Numerical simulation of Ge solar cells using D-AMPS-1D code

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ARTICLE INFO

Keywords:
Solar cells
Germanium
Numerical simulation

ABSTRACT

A solar cell is a solid state device that converts the energy of sunlight directly into electricity by the photovoltaic effect. When light with photon energies greater than the band gap is absorbed by a semiconductor material, free electrons and free holes are generated by optical excitation in the material. The main characteristic of a photovoltaic device is the presence of internal electric field able to separate the free electrons and holes so they can pass out of the material to the external circuit before they recombine. Numerical simulation of photovoltaic devices plays a crucial role in their design, performance prediction, and comprehension of the fundamental phenomena ruling their operation. The electrical transport and the optical behavior of the solar cells discussed in this work were studied with the simulation code D-AMPS-1D. This software is an updated version of the one-dimensional (1D) simulation program Analysis of Microelectronic and Photonic Devices (AMPS) that was initially developed at The Pennsylvania State University, USA, during the years 1988–1993 [2].

In AMPS the technique of finite differences and the Newton–Raphson iteration method are used to solve the Poisson and the continuity equations that are subject to appropriate boundary conditions [3]. The three unknowns were chosen as the quasi-Fermi levels $E_{FN}$ and $E_{FP}$ and the electron potential $\Psi$. The letter D stands for new developments that were introduced in recent years by the second author of this paper. For example, in order to properly model the recombination of electron–hole pairs in direct gap materials and in heavily doped crystalline semiconductors the mechanisms of band-to-band (direct) and Auger recombination were added to the already existing Shockley–Read–Hall formalism.

Structures such as homojunctions, heterojunctions, multijunctions, etc., resulting from stacking layers of different materials can be studied by appropriately selecting characteristic parameters. In this work, examples of cells simulation made with D-AMPS-1D are shown. Particularly, results of Ge photovoltaic devices are presented. The role of the InGaP buffer on the device was studied. Moreover, a comparison of the simulated electrical parameters with experimental results was performed.

1. Introduction

The electrical transport and the optical behavior of the solar cells discussed in this work were studied with the simulation code D-AMPS-1D [1]. This software is an updated version of the one-dimensional simulation program AMPS (Analysis of Microelectronic and Photonic Devices) that was initially developed at The Pennsylvania State University, USA, during the years 1988–1993 [2].

In AMPS the technique of finite differences and the Newton–Raphson iteration method are used to solve the Poisson and the continuity equations that are subject to appropriate boundary conditions [3]. The three unknowns were chosen as the quasi-Fermi levels $E_{FN}$ and $E_{FP}$ and the electron potential $\Psi$. The letter D stands for new developments that were introduced in recent years by the second author of this paper. For example, in order to properly model the recombination of electron–hole pairs in direct gap materials and in heavily doped crystalline semiconductors the mechanisms of band-to-band (direct) and Auger recombination were added to the already existing Shockley–Read–Hall formalism.

Structures such as homojunctions, heterojunctions, multijunctions, etc., resulting from stacking layers of different materials can be studied by appropriately selecting characteristic parameters such as the gap energy, carrier mobilities, absorption coefficients, and doping concentrations among others.

The code evaluates the external device characteristic curves such as the current density–voltage ($J$–$V$) under dark and under illumination, the quantum efficiency, the reflectivity, and internal quantities such as the electric field, the free and trapped carrier concentrations, the electron and hole currents, the recombination and generation rates, etc.

This work was the result of collaboration between the Solar Energy Department of the National Atomic Energy Commission (CNEA, Argentina) and the Solar Energy Institute of the Technical University of Madrid (UPM, Spain).

Nowadays, Ge solar cells have become important because they can be used both in homojunction and multijunction devices. An example of the first scenario is the case of devices for TPV (Thermophotovoltaics) applications [4] and an example of the second are the triple junction InGaP–GaAs–Ge cells for space or terrestrial applications [5].
2. Details of the simulated solar cell

The solar cell is composed by a single n-p junction formed by the diffusion of phosphorus to the p-type Ge substrate during the metalorganic vapor phase epitaxy (MOVPE) growth of an InGaP buffer layer. Ge wafers, 180 µm thick, (100) 6° off toward (111) have been used as substrates. The buffer layer is n-type doped with Si. A GaAs cap layer has been grown to ease the front ohmic contact. The back contact is carried out with Au, while the front contact was performed by deposition of the AuGe-Ni-Au system outside of a circular pattern made by photolithographic techniques. No antireflection coating (ARC) has been deposited. The area of the solar cells is a circle of about 1.53 mm of diameter. The main parameters used in the simulations are summarized in Table 1. The coefficient for radiative direct recombination was set to $1 \times 10^{-10}$ cm$^3$ s$^{-1}$ for InGaP [6]. The dependence of the mobility with respect to the doping level was taken into account in each device layer following the model used by Ghannam et al. [7].

The $J_S$ of InGaP was determined experimentally and it was found to be in agreement with the values reported in the literature for partially ordered InGaP [8,9]. Band offsets between InGaP and Ge were taken as type 1. In all cases the illumination source was the standard AM1.5G, spectrum taken from ASTM standards [10], since this was the spectrum available for the experimental measurements. A non-passivated surface was considered ($S_r=1 \times 10^6$ cm/s), as well as some band bending at the front surface.

3. Results

The Ge devices were electrically characterized in CNEA. The $I-V$ curve was measured with a commercial solar simulator with 1 kW Xe lamp, a customized optical filter for a better matching of the AM1.5G spectrum, and a data acquisition system. Irradiance was set with a c-Si reference cell previously calibrated. Then $I-V$ curves were corrected according to the short circuit current measured under the Sun, where global irradiance was monitored using a thermopile type radiometer. Finally, electrical parameters were extracted from the corrected $I-V$ curves.

The experimental and the simulated results are presented in Table 2. $J_S$ is the short current density, $V_{oc}$ is the open circuit voltage, $FF$ is the fill factor and $\eta$ is the conversion efficiency.

Table 3
Light $J-V$ parameters calculated for the Ge solar cell with ARC (AM1.5G).

<table>
<thead>
<tr>
<th>Material</th>
<th>Buffer</th>
<th>Emitter</th>
<th>Base</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_g$ (eV)</td>
<td>InGaP</td>
<td>Ge</td>
<td>Ge</td>
</tr>
<tr>
<td>Thickness (nm)</td>
<td>580</td>
<td>180</td>
<td>180,000</td>
</tr>
<tr>
<td>$N_i$ (cm$^{-3}$)</td>
<td>$3 \times 10^{18}$</td>
<td>$8.5 \times 10^{18}$</td>
<td>-</td>
</tr>
<tr>
<td>$N_e$ (cm$^{-3}$)</td>
<td>-</td>
<td>-</td>
<td>$1.5 \times 10^{17}$</td>
</tr>
<tr>
<td>Electron mobility (cm$^2$/Vs)</td>
<td>803</td>
<td>1000</td>
<td>2000</td>
</tr>
<tr>
<td>Hole mobility (cm$^2$/Vs)</td>
<td>40</td>
<td>200</td>
<td>700</td>
</tr>
<tr>
<td>Radiative recombination coefficient (cm$^3$/s)</td>
<td>$1 \times 10^{-15}$</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

The results show small differences in the electrical parameters when a Gaussian or an abrupt change in the concentration of the emitter doping is considered.

The predictive values of electrical parameters for the case of a cell with ARC on the front of the device are shown in Table 3. The anti-reflective coating consists of a bilayer MgF$_2$-ZnS. The results are consistent with those found in the literature [4].

Fig. 1 shows the external quantum efficiency (EQE) measured at the UPM and the simulated curve. It is important to note that when a high density of defects in the buffer (about $1 \times 10^{17}$ cm$^{-3}$) is considered, a better fitting for the EQE curve at low wavelengths is achieved. In this particular case, the short circuit current became $J_S=25.03$ mA/cm$^2$ that better approximates the experimental value. This could mean that there is a high density of defects in the material or at the InGaP-Ge interface, reaching the junction fewer electron–hole pairs generated in the InGaP.

Fig. 1. Simulated and experimental external quantum efficiency and reflectivity of the Ge cell.

Fig. 2. Reflectivity of the front of the Ge cell for different thickness of the InGaP layer.
On the other hand, the peaks of the simulated and experimental EQE were fitted varying the thickness of the InGaP. A better fit is achieved for a thickness of 840 nm InGaP but does not fully explain the positions of all peaks. For this reason it could be assumed that there are differences in the structure considered for the device respect to the real one.

To study the influence of the buffer layer on the optical properties of the cell, the reflectivity of the cell for different thicknesses of InGaP was calculated (Fig. 2). The worst case corresponds to not having the InGaP layer, because the device is more reflective. In his case the current decreases to 20.11 mA/cm².

Furthermore a study on the influence of the InGaP layer, thickness and doping, on the electrical parameters of the device was performed. The Fig. 3 shows the $J_{sc}$ vs. the InGaP thickness. There is a thickness for which the current is maximum, which is about 40 nm. Several factors might explain this: one is that as the thickness of InGaP increases, this material absorbs more and fewer photons reach the n-p junction of Ge, with the consequent fall in the $J_{sc}$. While the InGaP layer plays in some extent the role of anti-reflective coating, it is important to mention that also has a passivating role due to its high band gap with respect to Ge. A similar situation was studied for the case of a GaAs cell with InGaP window [11].

$J_{sc}$ and $V_{oc}$ vs. the buffer layer doping was calculated. It is not observed a pronounced change in the $V_{oc}$ but from the point of view of the $J_{sc}$ values seems to be convenient to keep the doping at low levels.

Fig. 4 shows the generation (G) and recombination rates (R) for the different device layers.

The region of the substrate where $R = G$, about 67 µm from the surface, is a dead zone in terms of collection of photocarriers that does not contribute to the current $J_{sc}$, i.e., it just plays the role of mechanical support.

4. Conclusions

Single junction n-p Ge solar cells for terrestrial concentrator applications were studied by numerical simulations. The results were compared with experimental curves of actual devices. The simulation results for the electrical parameters were consistent with the experimental data, indicating that the D-AMPS-1D code is a suitable tool for the analysis of these devices. However, some differences were found in the case of the external quantum efficiency, suggesting that the device structure considered for the simulation is not exactly the real one.

The predicted short circuit current shows a weak dependence with respect to the doping present at the InGaP layer and a more intense dependence on this thickness, which turns out to be optimum around 40 nm.

Depending on the application of an ARC and the final use of the cell, the thickness and doping level of the InGaP buffer layer should be lower than those actually used in the devices analyzed.

References