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Automated design of multi junction solar cells by genetic approach: Reaching the >50% efficiency target

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ABSTRACT

The proper design of the multi-junction solar cell (MJSC) requires the optimisation search through the vast parameter space, with parameters for the proper operation quite often being constrained, like the current matching throughout the cell. Due to high complexity number of MJSC device parameters might be huge, which makes it a demanding task for the most of the optimising strategies based on gradient algorithm. One way to overcome those difficulties is to employ the global optimisation algorithms based on the stochastic search. We present the procedure for the design of MJSC based on the heuristic method, the *genetic algorithm*, taking into account physical parameters of the solar cell as well as various relevant radiative and non-radiative losses. In the presented model, the number of optimising parameters is $5M + 1$ for a series constrained M-junctions solar cell. Diffusion dark current, radiative and Auger recombinations are taken into account with actual ASTM G173-03 Global tilted solar spectra, while the absorption properties of individual SCs were calculated using the multi band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. We predicted the efficiencies in case of $M = 4$ to be 50.8% and 55.2% when all losses are taken into account and with only radiative recombination, respectively.

1. Introduction

Among the third generation solar cell concepts, the multijunction solar cells (MJSC) are the only devices with the proven efficiency [1], which exceed the Shockley-Queisser limit [2], in the laboratory and small commercial set-ups. This is achieved due to much better spectrum matching than in the other SC concepts [1,3]. However, this concept still lacks the detailed theoretical descriptions and understanding of major factors influencing the operation and efficiency of such devices. The majority of MJSC models so far were based on principles of the detailed balance and thermodynamics [4–7], with recent attempts to address the real SC's material parameters [8]

The main conceptual message of the MJSC and a route to overcome the poor spectral matching of a single-junction SC is to introduce subcells with different energy gaps (E_g) into the device [9]. Such devices consisting of several solar cells (SC), i.e subcells, each of which with different E_g are capable of absorbing the photons from different part of the solar spectrum. Generally, this design is achieved by growing semiconductors with different E_g on top of each other. The upper subcells are grown with a higher E_g and absorb photons with higher energies. Each subcell is also transparent for the photons with energies lower than its E_g. Such a concept provides for the absorption of the higher energy photons in the upper subcells and prevents them from being absorbed in the subsequent subcells to reduce the thermal losses [10,11]. Increasing the number of subcells to the extreme, when the Sun spectrum is divided so that each subcell is illuminated almost with monochromatic light, conceptually will allow the extreme efficiencies [12–14]. The MJSCs with increased number of junctions, when compered to the single junction SC, have additional significant benefit of lowering the current density, and reduction of I^2R series resistance loss. This lowering of currents generated in subcells is due to spectra splitting between subcells.

In order to achieve the highest possible values of solar cell efficiencies, the design parameters have to be optimally selected and tuned. To find the optimal combination of these parameters, we used the drift-diffusion model, with all parameters of III-V semiconductors, like the effective masses, conduction band and valence band density of states, etc., calculated and scaled as a function of the energy gap. This way we have formed a generic material parameter set, which together with the detailed model of radiative and non-radiative (Auger) losses, provides reliable basis for the description of the underlying parameters of MJSC and its subcells. In our analysis we have optimised the *pn* junctions of an MJSC only. We assume the sufficiently good anti-reflective coating with neglected reflection. In order to find the optimal efficiency in such multi-dimensional phase space with conflicting requirements and constrained parameters, we employed the global

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optimisation strategies using the genetic algorithm as a *driver* to run the drift diffusion model as a *solver*.

The main advantages of the genetic algorithm (GA) over other, more conventional optimisation techniques based on gradient methods, is the robustness, stability, and ability to avoid being trapped (quenched) in a local maxima during the search for the global one. The GA does not make any presumptions about the objective function, and can be used safely when the objective function is discontinuous, stochastic, highly nonlinear or has undefined derivatives. Furthermore, the GA is applicable when the parameter space is constrained by highly complex and conflicting requirements or is *N*-dimensional. The GA is very quick in locating the area, in a multidimensional parameter space, around the optimal solution, however unlike gradient based methods, it takes them more time to reach the exact solution within the located area.

The MJSC design parameters which were optimised by the GA are: thicknesses, impurity concentrations, energy gaps and optimal current through the device under the current matching condition. In order to address effect of radiative and non-radiative losses on the MJSC efficiencies, the optimisation was conducted for three characteristic cases. First, with the radiative recombination only taken into account [15,16]. Next, with the radiative recombination and diffusion current [17]. And finally, with the Auger recombination together with the other two losses [18]. MJSCs were optimised as series constrained, which means optimal currents of individual cells in MJSC are equal. All predictions were carried out with the actual ASTM G173-03 Global tilted solar spectrum [19] while the absorption spectra for each subcell were calculated using the kppw parallel code [20]. Our results reveal the influence of each type of losses to the overall efficiency. The model based on the genetic algorithm predicts the efficiency of 55.2% and above in the case 4-junction SC in the radiative limit. This efficiency drops to 50.77% when all losses are taken into account in the case of series constrained MJSC.

2. Methodology

2.1. Theory

In the general form, the electron-hole pair generation in m^{th} solar cell of an MJSC can be written as:

$$\begin{aligned} g^{(m)}(\lambda, z) \;=\; & \Phi(\lambda)[1 - R(\lambda)](\textstyle\prod_{k=1}^{m-1}[1 - R_{\mathrm{k}}(\lambda)]) \\ & \times (\textstyle\prod_{k=1}^{m-1} e^{-\alpha_{\mathrm{k}}(\lambda)(z_{\mathrm{k}+1}-z_{\mathrm{k}})}) \\ & \times \alpha_{\mathrm{m}}(\lambda) e^{-\alpha_{\mathrm{m}}(\lambda)(z-z_{\mathrm{m}})} \end{aligned} \tag{1}$$

where $\Phi(\lambda)$ is the solar photon flux, $R(\lambda)$ is the reflection coefficient on surface of the MJSC, $R_{\mathrm{k}}(\lambda)$ is the reflection between two, k^{th} and $k+1^{\text{st}}$, subcell in MJSC, $\alpha_{\mathrm{k}}(\lambda)$ is the absorption of k^{th} subcell. In our procedure, we assumed $R(\lambda) = 0$ and all $R_{\mathrm{k}}(\lambda) = 0$, therefore the generations in the first, second,..., and m^{th} subcell, can be rewritten as:

$$g^{(1)}(\lambda, z) = \Phi(\lambda)\alpha_1(\lambda)e^{-\alpha_1(\lambda)(z-z_1)} \tag{2}$$

$$\begin{aligned} g^{(2)}(\lambda, z) \;=\; & \Phi(\lambda)e^{-\alpha_1(\lambda)(z_2-z_1)} \\ & \times \alpha_2(\lambda)e^{-\alpha_2(\lambda)(z-z_2)} \end{aligned} \tag{3}$$

$$\begin{aligned} g^{(m)}(\lambda, z) \;=\; & \Phi(\lambda)\left(\prod_{k=1}^{m-1} e^{-\alpha_k(\lambda)(z_{k+1}-z_k)}\right) \\ & \times \alpha_m(\lambda)e^{-\alpha_m(\lambda)(z-z_m)}. \end{aligned} \tag{4}$$

However, if the m^{th} subcell is not thick enough, not all the photons are going to be absorbed and some of the higher energy photons will pass to the $m+1^{\text{st}}$ subcell, Fig. 1. In such a situation, in addition to transmitted photons, the subsequent subcell absorbs photons with energies that are higher than its band gap and lower than upper subcell's E_g, and properly attenuated for the thickness of the preceding regions in the MJSC stack too, see Fig. 1. The absorptions coefficients $\alpha(\lambda)$ are calculated using

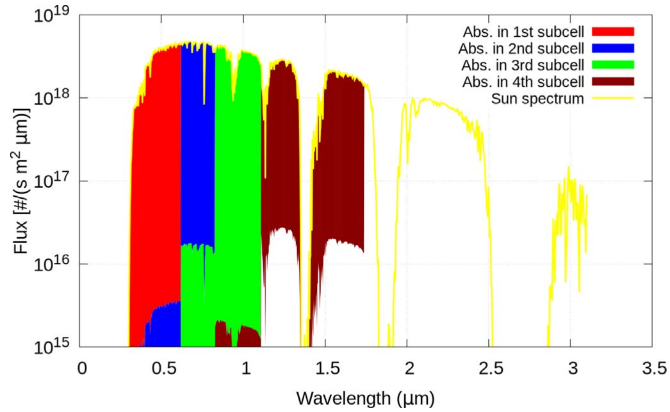

Fig. 1. ASTM G173-03 Global tilted solar spectra and attenuated portions of this spectra in each of 4 subcells in 4-junction MJSC. It corresponds to the 4-junctions MJCS analysed in Fig. 3(c).

the parallel kppw code [20]. Actual III-V material parameters, such as refractive index, relative dielectric constant, effective masses and effective density of states were calculated from the **k**·**p** theory and their functional dependence on E_g is given in the Appendix A.

The general expression for the current generated in m^{th} subcell is then:

$$J_\nu^{(m)} = q\int_{z_{m,l}}^{z_{m,u}}\int_{\lambda_l}^{\lambda_u} g^{(m)}(\lambda', z')d\lambda' dz'. \tag{5}$$

where $z_{m,l}$ and $z_{m,u}$ are the coordinates of the lower and upper edge of the m^{th} subcell and λ_l and λ_u are the lower and upper light wavelength absorbed in the m^{th} subcell; for ASTM G173-03 $\lambda_l = 280$ nm and $\lambda_u = 4000$ nm [19]. In Eq. (5) index $\nu \in \{n, \mathrm{dr}, p\}$, where n, dr and p represent minority carrier current in quasi-neutral $p-$ region, majority electron and hole current in depletion region and minority carrier current in quasi-neutral $n-$ region, respectively. The expressions for currents in different regions of MJSC depend on their geometry, material type, and impurities. For the *pn* homojunction, those are the textbook expressions, and together with the boundary conditions, can be found elsewhere [17,21–23].

Now the short circuit current in m^{th} subcell, $J_{\mathrm{SC}}^{(m)}$, can be calculated as:

$$J_{\mathrm{sc}}^{(m)} = J_n^{(m)} + J_{\mathrm{dr}}^{(m)} + J_p^{(m)} \tag{6}$$

where J_n is the electron minority current in the quasi-neutral p region, J_{dr} is the electron and hole majority current in the depletion region and J_p is the hole minority current in the quasi-neutral n region.

Various losses existing in the MJSC are accounted in the form of the diode equation:

$$J_0^{(m)} = J_{\mathrm{sat}}^{(m)}\left(e^{\frac{qV^{(m)}}{k_{\mathrm{B}}T}} - 1\right) \tag{7}$$

$$J_{\mathrm{sat}}^{(m)} = J_{0,\mathrm{Rad.}}^{(m)} + J_{0,\mathrm{Dark}}^{(m)} + J_{0,\mathrm{Aug.}}^{(m)} \tag{8}$$

where $J_{0,\mathrm{Rad.}}$ [15,16], $J_{0,\mathrm{Dark}}$ [17] and $J_{0,\mathrm{Aug.}}$ [18] are the diffusion dark current, the radiative recombination current and the Auger recombination current, respectively, given as:

$$J_{0,\mathrm{Rad}}^{(m)} = q[w_n^{(m)} + w_p^{(m)}]\frac{8\pi n_i^{(m)2}}{h^3c^2}\left[\int_0^\infty \frac{\alpha^{(m)}(h\nu)^2}{e^{\frac{h\nu}{k_{\mathrm{B}}T}}}d(h\nu)\right] \tag{9}$$

where, $\alpha^{(m)}(h\nu)$ is the absorption coefficient of relevant materials, $n_i^{(m)}$ is the intrinsics carrier concentration, and $w_n^{(m)} + w_p^{(m)}$ is the thickness of m^{th} subcell depletion region;