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Citation: Abdul Hadi, Sabina, Tim Milakovich, Mayank T. Bulsara, Sueda Saylan, Marcus S. Dahlem, Eugene A. Fitzgerald, and Ammar Nayfeh. "Design Optimization of Single-Layer Antireflective Coating for GaAs[subscript 1–x]xP[subscript x]x/Si Tandem Cells With x=0, 0.17, 0.29, and 0.37." IEEE J. Photovoltaics 5, no. 1 (January 2015): 425–431.

As Published: http://dx.doi.org/10.1109/JPHOTOV.2014.2363559

Publisher: Institute of Electrical and Electronics Engineers (IEEE)

Persistent URL: http://hdl.handle.net/1721.1/108586

Version: Author's final manuscript: final author's manuscript post peer review, without publisher's formatting or copy editing

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Design Optimization of Single Layer Anti-Reflective Coating for $GaAs_{1-x}P_x$ / Si Tandem Cells with x = 0, 0.17, 0.29 and 0.37

Sabina Abdul Hadi, Tim Milakovich, Mayank T. Bulsara, Sueda Saylan, Marcus S. Dahlem, Eugene A. Fitzgerald and Ammar Nayfeh

Abstract-Single layer anti-reflective coating (SLARC) materials and design for GaAs_{1-x}P_x/Si tandem cells were analyzed by TCAD simulation. We have shown that optimum SLARC thickness is a function of bandgap, thickness and material quality of top GaAs_{1-x}P_x subcell. Cells are analyzed for P fractions x=0, 0.17, 0.29 and 0.37 and ARC materials: Si₃N₄, SiO₂, ITO, HfO₂ and Al₂O₃. Optimum ARC thickness ranges from 65-75 nm for Si₃N₄ and ITO to ~100-110 nm for SiO₂. Optimum ARC thickness increases with increasing GaAs_{1-x}P_x absorber layer thickness and with decreasing P fraction x. Simulations show that optimum GaAs_{1-x}P_x absorber layer thickness is not a strong function of ARC material, but it increases from 250 nm for x= 0 to ~1 µm for x= 0.29 and 0.37. For all P fractions, Si₃N₄, HfO₂ and Al₂O₃ performed almost equally, while SiO₂ and ITO resulted in ~1% and ~2% lower efficiency, respectively. Optimum SLARC thickness increases as material quality of the top cell increases. The effect of ARC material decreases with decreasing GaAs_{1-x}P_x material quality. The maximum efficiencies are achieved for cells with ~1 μ m GaAs_{0.71}P_{0.29} absorber (τ =10 ns): ~26.57% for 75 nm Si₃N₄ SLARC and 27.62% for 75 nm SiO₂/60 nm Si₃N4 double layer ARC.

Index Terms— Anti-reflective coating, GaAs_{1-x}P_x, III-V on Si, Si₃N₄, ITO, SiO₂, Al₂O₃, HfO₂, Synopsys, TCAD, TMM.

I. INTRODUCTION

PERFORMANCE of solar cells can be greatly improved with optimized anti-reflective coating (ARC) that reduces amount of reflected incident light. Uncoated crystalline silicon (c-Si) surface (refractive index n-3.7) at interface with air (n-1) is shown to reflect between 31% - 48% of incident light [1]. The concepts of optimum ARC material, number of layers, layer thickness and surface texturing are continually being studied [1 - 7]. Ideally, the ARC should be abundant material, easily deposited, transparent to most of the solar spectrum and compatible with materials and processes commonly used in solar cell industry. Single layer ARC (SLARC) can minimize reflection at one specific wavelength (quarter-wave ARC). However, the remaining part of the solar spectrum is highly reflected. Hence, for optimum solar cell operation, SLARC is used to minimize wavelength with highest spectral intensity. Double and multilayer anti-reflective coatings can minimize reflection for more than one wavelength of interest, but the choice of the ARC materials is more constricted, due to refractive index constraints [2-4]. Different materials such as SiO₂, SiO_x, SiN_x, Si₃N₄, ZnO, ZnS, ITO, TiO₂, MgF₂/ZnS, etc. have been shown to have good ARC properties [1-7], but their performance depends on ARC design and solar cell application. Furthermore, reflectance can be greatly reduced by surface patterning, which is of most interest for concentrated solar cells with normal light incidence [2].

With growing development of tandem cell applications for high efficiency, ARC design specifically tuned to optimize multijunction (MJ) cell performance is needed. Subcells can be grown on top of each other or they can be fabricated separately and mechanically bonded. Theoretically, optimal efficiency of two junction solar cell can be achieved if bottom cell bandgap, E_g , is 1.1 eV, while bandgap of top cell is 1.7 eV [8]. Therefore Si (E_g =1.12 eV) based tandem cells with top GaAs_{1-x}P_x cell (E_g =1.42 - 2.22 eV for x = 0 - 1) are an attractive area of research for low cost MJ solar cells.

Main challenges for $GaAs_{1-x}P_x$ / Si tandem cell are lattice and thermal expansion mismatch between Si and GaAs_{1-x}P_x compounds. Nonetheless, high-quality GaAs solar cells were successfully grown on Si by using SiGe step-graded buffers in order to grow virtual Ge substrate that is latticed matched to GaAs [9, 10]. Furthermore, Ge fraction in step-graded buffers can be tuned to lattice match desired GaAs_{1-x}P_x compound [11, 12]. Unfortunately, due to its optical properties and decreasing bandgap, SiGe buffer layer would absorb light intended for bottom Si cell [13-15]. Another successful way to grow a defect-free III-V layer on silicon is based on the use of a GaP nucleation layer, followed by GaAs_{1-x}P_x graded buffer [16-19]. The method that would avoid use of graded buffer layers and its related optical losses is mechanical stacking of two sub-cells. In this work we present simulation of the structure that represents mechanically bonded $GaAs_{1-x}P_x$ and Si cells.

For optimum performance of MJ cells, current generated in all sub-cells need to match. Sub-cell with lowest optically

Date Submitted: July, 22nd, 2014.

This work was supported by Masdar Institute of Science and Technology (MIST), Abu Dhabi, UAE.

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generated current limits current flow in tandem cell, decreasing its overall efficiency. Hence, ARC for Si based MJ cells should be designed to maximize optical absorption in Si base cell, but also not to impair performance of the top cell significantly.

In this paper we analyze the design requirements for GaAs_{1-x}P_x/Si tandem cell for x= 0, 0.17, 0.29 and 0.37 in terms of optimum GaAs_{1-x}P_x absorber layer thickness and single layer anti-reflective coating (SLARC). Analysis is carried out for 5 different ARC materials: Si₃N₄, SiO₂, ITO, HfO₂ and Al₂O₃, that were chosen either based on their optical compatibility with GaAsP, their common use in PV application or convenience of the in-situ growth. Transfer Matrix Method (TMM) is used to estimate the range of optimum anti-reflective layer thicknesses, which are then analyzed by optical and electrical simulations using TCAD Synopsys [20-22]. Finally, results for optimized GaAs_{1-x}P_x/Si tandem cell with optimum SLARC design is compared to the equivalent cell with optimized SiO₂/Si₃N₄ double layer anti-reflective coating (DLARC) [4,23].

II. METHODOLOGY

Various ARC materials were analyzed to observe how well they satisfy quarter-wave film condition. Transfer Matrix Method (TMM) is then used to estimate SLARC thickness, d, with minimum reflection for Air/ARC/GaAs_{1-x}P_x/Si interface with varying GaAs_{1-x}P_x thickness, without taking into consideration the light absorption in each layer. In order to account for absorption and to find optimum ARC design for tandem cell, d is further varied in TCAD simulations. Moreover, $GaAs_{1-x}P_x$ layer thickness, t, is varied in order to find optimum tandem cell design with matching sub-cell currents. GaAs_{1-x}P_x / Si tandem cell is simulated for top cell thickness, t, and ARC thickness, d, for varying $GaAs_{1-x}P_x$ minority carrier lifetime, τ , in order to find an optimum tandem cell design with maximum efficiency. Moreover, the efficiency of the tandem cell is used to identify the optimum design that can be achieved. The efficiency is a performance parameter that encapsulates effects of all variables in this analysis, such as ARC material, ARC thickness, $GaAs_{1,x}P_x$ absorber layer thickness and lifetime. Finally, by means of TCAD simulations, SiO₂/Si₃N₄ DLARC is optimized for the most efficient GaAsP/Si tandem cell and compared to optimum SLARC design.

A. Selection of SLARC materials

Quarter-wave films are specially designed to reduce or completely eliminate reflection at the interface between two media of different refractive indices, n. In our ARC selection process, quarter-wave (QW) condition was analyzed for Air $(n_{Air}-1) / GaP (n_{GaP}-3)$ and Air / GaAs $(n_{GaAs}-3.4)$ interfaces, as shown in equation (1) [24], since QW condition for GaAs₁. _xP_x compounds should fall in between.

$$n_{ARC} = \sqrt{n_{Air} \cdot n_{GaAs_{1-x}P_x}} \tag{1}$$

Figure 1 shows refractive indices of selected ARC materials, QW conditions for GaAs/Air and GaP/Air interfaces (optical properties utilized from [25]) and solar spectral irradiance AM1.5 [26]. Optical parameters of GaAs_{1-x}P_x are obtained by measurements by J. A. Woollam Co. of MOCVD grown 2 μ m thick GaAs_{1-x}P_x layers on graded SiGe buffer [27]. In terms of reflection, SiO₂ performs poorly for the entire wavelength range and it is included in our further study due to its good surface passivation properties and DLARC applications [4, 23]. For wavelengths with highest spectral intensity ($\lambda \sim 400-600$ nm), Si₃N₄, ITO and HfO₂ satisfy QW condition for GaAs_{1-x}P_x compounds the best, while Al₂O₃ is close to QW condition of Air/GaP interface.



Fig.1. Refractive indices of analyzed ARC materials [25]. Also shown are quarter-wave conditions for Air/GaAs and Air/GaP interfaces as well as Solar Spectral Irradiance AM1.5(arbitrary units) [26].

B. Transfer Matrix Method

Transfer Matrix Method (TMM) is used to calculate the incident wave reflection with wavelength λ , propagating through multiple layers with refractive index n_i and thickness, d_i , without accounting for absorption in each medium. Wave transfer matrix used to describe propagation of the wave through homogenous i^{th} layer is defined in (2) and transfer matrix describing reflectance at the boundary of two layers with different refractive indices, n_i and n_{i+1} , is given in (3) [24].

$$M_{prop_{i}} = \begin{bmatrix} e^{-j\varphi_{i}} & 0\\ 0 & e^{j\varphi_{i}} \end{bmatrix}, \varphi_{i} = n_{i}d_{i}\frac{2\pi}{\lambda}$$
(2)

$$M_{i/i+1} = \frac{1}{2 \cdot n_{i+1}} \begin{bmatrix} n_{i+1} + n_i & n_{i+1} - n_i \\ n_{i+1} - n_i & n_{i+1} + n_i \end{bmatrix}$$
(3)

Wave propagating through N layers, assuming N+1 boundaries (sandwiched between two infinite media), can be described by matrix M, given in (4) [24].

$$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \prod_{i=1}^{N} (M_{i-1/i} \ M_{prop_i} M_{i/i+1})$$
(4)

Total intensity reflectance of wave propagation through N layers, from infinite region with n_0 to infinite region with n_{N+1} is then equal to [24]:

$$R_{0,N+1} = \left| -\frac{C}{D} \right|^2 \tag{5}$$

Figure 2 shows schematics of transfer matrix method applied to ARC optimization for $GaAs_{1-x}P_x$ / Si tandem cell.



Fig. 2. Schematics of TMM structure used in order to estimate optimum ARC for $GaAs_{1-x}P_x$ / Si tandem cell.

In order to find optimum SLARC thickness, reflectance intensity at each wavelength, $R_{0,N+1}$ (λ), is weighted by normalized spectrum intensity, $I(\lambda)$, and averaged over the spectrum, as shown in (6).

$$R_{average} = \frac{1}{\lambda_{end} - \lambda_{start}} \int_{\lambda_{start}}^{\lambda_{end}} R_{0,N+1}(\lambda) \cdot I(\lambda) d\lambda \tag{6}$$

Solar spectrum range from $\lambda_{\text{start}} = 300 \text{ nm}$ to $\lambda_{\text{end}} = 1100 \text{ nm}$ is taken into consideration since $\text{GaAs}_{1-x}P_x$ and Si optical responsevity fall within it. Analysis is repeated for varying $\text{GaAs}_{1-x}P_x$ thickness and P fractions of x = 0, 0.17, 0.29 and 0.37. Figure 3 shows minimum average spectral weighted reflectance, R_{average} as a function of P fraction (x), for each analyzed ARC material. $\text{GaAs}_{1-x}P_x$ thickness with minimum R_{average} varied with x and was equal to 2, 0.8, 2 (1.3 for SiO₂) and 1 µm for x = 0, 0.17, 0.29 and 0.37 respectively.



Fig. 3. Minimum average weighted reflectance, $R_{average}$ (%) as a function of P fraction, x, for different ARC material. GaAs_{1-x}P_x thickness with minimum Raverage shown above is equal to 2, 0.8, 2 (1.3 for SiO₂) and 1 µm for x = 0, 0.17, 0.29 and 0.37 respectively.

When absorption is not taken into account, optimum ARC thickness ranges roughly between 65 to 85 nm for all tested fractions of x and ARC materials, with exception of SiO₂. HfO₂ and Si₃N₄ show the lowest reflectance over the analyzed spectrum range (3.6 %). Si₃N₄ requires least ARC thickness to achieve minimum reflectance and is closely followed by HfO₂.

SLARC thickness with minimum average reflectance over the entire solar spectrum is selected for further device simulations in TCAD.

C. TCAD Simulation Model

Sentaurus TCAD by Synopsys [20-22] is used for electrical and optical simulation of the solar cell devices. Synopsys tools Sentaurus Structure Editor (SDE), Sentaurus Device (SDevice) and Inspect are used.

GaAs_{1-x}P_x / Si tandem cells are simulated for different ARC materials with varying ARC and GaAs_{1-x}P_x thickness, as well as GaAs_{1-x}P_x lifetime. Complex refractive indices for ARC materials, GaAs and Si are used from [25] while optical parameters of GaAs_{1-x}P_x (x=0.17-0.37) are obtained by measurements of MOCVD grown 2 μ m thick epi layer [27].

The Si solar cell is optimized such that absorber is 650 µm thick, lightly doped p-type Si substrate ($N_A = 10^{16}$ cm⁻³) and heavily doped ($N_D=10^{19}$ cm⁻³) 100 nm thick n-type emitter. GaAs_{1-x}P_x top cell is designed with variable absorber thickness and acceptor doping $N_A = 10^{18}$ cm⁻³ and 50 nm thick emitter with N_D= $5x10^{18}$ cm⁻³. Lifetime, τ , of Si is modeled as doping dependent in Physics section of SDevice Synopsys tool and its intrinsic value is set to 1 ms consistent with high quality c-Si wafer [28-30]. GaAs_{1-x}P_x lifetime is modeled as fixed value and it is varied from 10 ps to 1 µs, range of values reported for GaAs epi growth on SiGe graded buffers [31] and pure GaAs materials [32]. Values for energy bandgap for $GaAs_{1-x}P_x$ are utilized from [33], while for Si and GaAs default values from TCAD are used. Tunnel diode between two cells is simulated as a very thin, highly conductive region [34]. Optical and resistive losses in tunnel junction are not taken into consideration in these simulations. Effect of interface surface recombination is also ignored. Figure 4 shows a schematic crossection of simulated solar cell.



Fig. 4. Schematic cross-section of $GaAs_xP_{1\cdot x}$ / Si tandem cell simulated in TCAD.

By increasing P fraction, the bandgap of the top $GaAs_{1-x}P_x$ cell increases from ~ 1.43 eV for x=0 to ~1.88 eV for x=0.37 [33] resulting in lower photogenerated current in the top cell. In order to achieve matching currents of subcells, the optimum $GaAs_{1-x}P_x$ absorber layer thickness, as well as optimum SLARC thickness changes with increasing P fraction. Consequently, optimum SLARC thickness and material will differ from the values estimated by TMM analysis that did not

take into consideration the absorption or the tandem cell specific requirement for matching sub-cell currents.

III. RESULTS AND DISCUSSION

In order to show the effect of P fraction on the optimum SLARC and GaAs_{1-x}P_x absorber layer thickness, TCAD simulations were carried out for Si₃N₄ as a fixed ARC material, based on TMM results (shown in Figure 3 earlier). Figure 5 (a) shows maximum efficiency of GaAs_{1-x}P_x/Si tandem cell as a function of GaAs_{1-x}P_x absorber layer thickness at optimum Si₃N₄ ARC thickness for x=0, 0.17, 0.29 and 0.37, with GaAs_{1-x}P_x lifetime τ =10 ns. GaAs_{1-x}P_x absorber layer thickness for maximum efficiency increases from 250 nm for x = 0 to ~1 µm for x = 0.29 and 0.37. Tandem cell for x=0.29 preforms the best with maximum efficiency ~ 26.57%, closely followed by cells with x=0.37.



Fig. 5. (a) Maximum efficiency of GaAs_{1-x}P_x/Si tandem cell and (b) Optimum Si₃N₄ ARC thickness (nm) as a function of GaAs_{1-x}P_x absorber layer thickness for x=0, 0.17, 0.29 and 0.37 and GaAs_{1-x}P_x lifetime τ =10 ns.

Figure 5 (b) shows values for optimum Si_3N_4 ARC thickness at which maximum efficiency is achieved for varying $GaAs_{1-x}P_x$ absorber layer thickness and P fraction x. Maximum overall efficiency for all P fractions was achieved for Si_3N_4 thickness in the range between 65 - 75 nm. However, optimum ARC thickness increases with increasing $GaAs_{1-x}P_x$ absorber layer thickness. This is due to the fact that

more light is absorbed in the top cell with thicker absorber layer and photogeneration in bottom Si cell needs to be enhanced by favoring longer wavelengths. Furthermore, the trend in Figure 5 (b) shows that generally thicker ARC layer is required for cells with lower P fraction (x=0 and 0.17). This is due to the fact that cells with lower bandgap absorb more of the solar spectrum so the ARC thickness needs to be tuned such that performance of bottom cell is maximized. Similar analysis was repeated for other ARC materials. Optimum ARC thickness as a function of P fraction (x), and its corresponding optimum GaAs_{1-x}P_x absorber layer thickness for different ARC materials are shown in Figure 6 (a) for lifetime GaAs_{1-x}P_x = 10 ns. Figure 6 (b) shows maximum efficiency as a function of P fraction for GaAs_{1-x}P_x / Si tandem cells with optimized ARC and GaAs_{1-x}P_x absorber layer thicknesses.



Fig.6. (a) Optimum SLARC thickness for optimum $GaAs_{1-x}P_x$ absorber layer thickness for different ARC materials and (b) maximum efficiency as a function of P fraction x for optimized $GaAs_{1-x}P_x / Si$ tandem cells with $GaAs_{1-x}P_x$ lifetime τ =10 ns.

Results in Figure 6 show that optimum SLARC thickness is smallest for Si_3N_4 and ITO (65 -75 nm) and largest for SiO_2 (~100-110 nm). Optimum top absorber thickness is mostly unchanged with respect to different ARC materials, with the exception of ITO that resulted in slightly thinner GaAs_{1-x}P_x layer. In terms of efficiency, for all P concentrations, Si_3N_4 , HfO₂ and Al₂O₃ performed almost equally, while SiO₂ and ITO resulted in ~1% and ~2% lower efficiency, respectively. With respect to ARC performance and optimum thickness, TCAD simulations are in agreement with TMM results (Figure 3) except for ITO that was outperformed by SiO_2 . This is probably the result of larger absorption in ITO compared to SiO_2 , due to its higher extinction coefficients, k [25].

We have shown that optimum SLARC thickness changes with changing GaAs_{1-x}P_x absorber layer, due to the change in photogenerated current of both sub-cells. Similarly, optimum SLARC thickness changes with GaAs_{1-x}P_x material quality, which in this work is represented by minority carrier lifetime, τ . Optimum SLARC and GaAs_{1-x}P_x absorber layer thickness were studied for 10 ps $\leq \tau \leq 1$ µs. Since x=0.29 resulted in highest efficiency (for GaAs_{1-x}P_x absorber layer thickness between 950 nm -1 µm), the effect of GaAs_{1-x}P_x lifetime is shown here for that specific P fraction.



Figure 7 (a) Maximum efficiency and (b) optimum SLARC thickness as a function of $GaAs_{0.71}P_{0.29}$ minority carrier lifetime, τ , for $GaAs_{0.71}P_{0.29}$ / Si tandem cell with optimum $GaAs_{0.71}P_{0.29}$ absorber thickness.

Figure 7 (a) shows maximum efficiency of $GaAs_{0.71}P_{0.29}$ / Si tandem cell with optimized top cell absorber and ARC thicknesses, as a function of τ . The advantage of Si₃N₄, Al₂O₃ and HfO₂ materials decreases with lower material quality, with efficiency gain ranging from ~ 1.5 % at 10 ps to ~ 3% at 1 µs when compared with ITO. Figure 7 (b) shows optimum ARC thickness as a function of τ for GaAs_{0.71}P_{0.29} / Si tandem cell with optimum top cell absorber thickness. Optimum ARC thickness increases as material quality of the top cell increases, in an attempt to enhance photogeneration in bottom cell. Similarly, for poor lifetime in top cells, ARC thickness

decreases in favor of optical generation in top cell. The same trend is observed for all ARC materials and all P fractions (not shown here).

Figure 8 shows JV characteristics of GaAs_{1-x}P_x/Si tandem cells (x=0, 0.17, 0.29 and 0.37) with optimum SLARC and GaAs_{1-x}P_x absorber layer thicknesses with GaAs_{1-x}P_x lifetime equal to 10 ns. It can be noted that fill factor (FF) of cells with x=0.29 and x=0.37 is slightly higher, due to better match between subcell currents.



Fig.8. JV characteristics of $GaAs_{1-x}P_x/Si$ tandem cells (x=0, 0.17, 0.29 and 0.37) with optimum SLARC and $GaAs_{1-x}P_x$ absorber layer thicknesses with $GaAs_{1-x}P_x$ lifetime equal to 10 ns.



Fig.9. EQE (red) and Reflectance (blue) curves for 1 $\mu m~GaAs_{0.71}P_{0.29}$ /Si tandem cell with 75 nm Si_3N_4 SLARC (full line) and 75 nm SiO_2 / 60 nm Si_3N_4 DLARC (dashed line). GaAs_{0.71}P_{0.29} lifetime equals to 10 ns.



Fig.10. JV characteristics $GaAs_{0.71}P_{0.29}/Si$ of top, bottom and tandem cell for 75 nm Si_3N_4 SLARC (full lines) and 75 nm $SiO_2 / 60$ nm Si_3N_4 DLARC (dashed lines). $GaAs_{0.71}P_{0.29}$ lifetime equals to 10 ns.

Best preforming cell, with 1 µm thick GaAs_{0.71}P_{0.29} absorber, is further improved by using optimized 75 nm SiO₂/ 60 nm Si₃N₄ DLARC. Figure 9 shows comparison of reflectance and External Quantum Efficiency (EQE) for 1 µm thick GaAs_{0.71}P_{0.29} /Si tandem cell with 75 nm Si₃N₄ SLARC and 75 nm SiO₂ / 60 nm Si₃N4 DLARC. By using optimized SiO₂/Si₃N₄ DLARC overall reflectance is decreased, (for λ = 300-450 nm and λ > 700 nm). This results in improved spectral response of both cells, resulting in higher J_{sc} and ~1% efficiency gain, as shown in Figure 10.

IV. CONCLUSION

In summary, a simulation study was carried out in order to find the optimum ARC material and thickness for GaAs₁. $_{x}P_{x}/Si$ tandem cells. Optimum SLARC thickness is smallest for Si₃N₄ and ITO (65 -75 nm) and largest for SiO₂ (~100-110 nm). However optimum ARC thickness increased with increasing GaAs_{1-x}P_x absorber layer thickness. Furthermore, thicker ARC layer is required for cells with lower P fraction (x=0 and 0.17). The optimum $GaAs_{1-x}P_x$ absorber layer thickness increases from 250 nm for x = 0 to ~1 μ m for x =0.29 and 0.37. Maximum efficiency ~ 26.57% was achieved for cells with x=0.29 with optimized SLARC (75 nm Si_3N_4) and absorber layer thickness (~1 µm). For all P fractions, maximum efficiency was achieved for 65 - 75 nm thick Si₃N₄ SLARC. Finally, efficiency for ~1 µm GaAs_{0.71}P_{0.29} /Si tandem cell is increased to 27.62 % by using optimized 75 nm SiO₂/ 60 nm Si₃N4 DLARC.

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