]. The prototype developed by this team demonstrates the feasibility of such a concept: an optimization work becomes necessary in order to evaluate precisely and realistically the potentialities of this device. Some work has recently been done in that direction [15], using simplifying assumptions in order to pursue an analytical approach.

That is the reason why we propose, in this report and for the first time using a comprehensive numerical method, a detailed study of the potentialities of the InGaN Schottky technology as a viable alternative to the InGaN p–n junction solar cell. We used mathematical algorithms to study this new solar cell where usual approaches use one-by-one parametric analysis which is inherently inexact and quite tedious. Our mathematical optimization approach is novel in the area of solar cell devices, though relatively common in other applied physics areas such as mechanical engineering.

The following section describes the physical modeling of the InGaN Schottky solar cell structure and discusses its main adjustable parameters. The second section presents the detailed optimized results and a device analysis with respect to the main cell parameters.

2. Schottky solar cell modeling

2.1. Physical modeling

The InGaN Schottky solar cell schematic view is shown in Fig. 1.

The here proposed device could be realized in practice using the conventional growth of InGaN on insulating substrates such as sapphire [16] or Fe compensated GaN. To further ensure practical

* Corresponding author at: Université de Lorraine, Laboratoire Matériaux Optiques, Photonique et Systèmes, EA 4423, Metz F-57070, France.
E-mail addresses: sidi.hamady@univ-lorraine.fr (S. Ould Saad Hamady), abdoulwahab.adaine@univ-lorraine.fr (A. Adaine), nicolas@fressengeas.net (N. Fressengeas).

http://dx.doi.org/10.1016/j.mssp.2015.09.001
1369-8001/

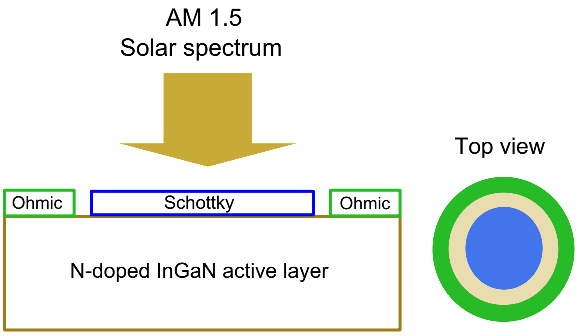

Fig. 1. InGaN solar cell device structure.

realization, we propose a coplanar device metallization.

Modeling this device implies taking into account the interactions of the basic transport equations, including the Poisson and continuity equations on electrons and holes. In this model, the current densities need to be calculated including both the drift and diffusion components.

Two of the main key parameters are the mobilities of electrons and holes. Their values can be deduced from temperature and doping using the Caughey–Thomas expressions [17]:

$$\mu_m = \mu_{1m}\left(\frac{T}{300}\right)^{\alpha_m} + \frac{\mu_{2m}\left(\frac{T}{300}\right)^{\beta_m} - \mu_{1m}\left(\frac{T}{300}\right)^{\alpha_m}}{1 + \left(\frac{N}{N_m^{\mathrm{crit}}\left(\frac{T}{300}\right)^{\gamma_m}}\right)^{\delta_m}}, \tag{1}$$

where m is either n or p, with μ_n being the electrons mobility and μ_p that of holes. T is the absolute temperature. N is the N-dopant (usually Silicon) density. N^{crit} and the n or p subscripted α, β, δ and γ are the model parameters which depend on the Indium composition [18].

In addition to the mobility model, we took into account the bandgap narrowing effect [19], the Shockley–Read–Hall (SRH) [20] and direct and Auger recombination models using the Fermi statistics [21].

Finally, the holes and electrons life time was taken equal to 1 ns [22] in GaN, InN and InGaN.

2.2. Material parameters

All these models include a number of material dependent parameters which can be determined for a given material either from experimental work or *ab initio* calculations. Their values are of course crucial for the numerical calculations to be meaningful, so as to give a good insight into the underlying physics and correctly pave the way to the realization of actual devices. Fortunately, many of the parameters have been intensively studied in the past [18,23,6,5] for GaN and InN binaries. Their values are summarized in Table 1.

As we will treat the x Indium composition in $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ as a free parameter for the optimization that will be undertook in Section 2.3, we will need the material parameters, as in Table 1, for all Indium composition: $\forall\, x \in [0, 1]$.

These values are yielded by the standard *modified Vegard law*. For the electronic affinity and the band-gap, the quadratic bowing factor is conventionally taken to be $b = 1.43$ eV [5]. However, some uncertainty remains concerning the actual value of b, as is discussed in Section 3.2. For all the others parameters, the bowing factor is assumed null.

In short, and provided the bowing factor is only taken in account for the band-gap energy and the electronic affinity, if A^{InN} and A^{GaN} are any one of the parameters in Table 1, the corresponding parameter for $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ will be deduced by

$$A^{\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}} = xA^{\mathrm{InN}} + (1-x)A^{\mathrm{GaN}} - bx(1-x). \tag{2}$$

The electron and holes mobility must be paid here a special attention: the linear interpolation of the parameters included in Eq. (1) implies that the mobility itself is *not* interpolated in a linear way.

Modeling the Schottky solar cell implies also the need for a detailed model of light absorption in the whole solar spectrum and for all x Indium composition. We propose to rely on a phenomenological model proposed previously [25] as

$$\alpha\ (\mathrm{cm}^{-1}) = 10^5\ (\mathrm{cm}^{-1})\sqrt{C(E_{ph}-E_g) + D(E_{ph}-E_g)^2}, \tag{3}$$

where E_{ph} is the incoming photon energy and E_g is the material band gap at a given Indium composition. Once C and D are known for a given Indium composition, the above Eq. (3) yields the absorption coefficient for the whole solar spectrum.

The values for C and D are again taken from the experimental measurement reported in [25] and summarized in Table 2. Their dependency on the Indium composition x is approximated by a polynomial fit, of the 4th degree for the former, and quadratic for the latter:

$$C = 3.525 - 18.29x + 40.22x^2 - 37.52x^3 + 12.77x^4$$
$$D = -0.6651 + 3.616x - 2.460x^2$$

For the refraction index we used the Adachi model [26], defined for a given photon energy as

Table 1
InN and GaN physical model parameters. Table 1(a) shows the band-gap E_g, the electron affinity χ, the effective density of states N_v and N_c in the valence and the conduction band respectively and the dielectric permittivity ε. Table 1(b) and (c) summarizes the parameters used to model the electron and hole mobilities in Eq. (1).

(a) Experimental data from Refs. [5,6,18,23]

	E_g (eV)	χ (eV)	N_c (cm^{-3})	N_v (cm^{-3})	ε
GaN	3.42	4.1			8.9
InN	0.7	5.6			15.3

(b) Experimental data from Refs. [6,24] except for α_n, β_n and γ_n which have been estimated to 1 in the absence of any experimental data

	μ_n^1 (cm^2/V s)	μ_n^2 (cm^2/V s)	δ_n	N_n^{crit} (cm^{-3})
GaN	295	1460	0.71	
InN	1030	14150	0.6959	

(c) Experimental data from Ref. [25] except for α_p, β_p and γ_p which have been estimated to be 1 in the absence of any experimental data

	μ_p^1 (cm^2/V s)	μ_p^2 (cm^2/V s)	δ_p	N_p^{crit} (cm^{-3})
GaN	3	170	2	1×10^{18}
InN	3	340	2	8×10^{17}

Table 2
Values for C and D in Eq. (3) as found by Brown et al. in [25].

Indium composition	C (eV^{-1})	D (eV^{-2})
1	0.69642	0.46055
0.83	0.66796	0.68886
0.69	0.58108	0.66902
0.57	0.60946	0.62182
0.5	0.51672	0.46836
0	3.52517	−0.65710