Triple-Junction Solar Cells (TJ-SC) – Support from MOCVD for Competitiveness through Improved Material Quality and Cost Reduction

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Abstract

Layer structures relevant for the growth of TJ-SC are being grown using a Metal-Organic Chemical Vapor Deposition (MOCVD) system. Advanced flow tuning using a three-fold inlet head is explored with focus on the performance at high growth rates.

INTRODUCTION

The increasing cost of fossil fuels and the threat of global warming from carbon-dioxide emissions in the long run demand alternative sources of energy generation. Solar cells demonstrating appropriate efficiency for space applications were developed and successfully used many years ago. Increasing efficiencies and the use of concentrating optics developed over the years made the solar cell panel more attractive as an alternative source of power supply for terrestrial applications as well. But this is still not sufficient for the solar cell to be competitive today against fossil resources. Further approaches for all involved disciplines in the device production process are necessary.

The key parameters for a cost reduction are the use of larger substrate sizes, the increase of precursor efficiency, the amount of user interaction and the reduction of the cycle time between subsequent production runs. Apart from the general requirements of high uniformities of all deposited layer properties, the durability and long-term stability of the reactor hardware (reactor inlet, ceiling, susceptor surface and exhaust) are of paramount interest, since the reactor cell will remain closed during the operator-free automated loading and unloading process.

NUMERICAL SIMULATION

Comprehensive simulation by computational fluid dynamics (CFD) was employed to optimize the reactor’s inlet area. A more flexible three-fold gas inlet with a group-III metal-organics inlet for Tri-Methyl-Alkyls (e.g. Alkyls of Ga, In or Al (TMGa, TMin, TMAl) sandwiched between upper and lower group-V hydride inlets for PH3 or AsH3 was designed. Fig. 1 shows a CFD-simulated flow field velocity pattern with unperturbed and parallel laminar flow. By adjusting the flows on the upper and lower group-V inlet an improved steering of the source reactants towards the growth surface is predicted.

This flow tuning also has a direct impact on the uniformity of the growth rate on the rotated wafer satellite. In addition to the total flow in the reactor, it offers an additional and independent degree of freedom for the tuning of the uniformity.

Fig. 2 shows numerically simulated growth rate profiles across the diameter of a 220 mm large wafer satellite. Four different upper/lower flow ratios QU/(U+L) of PH3 were calculated (0%, 15%, 30% and 50%). As can be seen the growth rate profile, and consequently the thickness profile, can be tuned from convex (QU/(U+L) = 0%) to concave (QU/(U+L) = 50%). It follows from reasoning that; thus, an optimum flow condition exists at which the uniformity is best.

EXPERIMENTAL VERIFICATION OF FLOW TUNING CAPABILITY

The above explained uniformity tuning by varying the
upper/lower inlet PH₃ ratio \(Q_{U/(U+L)}\) between 0% and 75% while keeping all other gas flows constant a clear effect on the growth of GaInP could be observed in experimental results. For instance the standard deviation of the thickness uniformity could be varied from 10% \(Q_{U/(U+L) = 0}\) down to 1% \(Q_{U/(U+L) = 50}\). This is accompanied by a photoluminescence uniformity yield improvement of up to 96% \(Q_{U/(U+L) = 20}\); measured area within \(\pm 1.5\) nm related to the target wavelength) and a monotonous decrease of the XRD-measured misfit from 190 ppm down to 30 ppm \(Q_{U/(U+L) = 75}\). These results show that the variation of \(Q_{U/(U+L)}\) provides an additional handle on thickness and Ga/In composition tuning independent from the TMGa/TMIn-ratio in the gas phase or the group-III total flow. This is especially important for the growth of strained materials commonly applied in TJ-SC grown on Ge.

For all further experiments \(Q_{U/(U+L)}\) was set to approx. 30%. By employing standard methods of flow tuning for GaInP a standard PL wavelength deviation of \(\sigma_\lambda = 0.59\) nm \((\lambda_{\text{mean}} = 659.5\) nm) was found and the intensity uniformity was 3.9%. The growth of \(Al_{0.14}GaInP\) material under similar growth conditions yielded \(\sigma_\lambda = 0.66\) nm at \(\lambda_{\text{mean}} = 598.3\) nm and an intensity uniformity of 10.9%. The standard deviation of the thickness uniformity was \(\sigma_t = 0.62\)% at a total thickness of 1.643 \(\mu\)m and a growth rate of 2.4 \(\mu\)m/h. The XRD peak of the \(AlGaInP\) material across the wafer varied from 1442 ppm (flat position) through 1443 ppm (center) to 1551 ppm (anti-flat position).

**LARGER WAFER SIZES**

The scaling to larger wafers, e.g. in the 5x8 inch configuration, requires special attention to the management of strain in the grown layer structures, as strain leads to wafer bow. This, in turn, can cause the wafer to lift up from the heated satellite. We will report on in-situ technologies and heating concepts to counter these effects. However, preliminary results using four 2 inch wafers across the diameter of the 8 inch satellite allowed an estimate of the transferability of the above mentioned results to 8 inch. For \(Al_{0.14}GaInP\) a max-min spread of the PL wavelength of \(\Delta\lambda = \pm 1.05\) nm at \(\lambda_{\text{mean}} = 605\) nm was achieved using 2 inch wafers. Similar results will be presented for other TJ-SC relevant layers.

**HIGH GROWTH RATES**

Another aspect of cost efficient production of TJ-SC is the growth rate of certain layers such as InGaAs. Fig. 3 shows experimental growth rate results determined from WLI measurements as a function of the group-III total MO flow varied between 138 \(\mu\)mol/min and 2944 \(\mu\)mol/min while keeping the indium to gallium ratio constant. The reactor total pressure was kept constant at 50 mbar. As can be seen the growth rate of the InGaAs material increases linearly with molar flow up to 15.2 \(\mu\)m/h.

The layer grown at 14.8 \(\mu\)m/h (see arrow in Fig. 3) was measured by XRD to determine its composition and crystalline quality. Fig. 4 shows an \(\Omega/2\Theta\) scan. The layer peak “L” and the substrate peak “S” can be seen. The layer peak “L” exhibits a Full-Width at Half Maximum (FWHM) of 16.95 arcsec indicating good layer quality for a 2.14 \(\mu\)m thick layer. The peak separation was measured to be -120.5 arcsec indicating an In-composition of 1.3% assuming a relaxed layer.

![Fig. 3: InGaAs growth rate as a function of group-III molar flow rate (symbols: experimental values determined by WLI; dotted line: trend line).](image)

![Fig. 4: XRD \(\Omega/2\Theta\)-scan of a 2.14 \(\mu\)m thick InGaAs layer grown at 14.8 \(\mu\)m/h.](image)
the growth of GaN. As can be seen, a linear increase of the growth rate of GaN was measured up to 9.5 µm/h for a total pressure of 200 mbar. Above 9.5 µm/h a roll-off of the growth rate can be seen (last data point of the 200 mbar trace in Fig. 5). This roll-off is more pronounced and starts at lower growth rates for the 400 mbar and 600 mbar cases, respectively (see Fig. 5). In the 600 mbar case even a decrease of the growth rate can be observed for high TMGa molar flows.

The dependencies suggest that gas-phase pre-reactions before the leading edge of the wafer set in when TMGa is abundant, thus depleting the total amount of TMGa available for direct growth on the wafer further downstream. The observed decrease of the growth rate in the 600 mbar case supports that explanation. Here the pre-reactions form particulates in the gas phase that serving as efficient (but non-preferred) nucleation centers that counteracts to any further increase regarding the supply of TMGa molecules into the reaction chamber as intended by the raise of TMGa flow-rates as established in the gas mixing system.

The nitride process, however, operates at much higher temperatures than the one established for the phosphide/arsenide regime, assumingly leading to an earlier onset of such pre-reactions due to the hotter entrance zone.

These comparative studies suggest that the growth rate also in the solar-cell process can not be raised infinitely. However, since this is a solely physico-chemical process dependent only on total pressure and amount of group-III and group-V precursors in the gas phase, it should be largely independent of the reactor type.

for AlAs/GaAs and GaInP, respectively. The TMAI and TMIn efficiencies were measured to 37.8% and 34.2% for the respective layers. For the 60x2 inch configuration an increase of the utilization efficiency of 1.3% on average for all precursors could be found. This is attributed to the increased coverage of wafers on the susceptor area.

CONCLUSIONS

The growth of TJ-SC related layers was shown in a novel and specially designed growth system. The introduction of the triple inlet already production-proven in nitride LED applications led to an additional degree of freedom in the flow tuning for the solar cell MOCVD reactor. Growth rates as high as 15.2 µm/h were achieved without any roll-off in linear dependency on the group-III molar flow. However, comparative studies conducted in the much hotter nitride process suggest that the growth rate can not be increased infinitely due to the onset of gas phase reactions.

The high growth rate in conjunction with group-III precursor efficiencies of about 40%, 37.8% and 34.2% for TMGa, TMAI and TMIn, respectively, facilitate a further decrease of the cost of ownership for the mass-production of terrestrial TJ-SC hopefully also contributing to the reduction of carbon-dioxide emission in the future.

ACRONYMS

CFD: Computational Fluid Dynamics
FWHM: Full-Width at Half Maximum
MO: Metal-Organic
MOCVD: Metal-Organic Chemical Vapor Deposition
PL: Photoluminescence
TJ-SC: Triple-Junction Solar Cell
TMAI: Tri-methyl-aluminum
TMGa: Tri-methyl-gallium
TMIn: Tri-methyl-indium
WLI: White Light Interference
XRD: X-Ray Diffraction

HIGH MATERIAL UTILIZATION

The material utilization was measured using AlAs/GaAs and GaInP test structures. For TMGa a utilization efficiency of 42.7% and 39.9% was measured...