Basic considerations, growth and interfacial issues around III-V high-efficiency solar cells

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In the meantime, the conversion efficiency of the current world record solar cell, a monolithic Ge/Ga(In)As/InGaP triple solar cell, fabricated by Spectrolab is about 39% under concentration at 236 suns, which can merely be improved insignificantly by another type of tandem or triple solar cell. Hence, the current research efforts of almost all research facilities working on III-V-PV cells with highest-efficiencies are focused on multi junction solar cells exceeding 3 sub cells, i. e. 4-, 5-, or even 6-junction solar cells, and are addressing a conversion efficiency towards 50%. Theoretical calculations show, that a band gap E_{gap} in the range of 1eV is highly desirable for solar cells with multiple junctions. The preparation of multi-junction solar cells based on the lattice constant of GaAs has either to exclude the band gap around 1 eV or to use nitrogen-containing, dilute III–V compounds like InGaAsN, which suffer from much too short diffusion lengths. In contrast, III–V semiconductors with band gaps in the range of 1 eV can be grown epitaxially on the lattice constant of InP. The challenge of material science arises here for the higher band gaps.



Figure 1: Left panel, shows the basic layer structure or rather a band scheme illustration of a InGaAs/InGaAsP low band gap tandem solar cell including a Esaki-diode-like tunnel junction. Right panel: I-V characteristic of an InGaAs/InGaAsP tandem solar cell measured under a full (blue curve) and a filtered (red curve, RG850) AM1.5g spectrum.

Nevertheless, it appears worthwhile to explore the possibilities of low band gap materials based on the InP lattice constant. A low band gap tandem and a high band gap tandem could then be combined via grading, wafer bonding, optical selection of different light energies (e.g. via a cassegrainian), etc. for preparing a high-performance multi-junction solar cell with four or more band gaps. Hence, aiming at the improvement of the conversion efficiency of a high-efficiency multi-junction solar cell different types of low band gap n/p solar cells were prepared on the lattice constant of InP via metal organic chemical vapor deposition (MOCVD) using only less-toxic, non-gaseous, so-called alternative precursors. New absorber materials were introduced on the lattice constant of InP and were compared to more established materials. In a next step these low band gap sub cells were combined to grow a

low band tandem solar cell involving band gaps around 0.7 and 1 eV and involving a new Esakidiode-like GaAsSb-InGaAs tunnel junction (Fig.1).

Another issue is the replacement of the expensive III-V-wafer by much cheaper Si substrates, which also combines III-V advantages with the mature Si-technology in general. Arsenic-terminated Si(100) surfaces have received as a potential substrate for subsequent III-V epitaxy and have been used to prepare thick (> 2μ m) state-of-the-art InP films on exactly oriented Si(100). In collaboration with NREL, clean, As-terminated Si(100) interfaces were prepared and theoretically modeled. Preparation was performed with H₂ carrier gas and AsH₃ and TBAs as precursors in our and in the NREL MOCVD reactors. InP(100) films were grown on Si(100) at HMI, TU Braunschweig, and NREL and film quality and interfaces were characterized with different techniques, i. e. in-situ RDS, STM, LEED, XPS, AES, and ex-situ XRD. The results were compared to each other, in particular with regard to the preparation of Si(100) single domain interfaces during nucleation prior to growth of InP. Issues are lower defect density for solar cells, reduced growth temperature, anti phase domains, reduced impurity concentration. In this regard, an STM and theoretical study was performed discovering an entire family of nano-scale trenches, ridges and steps that has been observed on AsH₃and TBAs-exposed Si(100) (Fig.2). These lines are very long and straight, and could even serve as templates for nanowires. Theoretical modelling shows that they are all built around a stress-relieving 5-7-5- ringed structure in which two 5-atom rings bracket a central 7-atom ring (Fig.3). These Asterminated surfaces were finally used as starting point for growing InP on exactly oriented Si(100).



Figure 2: This surface was annealed at 725°C under 42 mtorr AsH₃. '5-7-5' line structures partially relieve tensile stress generated by As-As dimers. Four representative structures have been labeled (corresponding to Fig. 2). Shallow craters form where AsH₃-etching of a terrace converts a step into a ridge ('e4' into 'f', for example). The subscripts '4' and '8' indicate step height in monolayers (1 ML = 1.36 Å).



Figure 3: Structures 'a' -'f': (a) Bulk-like type-A trench, (b) '5-7-5' type-A trench, (c) '5-7-5' 1-ML type-A step, (d) '5-7-5' type-B trench, (e) '5-7-5' type-B step, and (f) '5-7-5' ridge. As-As dimer bonds on the left-side terrace are either perpendicular (type 'A') or parallel (type 'B') to the line structure. All surface atoms are triplybonded As (dark gray). All sub-surface atoms are quadruply-bonded Si (light gray). (g) STM image, artificially illuminated from the right. Continuity of a '5-7-5' core structure is seen where AsH₃etching of the upper terrace has converted part of a type-B step into a ridge. To better show height differences, the ratio of height to width has been increased by 72%. $V_{sample} = -2.5 \text{ V}$, $I_{tun} = 0.04 \text{ nA}$.