Advances in preparing III-V multi junction solar cells

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***Short-Abstract*—Heterointerfaces are often the crucial part of high-performance optoelectronic devices. Examples are critical interfaces of multi junction solar cells, III-V on Si(100), or III-V on Ge(100). Until recently, III-V-compound based triple-junction solar cells demonstrated the highest conversion efficiencies worldwide reaching almost their practical limit. Thus, meanwhile research is also addressing four to five junction solar cells and lately a four-junction configuration with optimized band gaps including GaInP/GaAs and InGaAsP/InGaAs tandem cells has been realized yielding a new record efficiency of 44.7%. The paper discusses issues of critical epitaxial, MOVPE-based preparation and analysis routes including atomic scale control and minority carrier lifetime analysis.**

Since III-V semiconductor concentrator solar cells grown by metal organic vapor phase epitaxy (MOVPE) become actually more and more attractive for terrestrial applications, it is a major issue to increase efficiency and to reduce costs. Late, triple-junction solar cells based on III-V absorbers have displayed the highest solar-electric conversion efficiencies beyond 44%. However, they are finally reaching their practical limit [1] and, hence, research is also focusing towards multijunction solar cells involving more than three subcells. As of late, a four-junction configuration with optimized band gaps has been realized consisting of a GaAs-based GaInP/GaAs top-tandem that has been combined with an InP-based InGaAsP/InGaAs bottom-tandem cell (see Fig.1) via direct wafer bonding of the two tandems yielding a new record efficiency of 44,7% and having the potential to reach 50% and more [2]. Based on the latter two absorber materials, InGaAsP and InGaAs, a new low bandgap tandem solar cell with optimized bandgaps has been developed [3]. Since the diffusion length and thus the minority carrier lifetime is one of the key material parameters that determine solar cell performance, we report on suitable microscopic analysis and nondestructive time resolved photoluminescence (TRPL) measurements to identify the dependency on bulk and critical interface quality of the MOVPE-grown layers. We investigated the effect of different preparation routes for crucial interfaces on the abruptness, atomic configuration, lifetime, interface recombination velocity and its lateral interface homogeneity. Therefore, in situ monitoring and ultrahigh-vacuum (UHV)-based characterization was applied, and TRPL was correlated and and measured at double hetero structures (DHS) embedded between barriers such as $In_{0.53}Ga_{0.47}As$/InP. Another major issue of high-performance opto-electronics and multi junction solar cells is the delicate interface preparation of III-V-materials on IV-valent substrate materials, i.e. Ge(100) and Si(100). The handling of Ge(100)- based high-performance devices shows impressively that the common task, i.e. growing successfully polar III-V material on non-polar templates, can work out rather perfectly, even though the microscopic III-V/Ge(100) nucleation and its interface formation has not been described in detail so far and will be discussed in the paper. Triple junction solar cells with ultimate performance, can be grown with III-V compound semiconductors on Ge(100) substrates employing MOVPE on the highest level. A great landmark for solar cell-relevant breakthrough technologies is the merge of silicon and III-V technologies. This historic problem is still not solved, and even though a lot of studies of Si surfaces prepared in UHV have been published in the past, the challenge is the growth of III-V compounds on Si(100) surfaces without significantly deteriorating the opto-electronic properties of the III-V material. It is getting even more difficult, when regarding device structures prepared in MOVPE ambients, as the knowledge for these interfaces is much less and preparation conditions are more complex than in UHV due to the impact of hydrogen and other ingredients in the MOVPE-gas phase.

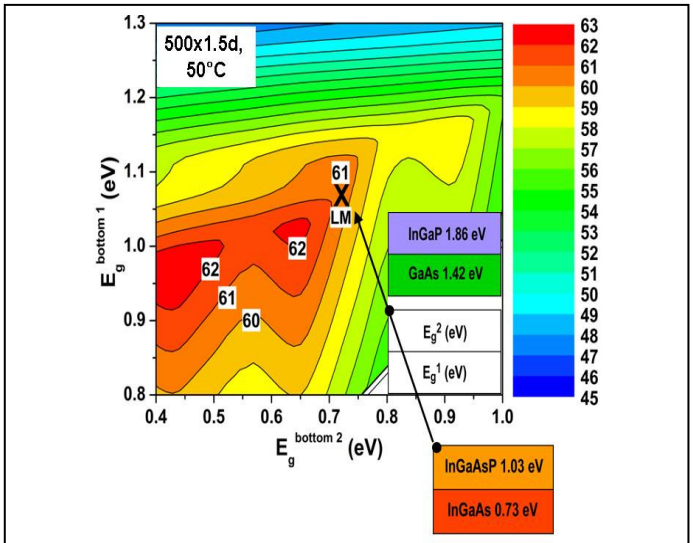

Fig.1 C*alculated limiting conversion efficiencies for an ideal 4-junction solar cell corresponding to an InGaAsP / InGaAs bottom tandem cell that has been realized under a InGaP / GaAs top cell via wafer bonding [2].*

Samples were prepared in an specific AIX-200 MOVPE reactor that is equipped with a LayTec EpiRAS 200 RA spectrometer and a contamination-free MOVPE-to-UHV transfer [4] that allows for photoemission measurements (XPS/UPS), low energy electron diffreaction (LEED), Fourier transform IR spectroscopy (FTIR, Bruker) and scanning tunneling microscopy measurements. Layer structures were grown employing trimethylindium (TMIn), triethylgallium (TEGa), tertiarybutylarsine (TBAs), and tertiarybutylphosphine (TBP) as III-V precursors, diethylzinc (DEZn) for p-type, and ditertiarybutylsilane for n-type doping.

Based on the thermodynamical detailed balance theory, a routine for calculating the limiting efficiencies and optimum band gap energies of multijunction solar cells can be applied [5]. It shows that the conversion efficiency of triple junction solar cells can be improved significantly if its bottom subcell is replaced with a more efficient tandem (two-junction) III-V solar cell as it was recently realized by wafer bonding [2]. The resulting four-junction configuration with optimum band gaps is displayed in Fig.1 and could principally be realized by means of grading, spectral beam splitting, mechanical stacking, or wafer bonding. For this purpose, low band gap InGaAsP/InGaAs tandem solar cells (1.03 eV, 0.73 eV) were grown monolithically and lattice-matched to InP (100) wafers. The two subcells were connected by a tunnel diode, which was composed of thin and highly doped n++-InGaAs and p++-GaAsSb layers. By means of surface sensitive measurement methods like RAS and LEED, a reproducible procedure was developed to prepare three different surface reconstructions {(4×3), (2×4) and (4×2)} on the InGaAs surface. XPS measurements showed that the growth of the thin GaAsSb layers on the As-rich, (4×3)-reconstructed InGaAs surface led to a much too low Sb-content in the first monolayers of the InGaAs/GaAsSb interface formation. Therefore, sharper InGaAs/GaAsSb interfaces in the tunnel junction were achieved when the GaAsSb layer was grown on the III-rich {(2×4) or (4×2)} InGaAs surface.

Via our experimental strategy, the MOVPE-growth of silicon and germanium and its (100) surface preparation have been studied in detail and approaches of growing III-Vs on Ge(100) have been compared to those of nucleating III-Vs on Si(100). One of the fundamental problems for III-V-on-Si growth relates to the difference in atomic structure which manifests itself in the polarity of the III-V material as opposed to the non-polar nature of the silicon substrate. As a consequence, the step structure of the substrate is vital for defect-free heteroepitaxy, with single layer steps on the substrate initiating anti-phase disorder in the III-V material, while a double-layer stepped substrate in principle enables anti-phase-free III-V growth. While UHV preparation of double-layer stepped Si(100) is well established, less is known about comparable preparation methods in the hydrogen-based MOVPE environment. Considered energetically least favorable on both the clean and the monohydride-terminated Si(100) surface, single domain surfaces with double layer steps in the unusual D_A configuration were recently prepared in MOVPE ambient. The D_A step formation in CVD ambient is suggested to originate in vacancy generation and diffusion on the terraces accompanied by preferential annihilation at the step edges. Here, we investigate Si removal and vacancy formation on Si(100) substrates with large terraces under CVD preparation conditions.

With in situ reflection anisotropy spectroscopy, we directly observe the domain formation in dependence of the preparation route. Oscillations in transient RAS measurements indicate layer-by-layer Si removal during annealing in hydrogen. Based on scanning tunneling microscopy results, we conclude that vacancy island formation and anisotropic expansion preferentially in parallel to the dimer rows of the terraces explains the layer-by-layer Si removal process. Afterwards, we studied the GaP/Si(100) interface formation *in situ.* Here, we can control and direct dimer orientations at the Si(100) surface by changing process conditions and in situ control and thereby choose the sublattice orientation of the GaP epilayers. Correlation of Si and P dimer orientations together with DFT calculations support an abrupt interface model with Si-P bonds (Fig.2).

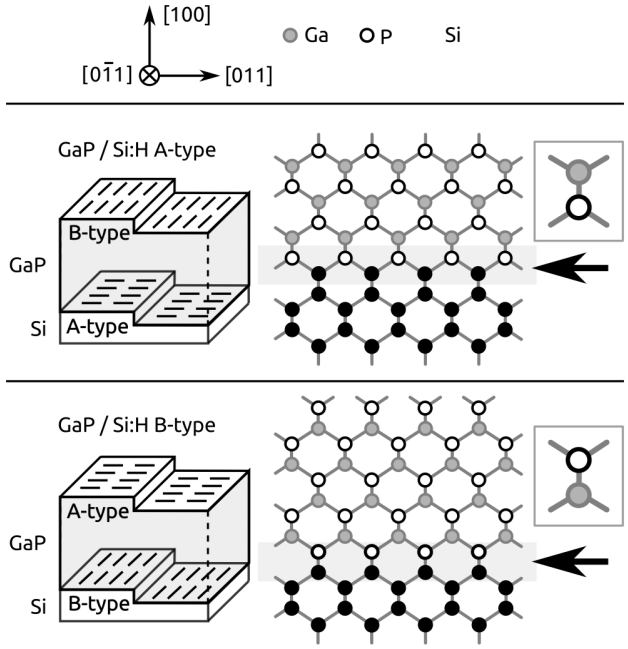

Fig.2 Interface structures for the abrupt interface model. The sublattice orientation (deduced from the P dimer orientation) is shown in the insets. Correlation to the Si dimer orientation prior to nucleation implies Si-P bonds both for growth on A-type and B-type Si(100).

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