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Development of Novel Thin Film Solar Cells: Design and Numerical Optimization

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ABSTRACT: *The development of cost effective solar cells requires on the one hand to master the elaboration techniques and, on the other hand, an adequate design to optimize the photovoltaic efficiency. These two research topics are closely linked and their association in the research work is the key in the development of novel thin film solar cells. The design associated with numerical optimization gives the set of optimal physical and geometrical parameters, taking into account the technological feasibility. This will allow elaboration to target the most efficient structures in order to speed up the final device realization. In this work, we used a new approach, based on rigorous multivariate mathematical global Bayesian algorithm, to optimize a Schottky Based Solar Cell (SBSC) using InGaN as the absorber. The obtained photovoltaic efficiency is close to the conventional structures efficiency while being less complex to elaborate. In addition, the results have shown that the optimized SBSC structure exhibits high fabrication tolerances.*

Keywords: Solar Cell, Photovoltaics, InGaN, Schottky, Simulation, Numerical Optimization.

1. INTRODUCTION

The optimization of thin film solar cells involve many physical and technological parameters such as the active layers' composition, doping, thickness, optical parameters, density of defects... The development of numerical optimization methods using all these parameters are crucial in the design and, *in fine*, the fabrication of cost effective solar cells. One main prerequisite for these methods is to take into account the solar cell parameters' interdependence. For instance, the optimal composition depends on the doping and the absorber thickness, while the optimal thickness depends on the optical parameters such as the absorption coefficient and the refractive index. To optimize the solar cell efficiency with respect to all these parameters, the so-called parametric analysis is usually used: only one parameter is varying at a time while the other parameters are kept constant.^{1,2} This standard procedure has two main drawbacks. It does not take into account the parameters' interdependence highlighted previously and, secondly, it does not give the absolute optimal efficiency. The new methodology based on a global Bayesian algorithm addressing these drawbacks is presented in the next section.

2. METHODOLOGY

As an alternative to parametric analysis, we developed a new methodology using nonlinear optimization algorithms to calculate the set of parameters maximizing the efficiency.³ This methodology permits to simultaneously optimize a large set of parameters taking automatically into account their interdependence while drastically reduce the computing time when compared to the parametric analysis. The developed code, SLALOM (SoLAR ceLL multivariate OptiMizer), implements this methodology and the including steps. Firstly, one define a set of crucial parameters to the solar cell operation (e.g. composition, doping concentration, layers thickness...). Then a semiconductor devices simulator is used to perform the numerical evaluation of the solar cell efficiency from its parameters using a mathematical algorithm designed to find the set of values that maximizes the efficiency using a numerical iterative procedure. The new implemented optimization method uses a global Bayesian algorithm.⁴ This global algorithm ensures that the found optimum is absolute and takes less computation time than the previously used methods.

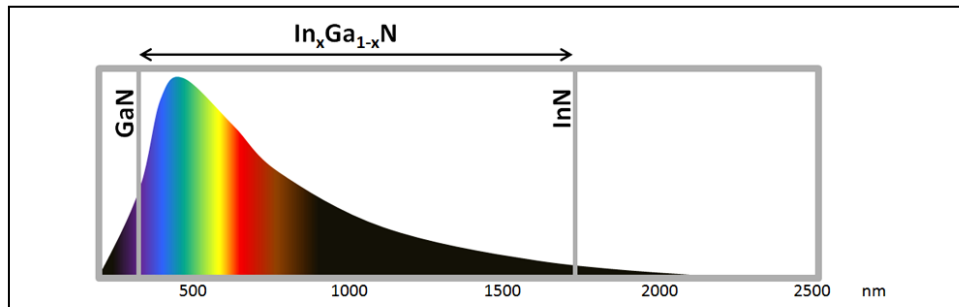


Figure 1: A schematic AM0 solar spectrum showing the matching with the InGaN bandgap with indium composition x varying from 0 (GaN) to 1 (InN).

The global Bayesian algorithm implemented in SLALOM is used in this work to optimize a Schottky Based Solar Cell (SBSC) using Indium Gallium Nitride (InGaN) as the absorber. InGaN has the potential to achieve high photovoltaic efficiency since its bandgap can cover the whole solar spectrum, as illustrated in figure 1, by changing the indium composition.⁵ In addition, this ternary alloy can potentially permit to fabricate cost effective and robust solar cells operating at high temperature and high light intensity, e.g. in concentrator solar cells. The main drawbacks of using this material are the difficulty to grow thin film with high indium composition, the difficulty of p-type doping and the realization of ohmic contacts.^{5,6} Using the SBSC technology is proposed to address the p-doping challenge. The InGaN SBSC structure is shown in figure 2. The main parameters used in the simulations, taken or extrapolated from experimental data, are summarized in table 1. The parameters to be optimized for this structure are the

Schottky contact workfunction, the indium composition in InGaN, the doping concentration and the layer thickness.

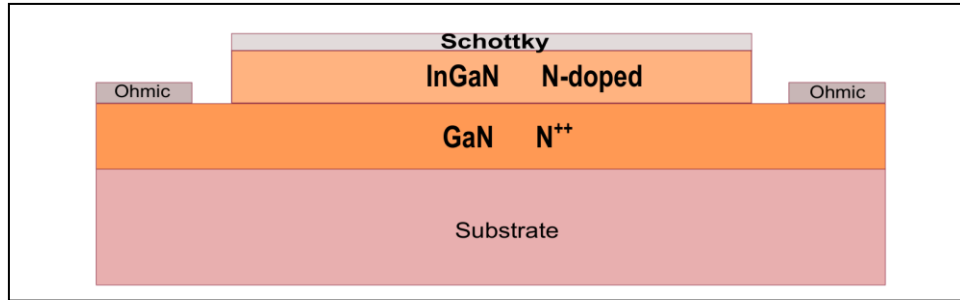


Figure 2: InGaN Schottky based solar cell structure. The InGaN layer is grown on a GaN template substrate on Sapphire. The role of the GaN is twofold. It is used as a substrate for the epitaxy growth of the InGaN absorber and to realize the back ohmic contact. It is heavily doped to reduce the ohmic contact resistance. The InGaN doping is $6.5 \times 10^{16} \text{ cm}^{-3}$ with a thickness of $0.86 \mu\text{m}$. The GaN layer doping is about 10^{19} cm^{-3} and its thickness is about $4 \mu\text{m}$.

| Parameters | InN | GaN |
|---|--|----------------------|
| Bandgap (eV) | 0.7 | 3.42 |
| Affinity (eV) | 5.6 | 4.1 |
| Carrier lifetime (ns) | 1 | 1 |
| Permittivity | 15.3 | 8.9 |
| Density of states in conduction band $N_c \text{ (cm}^{-3}\text{)}$ | 9.1×10^{17} | 2.3×10^{18} |
| Density of states in valence band $N_v \text{ (cm}^{-3}\text{)}$ | 5.3×10^{19} | 4.6×10^{17} |
| Absorption | Extracted from experimental data. ⁷ | |
| Mobility | Caughey-Thomas Model. ⁸ | |
| Refractive Index | Adachi Model. ⁹ | |

Table 1: The InGaN parameters used in the numerical simulations. Bandgap, affinity, density of states in valence and conduction bands, permittivity, absorption, SRH, Auger and direct recombination data are taken from literature or extrapolated from GaN and InN experimental data.

3. RESULTS AND DISCUSSION

Figure 3 displays the photovoltaic performances (efficiency, short-circuit current and open-circuit voltage) obtained using the global Bayesian optimization method. The total computation time, with high precision, is about 2 hours while it takes about 500 hours for the standard parametric analysis, and with lesser precision. The optimized parameters are shown in table 2. The InGaN SBSC exhibits an optimal efficiency of approximately 22 %, very close to the record efficiency obtained for the well-established thin film solar cells.¹⁰ This obtained result is

based on simulations using parameters extracted from experimental data, associated to a rigorous optimization global Bayesian algorithm. Therefore, we ensure that the obtained efficiency is optimal and not overestimated. This optimal efficiency is obtained for the following set of values: a layer thickness of $0.86 \mu\text{m}$, a doping of $6.5 \times 10^{16} \text{ cm}^{-3}$, a metal workfunction of 6.30 eV and an indium composition of 56% . The indium composition that is necessary for the optimal Schottky solar cell is still challenging. If we decrease the composition down to 30% , the efficiency decreases to around 10% . The simplicity of the SBSC structure, with only one n-doped layer, makes it very cost effective and robust when compared to the standard PN, PIN or multijunction structures.

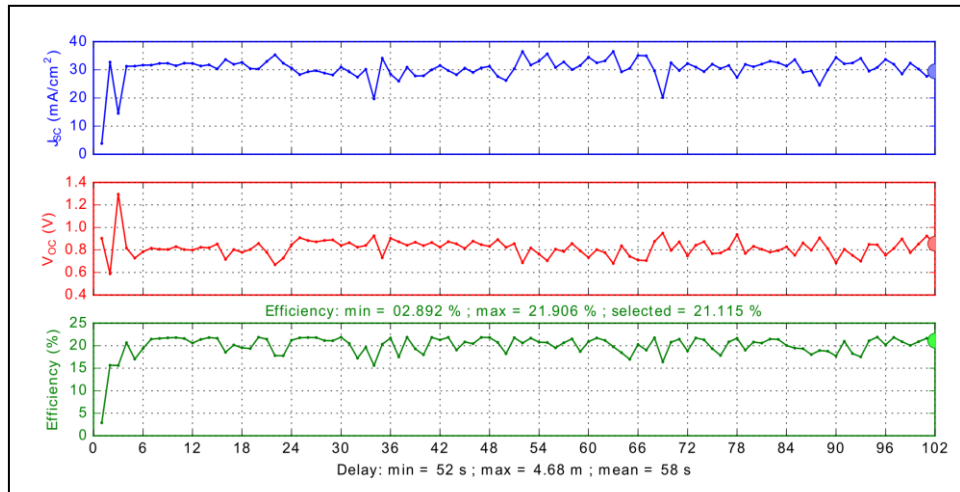


Figure 3: Evolution of the InGaN SBSC photovoltaic performances during the global Bayesian optimization process. The time (x-axis) is expressed in minutes. V_{OC} is the open-circuit voltage and J_{SC} the short-circuit current. The Bayesian algorithm iterates until the desired precision is obtained. In this case, the necessary time for convergence is about 102 minutes.

One aspect, crucial for the development of this technology, is the fabrication tolerance. The tolerance that is allowed on each parameter is the range in which this parameter can vary without decreasing the efficiency by more than 10% of its maximum.¹¹ This latter value is relative. For instance, if the optimized efficiency is 22% , then in the considered parameter's tolerance range the efficiency remains between 19.8% and 22% . Table 2 displays for each optimized parameter the corresponding tolerance range, showing that the proposed InGaN SBSC structure exhibits high fabrication tolerances. For instance, the layer thickness can vary between $0.53 \mu\text{m}$ and $1 \mu\text{m}$ with an efficiency between 19.8% and its optimal value of 22% . One of the main advantages of decreasing the layer thickness is the

possibility to grow epitaxial high quality layer using less material. In addition, the large tolerance in the doping can permit to use the residual InGaN n-doping without need to intentionally dope the layer.

| | InGaN Thickness (μm) | InGaN Doping (cm^{-3}) | Schottky Metal Workfunction (eV) | Indium Composition |
|-----------------|--------------------------------------|--------------------------------------|-------------------------------------|-----------------------|
| Range | [0.10 ; 1.00] | [10^{16} ; 10^{19}] | [5.50 ; 6.30] | [0.00 ; 1.00] |
| Optimum | 0.86 | 6.5×10^{16} | 6.30 | 0.56 |
| Tolerance range | [0.53 ; 1.00] | [10^{16} ; 3×10^{17}] | [6.15 ; 6.30] | [0.50 ; 0.72] |

Table 2: The optimized InGaN SBSC parameters and the corresponding fabrication tolerance range. The parameters to be optimized for this SBSC structure are the Schottky contact workfunction, the InGaN composition, doping concentration and layer thickness. The optimized efficiency is 22 %. In the considered fabrication tolerance range the efficiency remains between 19.8 % and 22 %.

These results pave the way to the actual fabrication of the optimized InGaN SBSC solar cell with two main planned steps. The first step involves the optimization of the InGaN MOCVD epitaxial growth for high indium composition.¹² The short-term objective is to grow an optimized InGaN layer with 20 % of indium and, in mid-term, to increase this composition up to 30 %. The second step is the fabrication of the semi-transparent Schottky contact using platinum. The final objective is to obtain the first InGaN SBSC with more than 20 % of indium.

4. CONCLUSION

In this paper, a new numerical optimization method is used to design a Schottky based solar cell using InGaN as the absorber. The global Bayesian algorithm used in this method takes into account the interdependence of the solar cell parameters and ensures the absoluteness of the optimized efficiency. The obtained results, based on using empirical parameters, precise physical models and rigorous optimization methodology, demonstrates the potential of this technology for cost effective and robust solar cells. The next step, based on this design and numerical optimization work, is the actual fabrication of the solar cell with the growth of the InGaN absorber and the realization of the semi-transparent Schottky contact in order to fabricate the first Schottky based solar cell using InGaN with more than 20 % of indium.

5. ACKNOWLEDGEMENTS

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