Design for strong absorption in a nanowire array tandem solar cell

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Semiconductor nanowires are a promising candidate for next-generation solar cells. However, the optical response of nanowires is, due to diffraction effects, complicated to optimize. Here, we optimize through optical modeling the absorption in a dual-junction nanowire-array solar cell in terms of the Shockley-Queisser detailed balance efficiency limit. We identify efficiency maxima that originate from resonant absorption of photons through the HE11 and the HE12 waveguide modes in the top cell. An efficiency limit above 40% is reached in the band gap optimized Al$_{0.10}$Ga$_{0.90}$As/In$_{0.34}$Ga$_{0.66}$As system when we allow for different diameter for the top and the bottom nanowire subcell. However, for experiments, equal diameter for the top and the bottom cell might be easier to realize. In this case, we find in our modeling a modest 1–2% drop in the efficiency limit. In the Ga$_{0.51}$In$_{0.49}$P/InP system, an efficiency limit of $\eta = 37.3\%$ could be reached. These efficiencies, which include reflection losses and sub-optimal absorption, are well above the 31.0% limit of a perfectly-absorbing, idealized single-junction bulk cell, and close to the 42.0% limit of the idealized dual-junction bulk cell. Our results offer guidance in the choice of materials and dimensions for nanowires with potential for high efficiency tandem solar cells.

The use of III–V nanowires for p-i-n junction solar cells is an emerging avenue for photovoltaics$^{1–6}$. Both single wire$^{4,7}$ and large-area nanowire array$^{5,9}$ devices show promise for next generation solar cells. Already for single nanowire systems, diffraction of light can lead to resonant coupling of light into the nanowire with several absorption peaks as a function of wavelength$^{10,11}$. Optimization of the geometry of the single-nanowire geometry is necessary to obtain maximum photocurrent$^{12}$ and open circuit voltage$^{12}$. The resonances can lead to a 20 times stronger absorption per volume semiconductor material in a III–V nanowire as compared to a bulk sample$^{13}$. An array of nanowires gives in turn access to large-area devices when higher output power is needed. For such arrays, an efficiency of 13.8% has been demonstrated using InP nanowires with a single p-i-n junction in the axial direction$^4$, and an efficiency of 15.3% has been reached with GaAs nanowires$^9$. However, the use of a single material gives an upper limit for the amount of sun light that can be converted into electrical energy$^{14}$, due to two reasons. First, the energy of photons with energy below the band gap energy of the semiconductor cannot be utilized since those low-energy photons cannot be absorbed. Second, a large part of the energy of absorbed high-energy photons is wasted due to thermalization. In this thermalization process, the photogenerated electrons and holes relax in energy to their respective band edges.

To reach higher efficiencies in solar cells, an avenue is to use multiple semiconductors, epitaxially grown on top of each other$^{15}$. See Fig. 1 for a system with two different semiconductor materials, where one material is used in the top cell and a different material in the bottom cell. The idea in such a tandem device is to absorb high energy photons in a high band gap top cell. In that top cell, the thermalization loss of the high energy photons is decreased compared to the single junction cell. The lower energy photons continue to the bottom cell where they are absorbed. Due to the lower band gap of the bottom cell than in the single junction cell, more photons are absorbed than in the single junction cell. In this way, the tandem cell can absorb more photons than the single junction cell, while at the same time having reduced thermalization losses. However, in planar cells, the crystal lattice constant between materials in adjacent subcells/layers should be matched to yield high-quality materials without performance limiting dislocations. Such requirements on crystal-lattice matching limit strongly the choice of materials for tandem cells.

Nanowire structures offer a clear benefit for multi-junction solar cells compared with planar cells. Efficient strain relaxation in nanowires allows for the fabrication and combination of dislocation-free, highly lattice-mismatched materials$^{16–19}$. Furthermore, III–V semiconductor nanowire arrays can in principle be fabricated on top of a Si substrate$^{19}$, giving the prospect of using the Si substrate as the bottom cell$^{2,20–23}$. Division of Solid State Physics and NanoLund, Lund University, Box 118, 22100 Lund, Sweden. Correspondence and requests for materials should be addressed to N.A. (email: nicklas.anttu@ftf.lth.se)
Thus, nanowires offer freedom for the material choice in multi-junction solar cells, making it easy to reach optimum material combinations to match the solar spectrum. Furthermore, the resonant absorption by designing the nanowire geometry holds the prospect of lower material usage than in thin-films. Therefore, to enable high-efficiency nanowire tandem solar cells, we need to understand the optimum choice of materials for the subcells as well as the optimum nanowire geometry to have the best absorption characteristics for photovoltaics. Already for single junction nanowire-array cells, we know that both the array pitch and the nanowire diameter need to be optimized simultaneously. At the same time, the optimum diameter depends on the band gap of the solar cell, that is, on the material choice.

Here, we perform optical modeling to calculate and optimize the absorption of light in a dual junction tandem nanowire solar cell (Fig. 1) with the scattering matrix method. This modeling allows us to perform a Shockley-Queisser detailed balance analysis to study and optimize the efficiency potential of the nanowire solar cell as a function of material choice and geometrical design of the nanowires. We show that an efficiency limit above 40% can be reached in the band gap optimized Al0.10Ga0.90As/In0.34Ga0.66As system when we allow for different diameter $D_{\text{top}}$ and $D_{\text{bot}}$ for the top and the bottom subcell. However, for experiments, the case of $D_{\text{top}} = D_{\text{bot}}$ might be easier to realize. In this case, we find a 1–2% drop in the efficiency. In the experimentally relevant Ga0.51In0.49P/InP system, an efficiency limit of $\eta = 37.3\%$ is reached for a nanowire length of 13 $\mu$m when using equal diameters of $D_{\text{top}} = D_{\text{bot}} = 160$ nm and a pitch $P = 380$ nm (we analyze also the effect of varying nanowire length, with results summarized in Table 1). These efficiencies for nanowire tandem cells are well above the 31.0% limit of an idealized, perfectly absorbing single-junction bulk cell and close to the 42.0% limit of the idealized, band gap optimized dual-junction bulk cell.

Material choice for the top and the bottom cell in a nanowire tandem solar cell

To choose the materials for the top and the bottom nanowire subcell, we perform the well-known Shockley-Queisser detailed balance analysis assuming first perfect absorption of above band gap photons in each subcell. This analysis corresponds to the case when each subcell absorbs optimally, without reflection losses. The specific assumption and technical details of the analysis can be found in the Supplementary Information.

Importantly, we assume that cell 1 absorbs all photons of energy above $E_1$, the band gap energy of cell 1. Cell 2 absorbs in turn all photons with energies between $E_1$ and $E_2$, the band gap energy of cell 2. We assume that $A_i(\lambda) = 1$ for $\lambda < \lambda_1bg$ and $A_i(\lambda) = 0$ otherwise. Here, $A_i(\lambda)$ is the absorption spectrum of cell 1 (2), that is, the fraction of incident light of wavelength $\lambda$ absorbed in cell 1 (2). Similarly, we assume that $A_i(\lambda) = 1$ for $\lambda_1bg < \lambda < \lambda_2bg$ and $A_i(\lambda) = 0$ otherwise. Here, $\lambda_1bg = 2\pi hc/E_1$ and $\lambda_2bg = 2\pi hc/E_2$. In this way, we find the materials that maximize the efficiency limit of the nanowire solar cell when the geometry is designed for optimum absorption (Fig. 2). Note that below, in the section Geometry Design, when considering the effect of the nanowire geometry on the absorption, we model the absorption spectra $A_i(\lambda)$ with sub-optimal absorption and varying reflection losses.

We find a maximum efficiency of 42.0% when the band gaps of the top and the bottom cell are $E_1 = 1.58$ eV and $E_2 = 0.95$ eV respectively (Fig. 2). Note that the results in the section Geometry Design are in good agreement with previous experimental results.
We use tabulated refractive index values for Al\(_{0.10}\)Ga\(_{0.90}\)As (band gap of 1.55 eV\(^2\)) and refractive index values available for the optics modelling. Among the ternaries for which such refractive index data were readily available, we identified Al\(_{0.10}\)Ga\(_{0.90}\)As, In\(_{0.34}\)Ga\(_{0.66}\)As (band gap of 0.95 eV\(^2\)), and refractive index data available for the InP substrate. Therefore, GaAs nanowires need dedicated surface passivation schemes,\(^a\) whereas the requirement on surface passivation is relieved for InP nanowires.\(^b\) Therefore, we chose to concentrate on an InP bottom cell. Here, a maximum efficiency of 38.6% is found with a top cell band gap energy of 1.86 eV (inset of Fig. 2). We note that Ga\(_{0.51}\)In\(_{0.49}\)P, for which refractive index data is available,\(^31\) has a band gap energy of 1.85 eV,\(^31\) giving an efficiency limit of 40.7% for perfectly absorbing subcells.

However, we could imagine that the fabrication of a dual-junction nanowire solar cell could benefit from the knowledge and control of the fabrication of single-junction nanowire solar cells. In this case, the natural candidates are the well-performing InP\(^a\) and GaAs\(^b\) systems. The band gaps of both these materials work well for the bottom cell (see inset in Fig. 2 for an InP bottom cell and Supplementary Figure S1 for a GaAs bottom cell). However, the surface recombination velocity of unpassivated GaAs can be five orders of magnitude higher than that of unpassivated InP\(^35\). Therefore, GaAs nanowires need dedicated surface passivation schemes,\(^a\) whereas the requirement on surface passivation is relieved for InP nanowires.\(^b\) Therefore, we chose to concentrate on an InP bottom cell. Here, a maximum efficiency of 38.6% is found with a top cell band gap energy of 1.86 eV (inset of Fig. 2). We note that Ga\(_{0.51}\)In\(_{0.49}\)P, for which refractive index data is available,\(^31\) has a band gap energy of 1.85 eV,\(^31\) giving an efficiency limit of 40.7% for perfectly absorbing subcells.

**Geometry Design**

After choosing the materials for the top and the bottom cell as described above (the nearly band gap optimized Al\(_{0.10}\)Ga\(_{0.90}\)As/In\(_{0.34}\)Ga\(_{0.66}\)As system as well as the technologically relevant Ga\(_{0.51}\)In\(_{0.49}\)P/InP system), we turn to the efficient analysis (RCWA)\(^4\) for the top cell and In\(_{0.34}\)Ga\(_{0.66}\)As (band gap of 0.95 eV\(^2\)), and refractive index from ref. \([29]\) for the bottom cell, which was found to be a good band gap combination with an efficiency limit of 40.7%.

To choose the III-V materials for the nanowire subcells, we calculated first the band gap for varying ternary compounds.\(^27\) After this, we investigated which ternary compounds have tabulated, experimentally determined, reliable refractive index values available for the optics modelling. Among the ternaries for which such refractive index data were readily available, we identified Al\(_{0.10}\)Ga\(_{0.90}\)As (band gap of 1.55 eV\(^2\)) and refractive index from ref. \([28]\) for the top cell and In\(_{0.34}\)Ga\(_{0.66}\)As (band gap of 0.95 eV\(^2\)), and refractive index from ref. \([29]\)) for the bottom cell as a good material combination with an efficiency limit of 40.7%.

Note that the optics modeling is done with the nanowires on top of an InP substrate (see Fig. 1). However, absorption of light in the substrate does not contribute to the current or voltage of the solar cell in our analysis. Thus, the substrate functions optically merely to partially reflect the light that reaches the substrate. Therefore, a change to a different substrate, like the less-expensive Si, with similar \(n \approx 3.5\) as the InP would give very similar absorption spectra.

We start by considering the case of Al\(_{0.10}\)Ga\(_{0.90}\)As (band gap of \(E_1 = 1.55\) eV) for the top cell and In\(_{0.34}\)Ga\(_{0.66}\)As (band gap of \(E_2 = 0.95\) eV) for the bottom cell, which was found to be a good band gap combination with efficiency limit of 40.7% for perfectly absorbing subcells.
It is known that the nanowire diameter affects strongly the absorption of light\(^1,5,7,8,13,35\). Therefore, to study the effect of the nanowire diameter on the absorption in the tandem cell, we fix \(P = 530 \text{ nm} \), \(L_{\text{bot}} = 2000 \text{ nm} \), and \(L_{\text{top}} = 2900 \text{ nm} \) [Fig. 3(a)]. As a main feature: the efficiency appears to be a function of just \(D_{\text{top}} \) when \(D_{\text{bot}} \) is large enough (typically when \(D_{\text{bot}} > 250 \text{ nm} \)). In this case of large \(D_{\text{bot}} \), two local maxima show up in the efficiency as a function of \(D_{\text{top}} \). To show these maxima clearly, we set \(D_{\text{bot}} \) to a fix value of 470 nm. Here, these two efficiency peaks show up at a top cell diameter of \(D_{\text{top}} = 150 \text{ nm} \) and \(D_{\text{top}} = 345 \text{ nm} \), respectively [Fig. 3(b)].

To understand the origin of these two efficiency maxima, we study the number of incident photons as a function of wavelength [blue line in Fig. 3(c,d)]. In the region 600 nm to 800 nm, the solar spectrum shows the highest number of incident photons as a function of wavelength. Since we assume that each absorbed photon contributes one charge carrier to the photogenerated current, strong absorption in this wavelength region is very important for \(j \) and consequently to the efficiency.

Therefore, we study the absorption spectrum in the top cell as a function of the diameter in the top cell around \(D_{\text{top}} = 150 \text{ nm} \) and \(D_{\text{top}} = 345 \text{ nm} \), respectively, where the two local maxima in \(\eta \) show up. In Fig. 3(c), when the diameter increases from 120 nm to 150 nm, we find an absorption peak in the spectrum, and it moves from about 600 nm to 700 nm\(^8,36,37\). This peak can be explained as resonant coupling of incident light into the HE\(_{11}\) waveguide mode of the individual nanowires. This resonant coupling leads to enhanced absorption in nanowire arrays\(^8\). When \(D_{\text{top}} \) increases further to 180 nm [red dotted line in Fig. 3(b)], the absorption peak has started to vanish since it red-shifts beyond the bandgap wavelength. This shifting and disappearance of the absorption peak leads consequently to a small decrease in the efficiency as \(D_{\text{top}} \) increases from 150 nm to 180 nm.

Similarly, in the case of \(D_{\text{top}} = 345 \text{ nm} \) we find again an absorption peak at \(\lambda \approx 700 \text{ nm} \) [Fig. 3(d)]. This time, the absorption peak originates from the higher order HE\(_{12}\) waveguide mode. This absorption peak has red-shifted beyond the band gap wavelength when \(D_{\text{top}} \) has increased to 375 nm [Fig. 3(d)], leading to a slight decrease in the efficiency. Thus, we find an efficiency maximum for the nanowire tandem solar cell [Fig. 3(a)] when \(D_{\text{top}} \) is optimized to place the HE\(_{11}\) or the HE\(_{12}\) absorption peak just below the bandgap wavelength. Very similar results have been reported for the diameter optimization of a single junction InP nanowire solar cell\(^8\).

To understand why the efficiency does not noticeably depend on \(D_{\text{bot}} \) for \(D_{\text{bot}} > 250 \text{ nm} \) [Fig. 3(a)], we study the photogeneration of charges in the top cell \((j_{\text{ph1}})\) and the bottom cell \((j_{\text{ph2}})\) [Fig. 3(e,f)]. Since \(j_{\text{bot}} = j_{\text{ph2}}\) and \(j_{\text{top}} = j_{\text{ph1}}\) (see Supplementary Information for details), the smaller one of \(j_{\text{bot}}\) and \(j_{\text{top}}\) is expected to limit the solar cell efficiency [Fig. 3(a)]. When \(D_{\text{top}} < 100 \text{ nm} \), the total current of the tandem cell is strongly limited by \(j_{\text{bot}}\). As the diameter of the top cell increases, \(j_{\text{bot}}\) can increase to about 20 mA/cm\(^2\). However, when the bottom cell diameter is larger than 250 nm, \(j_{\text{bot}} > 20 \text{ mA/cm}^2\). Thus, for \(D_{\text{bot}} > 250 \text{ nm} \), \(j_{\text{bot}} > j_{\text{top}}\) and the efficiency follows the absorption properties of the current-limiting top cell and therefore depends mainly on \(D_{\text{top}}\) and only very weakly on \(D_{\text{bot}}\).

We note that for the bottom cell, we find a pronounced maximum in \(j_{\text{bot}}\) as a function of \(D_{\text{bot}}\) for \(D_{\text{bot}} > 250 \text{ nm} \) when \(D_{\text{top}} \approx 0\). We assign this maximum in \(j_{\text{bot}}\) to the HE\(_{11}\) resonance in the bottom cell. We notice that in Fig. 3(f), that maximum is to a large degree overshadowed for \(D_{\text{bot}} > 0\) by the strong dependence of \(j_{\text{bot}}\) on \(D_{\text{top}}\). When we study the dependence of the efficiency on \(D_{\text{bot}}\) for a fixed \(D_{\text{top}}\) (see Supplementary Figure S2), we find that the maximum at \(D_{\text{bot}} = 250 \text{ nm} \) shows up also for \(D_{\text{bot}} > 0\) and broadens with increasing \(D_{\text{top}}\).

Thus, we have found above two clear local maxima for \(\eta\), one for \(D_{\text{top}} = 150 \text{ nm} \) and one for \(D_{\text{top}} = 345 \text{ nm} \) that originate, respectively, from resonant absorption through the HE\(_{11}\) and HE\(_{12}\) modes in the top cell. However, the results above were derived for a fixed \(L_{\text{bot}}, L_{\text{top}}, P\). Next, we optimize the efficiency limit for all these five parameters \((D_{\text{bot}}, D_{\text{top}}, L_{\text{bot}}, L_{\text{top}}, P)\) simultaneously. To make the optimization numerically feasible, we introduced a numerically efficient iteration process (See Supplementary Information for details). We choose to show the results in Fig. 4 as a function of top cell length \(L_{\text{top}}\). For tabulated values of the optimized geometry, see Supplementary Information Table S1. For a more complete dependence of the efficiency on the geometrical parameters, see Supplementary Figures S3–S14. Notably, with proper design, an efficiency limit above 40% can be reached by the use of Al\(_{0.10}\)Ga\(_{0.90}\)As for the top cell and In\(_{0.34}\)Ga\(_{0.66}\)As for the bottom cell [blue line, when \(L_{\text{top}} > 6 \mu\text{m}\), in Fig. 4(a)].

In this optimization, we can identify maxima in \(\eta\) to originate from the above discussed HE\(_{11}\) and HE\(_{12}\) resonances in the top cell [Fig. 4(a)]. In the region of \(L_{\text{top}} > 600 \text{ nm} \), the HE\(_{11}\) resonance of the top cell leads to a higher efficiency limit than that of the HE\(_{12}\) resonance. These results are in agreement with those for a single junction nanowire array solar cell where the HE\(_{11}\) resonance usually leads to the highest efficiency\(^8\). For the dual junction cell here, we call these maxima for brevity the HE\(_{11}\) and HE\(_{12}\) maxima/optimas.

For a single junction nanowire cell\(^8\), rough values for the optimum diameter were estimated as

\[
D_{\text{HE11(HE12)}} = \frac{\epsilon_{\text{HE11(HE12)}}}{\epsilon_{\text{bandgap}}} \approx \frac{\epsilon_{\text{HE11(HE12)}}}{\epsilon_{\text{bandgap}}} \geq \frac{\epsilon_{\text{HE11(HE12)}}}{\epsilon_{\text{bandgap}}}
\]

Here, \(\epsilon\) is the real part of the refractive index (at the band gap wavelength) and \(D_{\text{HE11(HE12)}}\) is the diameter that optimizes the wavelength position of the HE\(_{11}\) and HE\(_{12}\) resonance in order to maximize \(\eta\). The value for the constant \(\epsilon_{\text{HE11(HE12)}}\) can be extracted from the work on the single-junction nanowire solar cells\(^8\).

The diameter for the HE\(_{11}\) (HE\(_{12}\)) resonance of the top cell in Fig. 4(b) is \(D_{\text{top}} \approx 150 \text{ nm} \) (\(D_{\text{top}} \approx 345 \text{ nm} \)) in qualitative agreement with values from Equation (1) \([\text{about } 169 \text{ nm for } \text{HE}_{11}\text{ and } 394 \text{ nm for } \text{HE}_{12}\text{ resonance}]\). We find that \(D_{\text{bot}}\) fluctuates only slightly when \(D_{\text{top}} \approx 150 \text{ nm} \) to yield the HE\(_{11}\) maximum (blue dotted line in Fig. 4(b)). In contrast, \(D_{\text{bot}}\) fluctuates more at the HE\(_{12}\) maximum (green dotted line in Fig. 4(b)). This fluctuation in \(D_{\text{bot}}\) is understood from the fact that for the HE\(_{12}\) maximum at \(D_{\text{top}} \approx 345 \text{ nm} \), the efficiency shows a very broad maximum in \(D_{\text{bot}}\) (black dashed line in Fig. 3a and Supplementary Figure S2), which allows for large variations in \(D_{\text{bot}}\) when \(L_{\text{bot}}, L_{\text{top}}, P\) are optimized.

Similarly as for the single nanowire case\(^8\), we find that the optimum pitch \(P\) [solid lines in Fig. 4(b)] tends to increase with increasing nanowire length, that is, with increasing \(L_{\text{bot}}\) and \(L_{\text{top}}\). This behavior can be understood as
a competition between increased absorption and increased reflection with decreasing $P$. With increasing nanowire length, the absorption increases, and we can allow for a larger $P$ to decrease reflection losses.

In our results, we find that $L_{\text{bot}} > L_{\text{top}}$ [Fig. 4(f)]. However, the efficiency tends to increase as a function of $L_{\text{bot}}$ (see Supplementary Figures S3–S14), and therefore whether we end up in the case of $L_{\text{bot}} > L_{\text{top}}$ or in the case of $L_{\text{bot}} < L_{\text{top}}$ depends on how heavily we maximize the efficiency $\eta$ at the cost of increasing $L_{\text{bot}}$. We allowed the optimization to stop with respect to $L_{\text{bot}}$ when we reached a value of $d\eta/dL_{\text{bot}} < 0.001 \mu\text{m}^{-1}$ in our geometry optimization (see Supplementary Information). In this case, for all the considered $L_{\text{top}}$, the optimized value for $L_{\text{bot}}$ ended up slightly larger than $L_{\text{top}}$.

For fabrication purposes, it could be a benefit to consider $D_{\text{top}} = D_{\text{bot}}$, that is, nanowires of a single diameter $D$ throughout (see the red dashed line in Fig. 4a for the resulting efficiency). We found in this case large fluctuations in the optimum value of $L_{\text{bot}}$ when $L_{\text{top}}$ is increasing (the fluctuation in $L_{\text{bot}}$ could be larger than the value of $L_{\text{top}}$).

To be able to analyze this case as a function of $L_{\text{top}}$ we set an upper limit of $L_{\text{top}} + 1000 \text{ nm}$ for $L_{\text{bot}}$.
We find an interesting behavior for the optimized diameter $D$ for these single-diameter nanowires [red dashed line in Fig. 4(b)]. For the smallest considered $L_{\text{top}}$ of 500 nm, $D$ starts close to the $D_{\text{top}} \approx D_{\text{HE11}} \approx 150$ nm of the HE11 maximum for the case in which we allow for $D_{\text{top}} \neq D_{\text{bot}}$. When $L_{\text{top}}$ increases toward the largest considered value of 8000 nm, $D$ increases toward the value of the $D_{\text{bot}} \approx 200$ nm which optimizes the HE11 maximum in the $D_{\text{top}} \neq D_{\text{bot}}$ case. This behavior can be understood as follows. When $L_{\text{top}}$ is small, the absorption in the top cell is weak in relative terms, and photons also in the short wavelength region can reach the bottom cell due to insufficient absorption in the top cell. As a result, the current, and therefore the efficiency, of the solar cell is limited by absorption in the top cell. As a consequence, the optimum $D$ occurs when the absorption in the top cell is optimized for, which happens at $D \approx D_{\text{HE11}}$. In contrast, when $L_{\text{top}}$ is large, the absorption in the top cell is instead strong, and the performance of the solar cell becomes limited by the current-generation in the bottom cell, which is optimized for $D_{\text{bot}}$ in a similar way as when $D_{\text{top}} = D_{\text{bot}}$. Thus, for large $L_{\text{top}}$ $D$ goes toward the $D_{\text{bot}}$ that optimizes the HE11 maximum.

Since we find the optimum for $D$ close to the diameters found for the HE11 maximum in the $D_{\text{top}} = D_{\text{bot}}$ case, we find, not completely surprisingly, values for $P$ close to those of the HE11 case of $D_{\text{top}} = D_{\text{bot}}$. As an end result, we find that the efficiency for this case of $D = D_{\text{top}} = D_{\text{bot}}$ is typically 1 to 2% lower than when we allow for $D_{\text{top}} = D_{\text{bot}}$ [Fig. 4(a)].

We have also studied the efficiency of the InP based Ga0.51In0.49P/InP nanowire tandem system [Fig. 4(d–f)], with maximum efficiency of 38.5% for perfectly absorbing subcells, which should be set in relation to the limit of 42.0% for the idealized, perfectly absorbing, band gap optimized dual-junction bulk cell. Also for this material choice we reach an efficiency within 2% of this maximum, with $L_{\text{top}} > 6 \mu\text{m}$ and $L_{\text{bot}} > 7 \mu\text{m}$, when we allow for

| $L_{\text{top}}$ (nm) | $D_{\text{top}}$ (nm) | $D_{\text{bot}}$ (nm) | $L_{\text{bot}}$ (nm) | $P$ (nm) | η (%) |
|---------------------|---------------------|---------------------|---------------------|--------|--------|
| 500                 | 130                 | 130                 | 1500                | 190    | 29.7   |
| 1000                | 140                 | 140                 | 2000                | 220    | 33.6   |
| 2000                | 150                 | 150                 | 3000                | 270    | 35.5   |
| 4000                | 150                 | 150                 | 5000                | 360    | 36.6   |
| 8000                | 160                 | 160                 | 8800                | 420    | 37.5   |

Table 1. Optimized efficiency for varying $L_{\text{top}}$ for the Ga0.51In0.49P/InP dual-junction solar cell when the nanowire has a single diameter ($D_{\text{top}} = D_{\text{bot}}$), together with the corresponding geometrical parameters, as extracted from Fig. 4(d–f).
\( D_{\text{top}} = D_{\text{bot}} \). Also here, an additional drop by about 1% occurs with the constraint \( D_{\text{top}} = D_{\text{bot}} \). With Ga\(_{0.51}\)In\(_{0.49}\)P and InP as the material and \( D_{\text{top}} = D_{\text{bot}} \), we reach \( \eta = 35.5\% \) when \( L_{\text{top}} = 2000 \text{ nm} \) and \( L_{\text{bot}} = 3000 \text{ nm} \), considerably higher than the maximum 31.0\% possible in the single junction bulk solar cell case. To aid the reader, we show in Table 1 the values extracted from Fig. 4 for this case of \( D_{\text{top}} = D_{\text{bot}} \) (for the HE\(_{11}\) and HE\(_{12}\) maximum, we refer the reader to Supplementary Information Table S1).

**Conclusion**

We performed electromagnetic modeling to investigate theoretically the absorption properties of a dual junction nanowire array solar cell. We used then the Shockley-Queisser efficiency limit as a metric for optimizing the materials and geometry of the nanowires. The optimized geometries are presented in Fig. 4, Table 1, and Supplementary Information Table S1. The drop in efficiency limit when moving away from such an optimized geometry is presented in Supplementary Information Figures S3–S14. These results present a guideline for choosing a nanowire geometry that has promise for optimized absorption in a dual-junction nanowire array solar cell. In this way, our results can be used as a starting point for theoretical studies on the optimization of the electrical properties of dual-junction nanowire array solar cells. Our results can also guide in the choice of materials and dimensions for the fabrication of nanowires aimed for tandem solar cells.

**References**

1. Anttu, N. Shockley-queisser detailed balance efficiency limit for nanowire solar cells. *ACS Photonics* 2, 446–453 (2015).
2. Bu, S. et al. Optical and electrical simulations of two-junction III-V nanowires on Si solar cell. *Appl. Phys. Lett.* 102, 031106 (2013).
3. Kupec, J., Stoop, R. L. & Witzigmann, B. Light absorption and emission in nanowire array solar cells. *Opt. Express* 18, 27589–27605 (2010).
4. Sandhu, S., Yu, Z. & Fan, S. Detailed balance analysis and enhancement of open-circuit voltage in single-nanowire solar cells. *Nano Lett.* 14, 1011–1015 (2014).
5. Wällentin, J. et al. InP nanowire array solar cells achieving 13.8\% efficiency by exceeding the ray optics limit. *Science* 339, 1057–1060 (2013).
6. Sandhu, S., Yu, Z. & Fan, S. Detailed balance analysis of nanophotonic solar cells. *Opt. Express* 21, 1209–1217 (2013).
7. Nowzari, A. et al. A comparative study of absorption in vertically and laterally oriented InP core-shell nanowire photovoltaic devices. *Nano Lett.* 15, 1809–1814 (2015).
8. Anttu, N. & Xu, H. Q. Efficient light management in vertical nanowire arrays for photovoltaics. *Opt. Express* 21, A558–A575 (2013).
9. Aberg, I. et al. A GaAs nanowire array solar cell with 15.3\% efficiency at 1 sun. *IEEE J. Photovolt.* 6, 185–190 (2016).
10. Cao, L. et al. Engineering light absorption in semiconductor nanowire devices. *Nat. Mater.* 8, 643–647 (2009).
11. Hosseinnia, A. & Anttu, N. Absorption through a coupled optical resonance in a horizontal InP nanowire array. *Photon. Res.* 3, 125–128 (2015).
12. Kroghstrup, P. et al. Single-nanowire solar cells beyond the shockley-queisser limit. *Nat. Photonics* 7, 306–310 (2013).
13. Anttu, N. et al. Optical far-field method with subwavelength accuracy for the determination of nanostructure dimensions in large-area samples. *Nano Lett.* 13, 2662–2667 (2013).
14. Shockley, W. & Queisser, H. J. Detailed balance limit of efficiency of p-n junction solar cells. *J. Appl. Phys.* 32, 510 (1961).
15. Devos, A. Detailed balance limit of the efficiency of tandem solar–cells. *J. Phys. D.* 13, 839–846 (1980).
16. Caroff, P. et al. InAs heterostructure nanowires: MOVPE growth under extreme lattice mismatch. *Nanotechnology* 20, 495606 (2009).
17. Bjork, M. T. et al. One-dimensional steepchase for electrons realized. *Nano Lett.* 2, 87–89 (2002).
18. Gudiksen, M. S., Lauhon, L. J., Wang, J., Smith, D. C. & Lieber, C. M. Growth of nanowire superlattice structures for nanoscale photonics and electronics. *Nature* 415, 617–620 (2002).
19. Mårtensson, T. et al. Epitaxial III–V nanowires on silicon. *Nano Lett.* 4, 1987–1990 (2004).
20. Hu, Y., Li, M., He, J. J. & LaPierre, R. R. Current matching and efficiency optimization in a two-junction nanowire-on-silicon solar cell. *Nanotechnology* 24, 065402 (2013).
21. LaPierre, R. R. Theoretical conversion efficiency of a two-junction III-V nanowire on Si solar cell. *J. Appl. Phys.* 110, 014310 (2011).
22. Huang, N. F., Lin, C. X. & Povinelli, M. L. Limiting efficiencies of tandem solar cells consisting of III–V nanowire arrays on silicon. *J. Appl. Phys.* 112, 064321 (2012).
23. Benali, A. et al. Optical simulation of multijunction solar cells based on III–V nanowire arrays on silicon. *Energy Procedia* 60, 109–115 (2014).
24. Anttu, N. et al. Crystal phase-dependent nanophotonic resonances in InAs nanowire arrays. *Nano Lett.* 14, 5650–5655 (2014).
25. Anttu, N. & Xu, H. Q. Scattering matrix method for optical excitation of surface plasmons in metal films with periodic arrays of subwavelength holes. *Phys. Rev. B* 83, 165431 (2011).
26. Strandberg, R. Detailed balance analysis of area de-coupled double tandem photovoltaic modules. *Appl. Phys. Lett.* 106, 033902 (2015).
27. Vurgaftman, I., Meyer, J. E. & Ram-Mohan, L. Handbook series on semiconductor parameters Vol. 2: Ternary And Quaternary III-V Compounds (World Scientific, 1996).
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Author Contributions

Y.C. performed the simulations, analyzed and interpreted the results, and wrote the paper. M.E.P. and N.A. initiated and supervised the study and interpreted the results. All authors contributed to writing and editing the manuscript.

Additional Information

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