Numerical Analysis of GaInP Solar Cells:
Toward Advanced Photovoltaic Devices Modeling

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Abstract

Simulation capacities of GaInP solar cells were studied with a special emphasis on material and structural parameters. The comparison between experimental and numerical results allowed to validate the models used for such a device and permitted to extrapolate the layers structure. With this method we proved the role of the substrate in the simulation and thus its importance in the optimization process. This study is an important previous step to validate the numerical approach for multi-junction solar cell simulation in 3D.

I. Introduction

In the last decade, a great activity is being carried out worldwide to achieve commercial PV based on concentrator III-V solar cells modules for terrestrial applications. Despite current concentrator products are based on silicon cells, III-V multi-junction solar cells have a tremendous potential for increasing efficiency and also to operate at higher concentration levels than silicon. Both aspects, high efficiency and high concentration, are determinant in order to achieve low cost [7]. Multi-junction solar cells including GaInP, (In) GaAs and Ge are known as super-high efficiency and are now in the main stream for terrestrial use under concentration. The high cost of these materials require concentration about 1000 suns to reduce the energy cost and a two or three junctions design for a better use of the solar spectra [1]. Efficiencies about 30% at 1000 suns [8] and 39% at 236 suns [5] have been reached and efficiencies about greater than 40% are hoped for the next years. This activity, which is in the search of a real breakthrough, is requiring very accurate models for concentrator solar cells that conduct to the highest efficiency of PV modules [2]. In order to increase the performance of such concentrator solar cells, a modeling as accurate as possible is necessary to guide the technological approaches. In this paper we will focus on the GaInP solar cell. By using a numerical analysis, we could calculate the external quantum efficiency and the performance of the device taking into account many material and structure parameters. We can analyze the behavior of the device over a wide range of wavelengths and by fitting the calculated data and the experimental ones we can extract the exact layers structure further confirmed by SEM measurements. This process will be very useful to validate the simulation input parameters, to explain the behavior of a device and then to optimize the layers structure according to the requirements of this top cell into the multi-junction solar cells.

II. The Simulation Tools

Traditionally, the simulated electronic devices were of micrometric scale while solar cells had always been too big to be modeled. In our case we are simulating concentrator solar cells, this means we reduce the cell area using an optic focusing the light on a smaller surface (see Figure 1) [6]. The typical concentration we use is about 1000 suns, which is the same as saying that the optic has an area a thousand times greater than the cell, so our active area is reduced to 1 mm². Solar cell size is a key aspect in concentration applications that is not usually taken into account. In fact, there are not in literature specific values for the solar cell size following optimization criteria. Therefore, we determined the optimum size for a GaAs solar cell operating at 1000 suns [7]. It is about 1 mm² and it appears as a trade-off between the influence of series resistance and perimeter recombination. More-
over, a III-V concentrator solar cell has a very simple structure which consists of a superposition of layers; this means that we have, excepting of the metallization grid, a one dimension device. And the metallization grid has a two axis symmetry, this allow us to simulate only half of the cell in 2D (or a quarter of the cell in 3D). For this reasons it is easier to model concentrator solar cell than standard solar cell with a traditional device simulator.

The Silvaco Software Package is a simulation software targeting the area of electronic design. This is a large suite of highly sophisticated tools that aid in the design and development of all types of semiconductor devices. The phenomena modeled start from simple electrical properties and extend to optical properties, thermal heating, interface recombination effects etc. A big variety of detailed layer growth processes and material parameters (mobilities, recombination parameters, ionization coefficients, optical parameters, etc) add accuracy to the simulation [2] and give a great versatility to the software.

III. The Solar Cell Model

Silvaco ATLAS is a physically-based device simulator which predicts the electrical characteristics that are associated with specified physical design and bias conditions. By applying a set of differential equations, based on Maxwell's laws, we can simulate the transport of carriers through a device [3]. Physically-based simulation is very different from analytical modeling which provides efficient approximation and interpolation [4] but does not provide insight, or predictive capabilities, or encapsulation of the theoretical knowledge.

To calculate a solar cell structure, ATLAS solves Poisson’s equation, carrier continuity equation, the drift-diffusion transport model and the energy balance transport model.

The previous step in order to provide accurate simulation is the insertion of specific parameters in the material related models. Indeed, depending on the growth conditions, material properties can reach a wide range of values. So we characterized intensively our materials to supply an accurate input to the simulation tool. The indispensable material related models we introduced are doping dependent mobility, doping dependent bandgap narrowing, doping and temperature dependent recombination rates. It is also important to note that a solar cell has to work over a wide range of wavelengths, and for each wavelength and doping concentration, materials have different sets of (n, k) which implies that the simulation has to allow a complete customization of the photogeneration rate, depending on the optical properties of the grown layers. The photogeneration is given by,

$$G = \eta_0 \frac{P h c}{\lambda} \alpha e^{-\alpha y}$$

with G being the photogeneration rate, P the cumulative effects of reflections, transmissions, and loss due to absorption over the ray path, $\eta_0$ the relative distance for the given ray, $h$ the Planck’s constant, $\lambda$ the wavelength, $c$ the speed of light and $\ell$ the absorption coefficient calculated for each set of (n, k) value.

By creating a doping, wavelength and material dependent (n,k) model, we can numerically reproduce the behavior of the solar cell all over the wavelength range of the solar spectra.

IV. The Virtual Cell

Ga$_{0.51}$In$_{0.49}$P (lattice matched to GaAs) solar cells were grown on GaAs substrates. A typical method is to simulate and optimize the cell without taking into account the substrate (so only considered as a mechanic support.). This substrate implies several changes in the infrared behavior of the device because of the smaller bandgap of GaAs. In fact, this is that we could call an “anti-BSF” effect. Consequently, if we want to correctly model the top cell we have to consider this phenomena, if not, we risk to make a erroneous adjustment and extrapolate wrong material parameters because we characterized a GaInP cell on a GaAs substrate to compare it with a simulated GaInP cell without GaAs substrate, which doesn't count with the EQE reduction implied by the substrate in the infrared. For this we chose to virtually 'grow' the structure shown in Figure1 to compare the measurements with the numerical study.
Moreover, in a double or triple junction solar cell the GaInP cell is supposed to be over a tunnel diode made of a smaller bandgap material such as GaAs or AlGaAs[5]. So, the optimization process of the top cell has to consider the presence of a smaller bandgap material layer under the PN junction and its effects on the band diagram (Figure 3).

V. Results

We modeled the characteristics of the top cell using the structural and material parameters of the grown device. Then we started an iterative routine to adjust the simulated EQE to the real one, the results are shown in Figure 4. The correlation between measured and simulated results is fairly good and we clearly see the substrate lowers the EQE for wavelengths between 500 nm and 600 nm because of the electric field created by the presence of the substrate (Figure 3). The only mismatch between the two curves appears for wavelengths greater than 620 nm, further experimental data revealed the formation of an undesired quaternary alloy (InAsGaP) coupled with an optical bandgap narrowing effect explaining this difference, however we think we could model this phenomena soon.

To adjust measurements and simulations we needed to modify some structural parameters such as layers thickness in the device property file. After such adjustments the results agreed but we still needed to legitimate the simulation with the substrate. So we further made some SEM, SIM and XPS measurements to know the exact characteristics of the grown device. From SIM analysis we confirmed the doping profile of the layers and the SEM gave new information about the layer thicknesses. We put in evidence the numerically predicted thicknesses agreed very well with the SEM measured values, better than the theoretically grown ones (Table 1).

Modeling with the substrate allowed to well determine the real structure of the device and by fitting many experimental curves we confirmed the validity of the GaAs, GaInP and AlInP parameters and equations used in the simulation software and we proved that it is necessary to model the device with the GaAs substrate in order to well analyze the structure of a device.

This numerical analysis is revealed to be very powerful to extrapolate some device parameters from experimental results. In fact, once the material parameters are well defined it is possible to determine the layers thicknesses as well as to detect the eventual formation of an undesired material during the growth process. Thus the GaInP top cell is aimed to be over a GaAs tunnel diode in a triple junction solar cell device, modeling with the substrate seems to be right way to optimize such a structure taking into account the change in the band diagram due to the GaAs layer.

Although we are still simulating in 2D, it is necessary to detect the pending issues in the modeling of concentrator solar cells when considering the situations appearing in their real operation. In our opinion, the most influencing ones are: different illumination spectra due to the optic, Inhomogeneous illumination distribution on the solar cell because of the focusing of the light, temperature gradients and the light impinging the cell within a cone [2]. These conditions requires a 3D simulation and, viewing the last achievements in 2D simulation of GaAs...
and GaInP solar cells, we are ready to begin 3D modeling of GaAs, GaInP and double junction solar cells under real operation conditions.

VI Conclusion

The GaInP solar cells was modeled and compared with measurements. The substrate effect on the band diagram was shown to be relevant in the results of the simulation. Taking into account this effect we generate the EQE, by adjusting the layers parameters we achieved to match the experimental and simulated results. SEM measurements were done to determine layers thicknesses and it revealed that the software predicted thicknesses were closer to the real ones than the foreseen thicknesses. By fitting many curves we validate the materials and physicals models used. We put in evidence that using the substrate in the numerical process was important in order to achieve a reliable analysis of the structure. Viewing the substrate effect we also saw it has to be include in the optimization process to consider the effect will have the tunnel diode on the band diagram of the GaInP cell. We demonstrate a modeling tool can be of great interest to deduce structural parameters of a grown device once we have completely defined the materials parameters and models.

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<th>Foreseen thickness</th>
<th>Measured thickness</th>
<th>Simulation deduced thickness</th>
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<td>Total window/emitter/base thickness in nm</td>
<td>1178</td>
<td>1231</td>
<td>1232</td>
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Table 1 Comparative of the foreseen, measured and simulation deduced thickness.

References
