"Reflection difference spectroscopy for the improvement of interfaces of a III-V multijunction solar cell"

U. Seidel[1], H. Döscher[1], N. Szabo[1], B.E. Sağol[1], B. Kunert[2], K. Volz[2], W. Stolz[2], K. Schwarzburg[1], T. Hannappel[1]

[1]Hahn-Meitner-Institute, Solar Energy (SE-4), Glienicker Str. 100, Berlin D-14109 Germany
[2]Philipps-Universität, Hans-Meerwein-Strasse 100, D-35032 Marburg, Germany

A next generation multijunction cell with four or more junctions and optimized band gaps is expected to break the present record efficiency surpassing the 50% mark. For that, the required low band gap combinations containing a band gap around 1eV are still to be improved [1]. We have developed a low band gap tandem solar cell lattice matched to InP. For the top and bottom subcells InGaAsP (Eg = 1.03 eV) and InGaAs (Eg = 0.73 eV) were utilized, respectively. A new interband tunnel junction was used to connect the subcells, including thin and highly doped layers of n-type InGaAs and p-type GaAsSb.

Typical deposition conditions in the metal-organic chemical vapour deposition (MOCVD) reactor require optical in-situ techniques instead of e.g. probing with electron beams. In our work, the delicate MOCVD preparation of critical interfaces was monitored with in-situ reflectance difference/anisotropy spectroscopy (RDS/RAS). RDS probes the normalized difference of reflection of light polarized in two perpendicular directions of the surface in normal incidence geometry $\Delta r / r$ [2]. In materials with inversion symmetry the bulk does not contribute to the sample's anisotropy, in these cases causing the desired surface sensitivity of RDS. By means of RDS, a reproducible procedure was developed for preparing three different surface reconstructions on the InGaAs surface via MOCVD. After a contamination-free transfer, the RDS signals were then benchmarked in UHV with surface science techniques like LEED, XPS and STM. XPS measurements revealed that the sharpest InGaAs / GaAsSb interface was achieved, when the GaAsSb layer in the tunnel junction of the solar cell was grown on III-rich (2×4)- or (4×2)-reconstructed InGaAs(100) surfaces. The improved interface preparation had a positive impact on the overall performance of the tandem cell, where higher efficiencies were observed for the cells with the III-rich-prepared tunnel junction interfaces. Efficiencies of about 8% were achieved for the tandem solar cells below an GaAs filter without anti-reflective coatings (ARCs) [3]. These values are considerably higher than 4.6%, which was the best ever reported efficiency for a Ge subcell below GaAs.

RDS was also used for the quantification of anti-phase domains on surfaces of thin III-V films deposited onto Si(100) by MOCVD. The prospect of high-efficiency multijunction solar cells on silicon substrates has long been a dream of researchers in the field of photovoltaics. However, the integration of optoelectronic devices like high-efficiency solar cells on Si(100) substrates requires a significant reduction of the defect concentration induced by the III-V/Si(100) hetero interface. Well-ordered GaP/Si(100) surfaces formed by hetero-epitaxial deposition could potentially serve as quasi-substrates for the integration of III-V-based devices on Si(100) substrates. Here, the challenging preparation of the polar on non-polar interface is the major source of defects. Since GaP and Si are almost lattice matched to each other, the latter was studied here on pseudomorphic GaP/Si(100) films that were prepared epitaxially on Si(100). Although the crystal structures are analogous, zinc blende GaP exhibits a reduced symmetry to diamond cubic Si due to its bipolar motif.

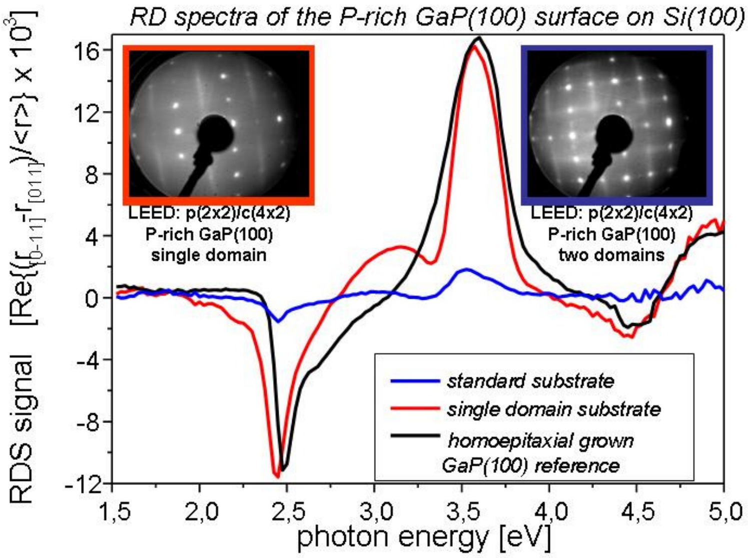

Fig. 1 *In-situ monitoring of the domain structure of GaP MOCVD-growth on Si(100)*

Inverse GaP domains are separated by odd-numbered atomic surface steps of the Si(100) substrate. By the time these anti-phase domains (APDs) adjoin, characteristic lattice defects occur and anti-phase boundaries (APBs) are formed, which, usually, propagate in growth direction. Hence, a significant reduction of defect concentration required for the fabrication of high-performance optoelectronic devices can only be achieved if anti-phase disorder is suppressed. The successful preparation of a single domain GaP/Si(100) surface was determined in-situ via the analysis of RDS peak intensities in reference to the well-known P-rich surface reconstruction of homo-epitaxially grown GaP(100) [4] (Fig.1). Both, pre-processed Si(100) substrates and MOCVD as-grown GaP/Si(100) films were also characterized ex-situ by atomic force microscopy to identify the formation of mono- and diatomic surface steps and the distribution of anti-phase domains, respectively. However, standard Si(100) surfaces typically exhibit two-domain (2x1)/(1x2) reconstructions due to alternating dimer orientation at single-atomic step edges. The energetic difference between the fundamental types of steps allows for the preparation of a single-domain Si(100) surface with di-atomic type B steps [5] in UHV. In contrast, a similar substrate preparation has not been established in the MOCVD environment. Single phase GaP/Si(100) is conceivable either starting GaP growth with a substrate surface terraced by even-numbered steps or by a procedure ensuring complete APB self-annihilation in the GaP/Si(100) buffer layer [6]. In this work, single domain GaP(100) surfaces grown on silicon substrates were realized via both preparation of preferentially single domain Si(100) and APB self-annihilation. These results show an approach how to verify the domain structure of III-V films grown on non-polar substrates on the example of GaP/Si(100) via the quantification of APDs on a macroscopic scale. Optical in-situ control with RDS was employed and the linear combination of signals of the different domains was analyzed in terms of the RDS peak intensity. These peaks well-known from former experiments and calculations can be regarded as surface sensitive fingerprints and can be employed for benchmarking domain-analysis of surfaces via homo-epitaxial prepared reference samples.

[1] A. Marti, G.L. Araujo, Sol. Energy Mat. & Sol. Cells 43 (1996) 203.
[2] D.E. Aspnes, J.P. Harbison, A.A. Studna, L.T. Florez, J. Vac. Sci. Technol. A 6 (1988) 1327.
[3] B. E. Sagol, U. Seidel, N. Szabó, K. Schwarzburg, T. Hannappel, Chimia 61 (2007) 775
[4] L. Töben, T. Hannappel , K. Möller et al., Surf. Sci. 494 (2001) L755
[5] D. J. Chadi, Phys. Rev. Lett. 59 (1987) 1691
[6] B. Kunert, I. Németh, S. Reinhard, K. Volz, W. Stolz, (2008) in print