Advances in Epitaxial GaInP/GaAs/Si Triple Junction Solar Cells

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***Abstract*— Epitaxial III-V on silicon multi-junction solar cells allow to increase the conversion efficiency of single-junction silicon devices. We report progress on the development of high-efficiency GaInP/GaAs/Si triple-junction devices over the last two years. The AM1.5g conversion efficiency has been increased from 19.7 % to 22.3 %, 24.3 %, and finally a value of 25.9 % could be achieved. The improvement was enabled by a reduction of nucleation-related crystal defects in the silicon to gallium phosphide transition and a reduction of parasitic absorption within the metamorphic GaAsP buffer structure which was limiting the current in the silicon subcell. By increasing the bandgaps in the graded buffer structure, a ~2x reduction of the threading dislocation density was observed and the short-circuit current density increased by 22 % relative. A majority barrier was identified and could be suppressed to obtain a new record conversion efficiency of 25.9 % with an open-circuit voltage of 2.647 V, a short-circuit current density of 12.2 mA/cm² and a fill factor of 80.2 %.**

Keywords—III-V on Si, multi-junction solar cells, MOVPE

I. Introduction

Tandem solar cell devices are known to achieve the highest conversion efficiencies. Combinations of III-V or perovskite top absorbers with silicon are currently investigated for high performance terrestrial PV applications. Both perovskite/Si and III-V/Si tandem cells have already surpassed the conversion efficiency of the best Si single-junction solar cell [1]. However, differences are found in stability which is in favor of III-V tandems and cost which is in favor of perovskite tandems. Essig et al. achieved an efficiency of 35.9 % for a mechanically stacked GaInP/GaAs/Si triple-junction cell in four-terminal operation mode [2]. For a two-terminal configuration the highest value of 34.1 % was enabled by direct wafer-bonding of GaInP/AlGaAs and Si solar cells by Fraunhofer ISE [1]. However, both fabrication techniques rely on the use of a GaAs substrate for the lattice matched growth of the GaInP/(Al)GaAs upper cells. This leads to high costs unless the substrate can be recycled many times, which is yet to be demonstrated. Direct epitaxial growth of the III-V materials onto the silicon bottom cell avoids additional III-V substrates, simplifies the process flow and therefore has better chances to reach the cost targets of 1-sun terrestrial PV. The main challenge of this approach is the lattice mismatch of ~4 % between GaAs and Si for the case of a GaInP/GaAs/Si triple-junction device. It leads to the formation of misfit and threading dislocations which limit the diffusion length for minority charge carriers in the III-V absorber layers. The transition from the non-polar Si to the polar III-V crystal easily induces additional defects like anti-phase domains, and the difference in thermal expansion coefficients between III-V materials and silicon can lead to the formation of cracks. In 2017, the authors demonstrated a Gen I GaInP/GaAs/Si device featuring a conversion efficiency of 19.7 % [3] which was followed by an improved Gen II design with 22.3 % conversion efficiency in 2019 [4]. In this work we show the individual improvements which enabled this increase and present recent advances which led to Gen III and Gen IV triple-junction solar cells with verified record conversion efficiencies of 24.3 % and 25.9 % under AM1.5g spectral conditions.

II. Experimental Approach

The Si bottom cells have been prepared by an *ex-situ* phosphorous diffusion or implantation process on 100 mm boron-doped float-zone Si substrates with a resistivity of 1-5 Ωcm (Gen I, II, III) or 12-28 Ωcm (Gen IV). The [001] oriented surface is miscut by 2° (Gen I, II, III) or 6° (Gen IV) towards (111) to ease the formation of double-steps on the surface. The GaP nucleation on Si is carried out in a CRIUS CCS MOVPE reactor from AIXTRON using a flow-modulated epitaxy process with TBP and TEGa as precursors. Details of the nucleation process are published elsewhere [5]. The growth of the step-graded $GaAs_yP_{1-y}$ (Gen I, II) or $(Al_x)Ga_{1-x}As_yP_{1-y}$ (Gen III, IV) buffer, consisting of 14 layers with a thickness of 160 nm respectively and homogeneous composition steps, was performed in a separate process in the CRIUSS CCS reactor. For the Gen III & IV devices aluminum was added in the last 5 layers to keep the bandgap of all individual buffer layers above 1.8 eV. The following $Al_xGaIn_{0.04}As$ overshooting layer (x=0.1 for Gen I & II, x=0.3 for Gen III & IV) and GaInP/GaAs dual-junction structure including two tunnel junctions were

deposited in a G4-TM reactor from AIXTRON. The thicknesses of the active absorber layers have been optimized from Gen I to Gen IV with the aim to achieve current matching among the subcells. The solar cells were characterized under calibrated AM1.5g spectral conditions in the Fraunhofer ISE CalLab.

III. Results and Discussion

In figure 1 the IV-characteristics of the triple-junction GaInP/GaAs/Si solar cells under AM1.5g conditions are shown.

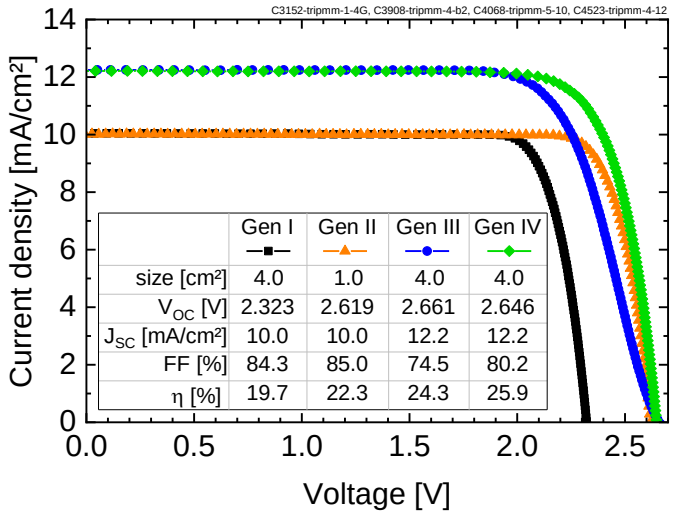

Figure 1: IV-characteristics of the GaInP/GaAs/Si triple-junction solar cells under calibrated AM1.5g spectral conditions.

The open-circuit voltage increase by 296 mV from Gen I to Gen II can be attributed to the following changes. The dopant concentration in the n-Si emitter has been increased significantly leading to a reduction of its sheet resistivity from 120 Ω/sq to 20 Ω/sq. As the recombination velocity at the GaP/Si interface was found to be high (>10^5 cm/s) [6], the higher-doped emitter leads to an increased voltage output of the Si bottom cell by ~+80 mV to ~630 mV (extrapolated from subcell voltage data). The composition of the GaInP top cell has been modified in Gen II (& III,IV) to achieve better lattice matching which resulted in an increased bandgap (~+30 meV). The remaining ~185 mV difference in open-circuit voltage at AM1.5g conditions can be attributed to the threading dislocation density (TDD) which could be reduced from 1.4×10^8 cm^{-2} to 2.2×10^7 cm^{-2}. This improvement was enabled by an extensive analysis and optimization of the GaP nucleation layer. It was found that during the pulsed GaP growth a high density of crystal defects (~10^8 cm^{-2}) like stacking faults, stacking fault pyramids and stacking fault trapezoids is formed. It was found that they act as blocking sites for dislocation glide and thus lead to an increased TDD. By optimizing the GaP nucleation process, the density of stacking fault pyramids could be decreased by three orders of magnitude to <10^5 cm^{-2}. From Gen II to Gen III the parasitic absorption in the $GaAs_yP_{1-y}$ step graded buffer structure was reduced by increasing the bandgap of each individual layer to ≥1.8 eV. This was achieved by adding the corresponding aluminum content up to a concentration of $Al_{0.29}Ga_{0.71}As$ for the last layer. The reduced parasitic absorption led to an increase in short-circuit current density of +2.2 mA/cm². Additionally, we found a decrease of the TDD by a factor of ~2× compared to the non-Al-containing buffer structures both on GaP and on GaP/Si substrates. As a result the V_{OC} increased slightly from Gen II to Gen III. However, as can be seen in figure 1 the IV-characteristics of the Gen III device show a charge carrier transport issue starting at $V=V_{OC}$, limiting the fill factor and thus the efficiency. It was found that this was caused by a majority barrier which was induced by the oxidation of the final $Al_{0.29}Ga_{0.71}As$ layer of the graded buffer structure before being overgrown with the GaInP/GaAs cell structure in a different reactor. For the Gen IV device the oxidation was successfully suppressed and no sign of charge carrier transport issues is observed, enabling a conversion efficiency of 25.9 % for the 4 cm² solar cell under AM1.5g conditions.

Figure 3 shows the external quantum efficiency of the latest Gen IV cell with integrated current densities (@AM1.5g) for each subcell. The orange dots depict the sum of the individual EQEs. For comparison, the current densities of the Gen I,II,III cells are listed in table 1.

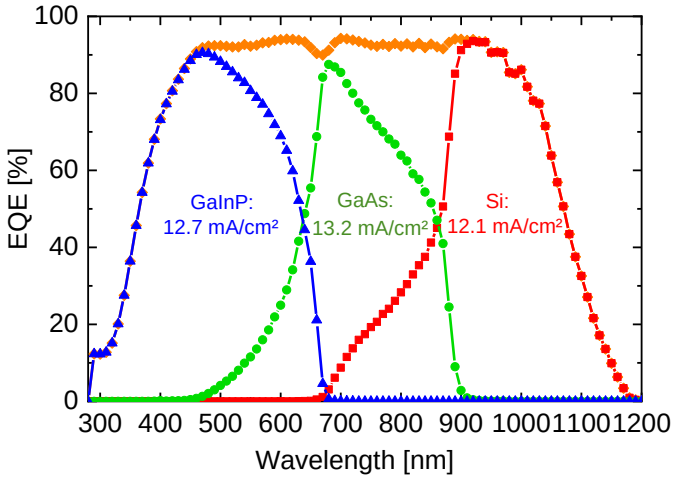

Figure 2: External quantum efficiency (EQE) of the latest Gen IV GaInP/GaAs/Si triple-junction solar cell. Stated current densities have been calculated for the AM1.5g spectrum.

Table 1: Calculated subcell current densities in mA/cm² for the triple-junction solar cells under AM1.5g conditions.

	Gen I	Gen II	Gen III	Gen IV
Si bottom cell	10.0	10.0	12.3	12.1
GaAs middle cell	11.1	12.8	12.2	13.2
GaInP top cell	13.0	12.2	12.6	12.7
Sum	34.1	35.0	37.1	38.0

The sum of the EQEs in figure 2 (orange) peaks at 94 % and does not show any sign of parasitic absorption in the range from 700 nm to 950 nm. The GaInP and GaAs subcells show an enhanced quantum efficiency compared to the previous

generations due to adjustments in the cell structure to account for the high TDD. The distribution of the currents is non-optimal and can be improved in future devices, opening the potential for >27 % conversion efficiency.

IV. Conclusion and Outlook

Recent developments of epitaxial triple-junction GaInP/GaAs/Si solar cells at Fraunhofer ISE have been presented. A new AM1.5g record conversion efficiency of 25.9 % has been achieved by improving individual components of the device. A reduction of nucleation-related crystal defects enabled an increase of >300 mV in V_{OC} and the reduction of parasitic absorption within the structure resulted in a 22 % relative increase in short-circuit current density. Future triple-junction solar cells can achieve >27 % by improving the current matching.

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