Optimal bandgap of GaInAsN for integration in a space four-junction photovoltaic cell

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***Abstract*—We use Poisson-Drift-Diffusion simulations to optimize a dilute nitride subcell architecture for an integration in a monolithic lattice-matched 4-junction multijunction solar cell under 1-sun AM0 spectrum. We explore a way to systematically explore how a variation of the subcell bandgap changes the power conversion efficiency of the whole multijunction cell. We first compare our Poisson-Drift-Diffusion results to approximate analytical solutions. Then, we compute the dilute nitride material bandgap-dependent absorption coefficients used as input values for the device simulation. We finally derive the evolution of the multijunction cell power conversion efficiency with regards to the dilute nitride subcell bandgap.**

***Index Terms*—dilute nitride, photovoltaic, multijunction**

I. Introduction and Objectives

GaInAsN alloys are particularly interesting for spatial lattice-matched multi-junction solar cells (MJSCs) [1]. Owing to the alloy nature of this compound, one can select independently the bandgap of $GaIn_xAsN_y$, predicted by the band-anticrossing (BAC) framework [2], and its lattice constant, predicted by the ratio x/y. It allows to increase the number of junctions from 3 to 4 ($GaInP_2$ - GaAs - GaInAsN - Ge) while choosing the added subcell bandgap to perfectly match Shockley-Quiesser's efficiency optimum and keeping the structure lattice-matched to GaAs. The ideal bandgap of GaInAsN subcells in a 4-junction architecture next to $GaInP_2$, GaAs and Ge has been predicted to be 1eV, reaching $\approx$ 40% power conversion efficiency (PCE) [3]. However, no four-junction solar cell made from these materials has yet reached the desired efficiency levels, due to low diffusion lengths in the dilute nitride layers. This can be circumvented by using a double-heterostructure solar (sub)cell (DHSC) architecture, but it has proven difficult to predict its optimal design, as it results in a trade-off between photogeneration and field-assisted carrier collection. As a consequence, the multi-junction cell performance and its optimal design are dependent on the dilute nitride material parameters [4], [5]. In a recent paper, we used a Poisson-Drift-Diffusion (PDD) framework on top of Transfer-Matrix-Method optics and BAC theory to compute the 4-junction cell performance under 1-sun AM0. We showed that the 1eV absorption coefficient of [6] was insufficient to provide the necessary short-circuit-current for MJSC integration (≈ 18 mA/cm^2) for realistic GaInAsN layer thicknesses and SRH lifetime [5].

In the present paper, we explore how the multi-junction cell performance depends on the bandgap of the GaInAsN layer E_g. We hypothesize that decreasing E_g would alleviate the constraints on the GaInAsN layer thickness needed for equal output short-circuit current. In turn, this could help move the optimal subcell design window towards lower minority carrier lifetimes, which are hopefully experimentally attainable. Calculating how the MJSC PCE evolves thus requires to derive the change in the GaInAsN absorption coefficient and its impact on the device main factors of merit (V_{OC}, J_{sc}, P_{MPP}). As the PDD scheme can prove too computationally expensive to allow a quick exploration of the whole parameter space, we first assess the analytical model of [4]. Indeed, such an analytical model can be extremely useful to provide first estimations before performing PDD simulations or to fit experimental data. At each GaInAsN bandgap, BAC theory provides the input absorption coefficient used by the simulation tool to compute the cell PCE. We use those results to further optimize the MJSC design under the AM0 spectrum.

II. Methods and preliminary results

The analytical model of [4] gives precious insights on the effect of the field on the photocollection of minority carriers in the i-GaInAsN layer. Using the same parameters for minority carriers and the same absorption coefficient than in our PDD simulation, and integrating the analytically derived QE, we compare our PDD simulations with the model. To do so, we use parametric curves of varying short-circuit currents with varying SRH lifetime, residual doping, and i-layer thickness. For example, we simulated the short-circuit currents of a n-p-p 1eV GaInAsN (with the absorption coefficient from Kurtz et al. [6]) with varying i-layer SRH lifetime, and compared it with the analytical QE integrated between 875 and 1270 nm (figure 1).

Reiterating the same work as in Fig. 1 at various residual dopings shows that, as in Wolf's original article [7], variations in the magnitude of the electric field in the QE model can

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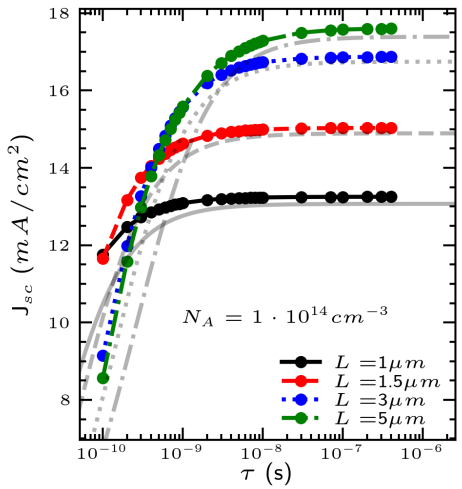

Fig. 1. Comparison of short-circuit currents obtained from PDD simulations for a n-p ($1e14$ cm^{-3})-p subcell (dotted, colored lines) with the short-circuit currents obtained from the analytical quantum efficiency model and a homogeneous electric field of $E = 0.75V/L$ (grey lines).

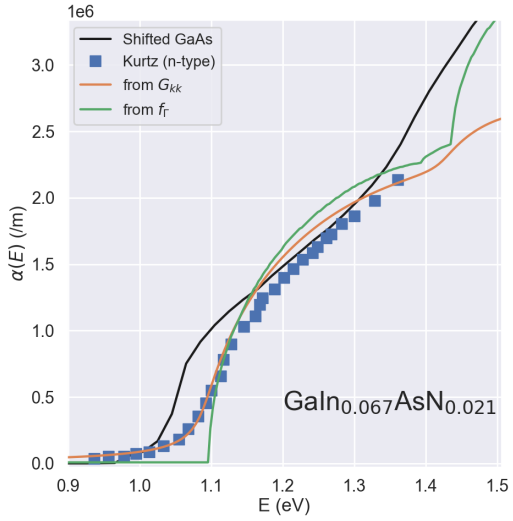

Fig. 2. Comparison of our calculations with experimental n-type 1eV GaInAsN of [6] as well as 0.315 eV red-shifted GaAs absorption coefficient.

explain the photocollection gain as the residual doping in the intrinsic layer decreases.

We propose computing the bandgap-dependent absorption coefficient α of near-1 eV GaInAsN from a minimal set of parameters. This method is as follows:
- Compute a realistic bandstructure for the dilute nitride material,
- Calculate the joint density of states (JDOS) between each of the valence subbands and each of the conduction bands,
- Recombine all of the interband contributions to compute the final $\alpha(E)$.

Here, we try to take two different routes, either following a calculation of the fractional Γ character of the BAC model using the approach of Seifikar et al. [8], or directly constructing a Green's function with for a single N level and calculating the absorption coefficient from it, following the approach of Wu et al. [2]. The first step for computing the absorption coefficient is to construct a realistic description of the conduction and valence bands. In Seifikar's model [8], this is done by constructing and diagonalizing a 5-level $\mathbf{k} \cdot \mathbf{p}$-like hamiltonian, and the topmost valence band is replaced with the Light-Hole (LH) and Heavy-Hole (HH) bands. In Wu's approach [2], the hamiltonian is constructed from a simple 2-level BAC approach and augmented with the LH, HH and Split-Off (SO) valence bands. The JDOS is then computed numerically, either defining a Green's function $G_{kk}(E)$ with broadening $i\Delta_N$ (Wu's approach), or using an expression of the fractional gamma character $f_\Gamma(E)$ (Seifikar's approach). The absorption coefficient is then calculated from the sum of the JDOS of all transitions between valence band i and conduction band j multiplied by their transition strength $a_{i\to j}$. We compare our predictions with the experimental values taken from the litterature for near-1eV GaInAsN. For example, in Fig. 2, the absorption coefficient of n-type GaInAsN from Kurtz et al. [6] seem to be well-fitted with a bandgap slightly above 1eV (1.087 eV). Although both methods give similar results, the broadening $i\Delta_N$ in Wu's approach allows to better match near-bandgap absorption smoothness than Seifikar's approach.

Finally, we use all the ingredients of our study together to compute the efficiency maps of $GaInP_2$ - GaAs - GaInAsN - Ge photovoltaic cells, using the optical absorption coefficients provided by the models. This demonstrates that the absorption coefficient also has an important impact on the optimal design of the multi-junction cell, and that achieving short-circuit currents of up to 18 mA/cm^2 is difficult. Our preliminary results indicate that the best efficiencies computed so far are approximatively 37-40 %, in accordance with [3]. However, for a given cell performance, equivalent or even superior designs can be found by decreasing both the bandgap and the thickness of the GaInAsN layer simultaneously.

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