III-V MULTI-JUNCTION SOLAR CELLS - SIMULATION AND EXPERIMENTAL REALIZATION

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Key words: Multi-junction solar cells, numerical modelling, record solar cell

Abstract: III-V multi-junction solar cells are the state-of-the-art approach for high-efficiency photovoltaic energy conversion. Due to the structural complexity of these devices numerical modelling and simulation for analysis and optimization has found increasing attention in recent years. This work presents an overview of the modelling techniques for III-V multi-junction solar cells applied at the Fraunhofer Institute for Solar Energy Systems (ISE). These are in particular the detailed balance model used in the program "etaOpt", the numerical semiconductor simulation using Sentaurus TCAD from Synopsys as well as classical network simulations. Our latest modelling results, the capabilities of the different approaches as well as their limitations are discussed. In addition, a focus is set on a recent record triple-junction solar cell with an efficiency of 41.1 % at a concentration ratio of 454 suns. Its key design factors are indicated and it is shown in which aspects numerical modelling supported this development and what extensions will be needed in the future.

III-V večspojne sončne celice – simulacije in praktične izvedbe

Kjučne besede: večspojne sončne celice, rekordna sončna celica, numerično modeliranje

Izvleček: III-V večspojnespoje sončne celice so trenutno najboljši pristop za doseganje visoke učinkovitosti pretvorbe. Zaradi strukturne kompleksnosti teh celic se je v zadnjih letih izredno povečalo zanimanje za njihovo numerično modeliranje, simulacijske analize in optimizacijo.V članku je predstavljen pregled tehnik modeliranja II-V sončnih celic, ki jih uporabljajo na Fraunhofer Institute for Solar Energy Systems (ISE).Te tehnike so: ravnovesni model, ki ga uporablja program "etaOpt", numerične polprevodniške simulacije z uporabo programa Sentaurus TCAD od Synopsysa, kakor tudi klasične mrežne simulacije. Predstavljeni so naši zadnji rezultati, kakor sposobnosti in omejitve posameznih pristopov. Dodatno je v članku povdarek na trenutni rekordni trispojni sončni celici z izkoristkom 41.1 % pri koncentraciji 454 sonc. Predstavljeni so ključni dejavniki pri razvoju strukture, podpora numeričnega modeliranja in kakšne nadgradnje bodo potrebne v prihodnosti.

1 Introduction

Monolithically stacked multi-junction solar cells based on III-V semiconductor materials, such as the GaInP/GaInAs/Ge triple-junction solar cell, are the state-of-the-art approach for high-efficiency photovoltaic energy conversion. Consisting of stacked p-n junctions with different band gap energies, these devices can exploit the solar spectrum very profitably. Just recently an efficiency of 41.1% was achieved for a metamorphic $Ga_{0.35}In_{0.65}P$/ $Ga_{0.83}In_{0.17}As$/Ge triple-junction solar cell under the standard AM1.5d ASTM G173-03 spectrum and a concentration of 454 suns /1,2/.

A multi-junction solar cell structure consists of a high number of layers of different III-V compound semiconductor materials. Due to the complex electrical and optical interactions between the different layers, a pure experimental optimization of these sophisticated structures would be very expensive and protracted. An accurate and reliable modelling is desirable in order to accelerate the optimization procedure considerably.

In recent years the use of numerical modelling and simulation of III-V multi junction solar cells has found increasing attention. Different approaches and tools are in use. The following seem to be most common: Very prevalent is the evaluation of theoretical efficiencies for specific structures. A good overview of the different approaches is presented in Ref. /3/. Several groups use semiconductor simulation environments for the analysis and optimization of the semiconductor layer structure, e.g. /4-8/. For the optimization of the front contact grid, network simulations were repeatedly used, e.g. /9,10/. In addition, some specialized programs for solar cell modelling have been developed of which the most common ones - such as PC1D and AMPS - are reviewed in Ref. /11/. These programs have also been used for III-V solar cells, e.g. /12-14/. Thus, numerical modelling and simulation have become common methods in the development of III-V multi-junction solar cells.

At Fraunhofer ISE different simulation techniques are used for the analysis and optimization of III-V multi-junction solar cells. The aim of this paper is to present an overview of the three modelling approaches applied and to present our recent findings. The capabilities and limitations of the models are also discussed. Concerning the current status of the experimental realization the focus is set on a recent highlight, which is the development of a metamorphic triple-junction solar cell with an efficiency of 41.1% /1/ under the AM1.5d ASTM G173-03 spectrum and 454 kW/m^2. It is shown in which aspects numerical modelling supported this development and what extensions will be needed in the future.

2 Numerical modelling

The parameter space for the structure optimization of III-V multi-junction solar cells is very large. In principle, the number of subcells, the layer structure and the materials in each subcell as well as the thickness and doping level of each semiconductor layer need to be determined. In addition, the front contact grid layout needs to be optimized in respect to the designated concentration and concentrating system. Obviously an experimental procedure would be very time-consuming and expensive. However, a numerical modelling tool that is able to search the whole parameter space does not yet exist. Therefore, different modelling tools are used for the analysis of the parameter space. In the III-V group at Fraunhofer ISE three different approaches are used. The optimal number of band gaps and the ideal band gap combination is evaluated with a modelling tool described in Section 2.1, which is based on the Shockley-Queisser limit. We analyze the semiconductor layer structure with the commercially available semiconductor simulation environment Sentaurus TCAD from Synopsys (see Section 2.2). Finally, the grid design is optimized with the circuit simulator LTSpice from Linear Technology Corporation /15/ described in Section 2.3.

2.1 Ideal efficiency calculation

One of the central benefits of using III-V semiconductors as material for solar cells is the wide choice of band gaps that can be experimentally realized and stacked. A valuable guidance for finding the most efficient set is the evaluation of ideal efficiencies, which could be realized without any, but the physically inevitable losses. At Fraunhofer ISE the program "etaOpt" was developed to calculate these ideal efficiencies /16/.

2.1.1 Modelling approach

The model used in "etaOpt" is based on the detailed balance method first introduced by Shockley and Queisser /17/, i.e. only radiative recombination is considered. All subcells have an external quantum efficiency (EQE) equal to one and it is assumed that photocurrent from upper subcells can be transferred to lower ones to improve current-matching. In reality this is achieved by thinning the absorbing layers.

2.1.2 Results for triple-junction solar cells

This section focuses on triple-junction solar cells as they currently have the highest efficiencies realized for terrestrial as well as for space applications. Figure 1 shows the optimal band gap combinations for triple-junction solar cells under the extraterrestrial AM0 spectrum (1367 W/m^2, 298 K) as well as under the terrestrial AM1.5d ASTM G173-03 spectrum with a concentration ratio of 500 suns (500 kW/m^2, 298 K). Optimal band gap combinations with efficiencies above 48% (AM0) or 60.5% (AM1.5d) are marked with black dots, while the grey dots represent structures with efficiencies of 48 to 49% and 59.0 to 60.5% respectively. Due to the homogeneous extraterrestrial AM0 spectrum, a large compound field of optimal band gap combinations is formed, whereas the absorption band of atmospheric water and carbon dioxide lead to the formation of two local maxima under AM1.5d.

The band gap combinations of five specific triple-junction solar cell structures, for which efficiencies of over 40% under the concentrated AM1.5d spectrum have already been experimentally realized, are indicated: lattice-matched $Ga_{0.5}In_{0.5}P$/ $Ga_{0.99}In_{0.01}As$/Ge (LM) /18-20/; metamorphic $Ga_{0.44}In_{0.56}P$/$Ga_{0.92}In_{0.08}As$/Ge (MM1) /18/; metamorphic $Ga_{0.35}In_{0.65}P$/$Ga_{0.83}In_{0.17}As$/Ge (MM2) /1/; inverted metamorphic $Ga_{0.5}In_{0.5}P$/GaAs/ $Ga_{0.73}In_{0.27}As$ (Inv1), inverted (double) metamorphic device $Ga_{0.63}In_{0.37}As$/$Ga_{0.96}In_{0.04}As$/GaAs (Inv2) /21/. A more detailed discussion of the particularities of these designs can be found in Ref. /1/.

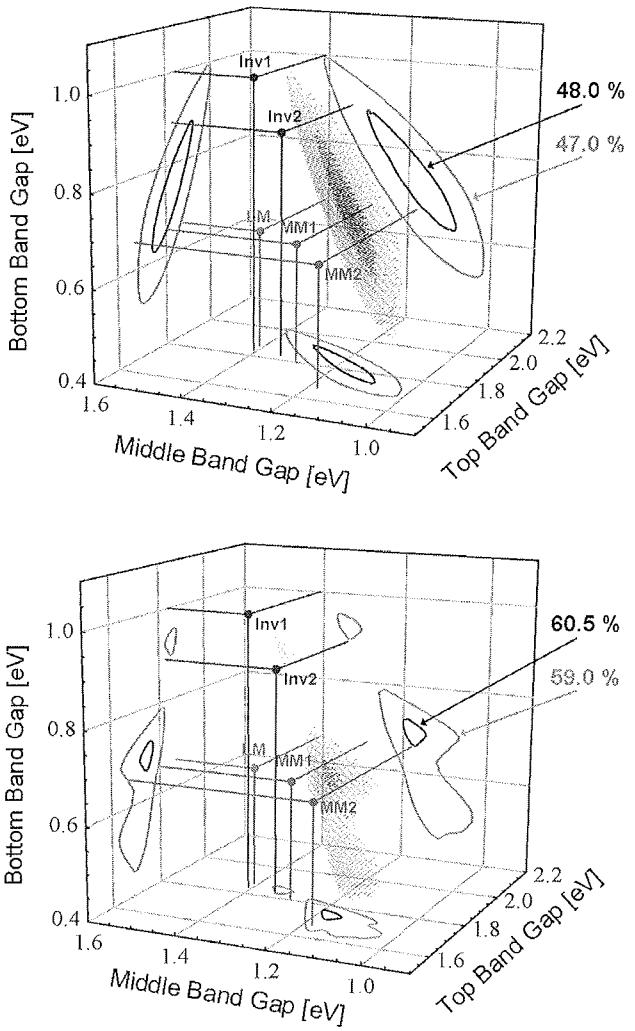

Fig. 1: Ideal efficiencies of triple-junction solar cell structures calculated with etaOpt under the AM0 (top) and the AM1.5d ASTM G173-03 spectrum with a concentration ratio of 500 suns (bottom, after Ref. /1/).

2.2 Numerical modelling of the cell structure

After the identification of the optimal band gap combinations using "etaOpt", the realistic cell structure with real material properties has to be designed. The optimization of the semiconductor layer structure is highly complex due to the high number of layers and the strong optical as well as electrical interactions between the layers. At Fraunhofer ISE the commercially available semiconductor simulation environment Sentaurus TCAD from Synopsys is used to analyze and optimize the layer structure.

2.2.1 Modelling approach

For the simulations presented here, different tools of the simulation environment Sentaurus TCAD are used. After defining the solar cell structure and meshing it with the tools Sentaurus Structure Editor and Mesh, the calculation of the optics and the electrical features are performed with the device simulator Sentaurus Device /22/.

We model the smallest two-dimensional symmetry element of the solar cell, which is constructed by a cut through the layers from cap to substrate perpendicular to the grid fingers. The element covers a width corresponding to half of the finger spacing. This ensures that series resistance effects caused by lateral current flow in the device are taken into account.

Realistic simulations with Sentaurus TCAD have two prerequisites: Firstly, the necessary models describing the occurring physical phenomena need to be implemented and validated. Of particular importance for solar cell modelling are optical interference effects, optical generation and recombination of minority carriers, carrier transport at hetero-interfaces and tunnelling effects. Secondly, material parameters such as optical constants, carrier mobilites, band gap energies, electron affinity and parameters for radiative, Auger, Shockley-Read-Hall as well as interface recombination are required for each semiconductor layer in the structure. In the following it will be shown that both prerequisites are satisfactory fulfilled for the materials used in our GaAs single-junction solar cells as well as in our lattice-matched GaInP-GaAs dual-junction solar cells. However, for other materials especially those in metamorphic III-V multi-junction solar cells the lack of material data limits the modelling capabilities.

2.2.2 Results for single-junction solar cells

In the past excellent results have been obtained for the modelling of III-V single-junction solar cells using numerical semiconductor simulation tools, e.g. /4,12,23/. Thereby, it was shown that the particular physical phenomena in III-V solar cells, such as carrier transport at hetero-interfaces as well as optical interference effects, are well described. However, the application of these relatively new models for design optimization has rarely been reported. In the following we present first optimization results for single-junction GaAs solar cells. Details about the underlying model and the material parameters can be found in Ref. /4/. Figure 2 shows a comparison between measured and simulated EQE and reflection of two GaAs solar cells with different material for the window (FSF) layer. All parameters of the solar cell except for the window layer have been identical.

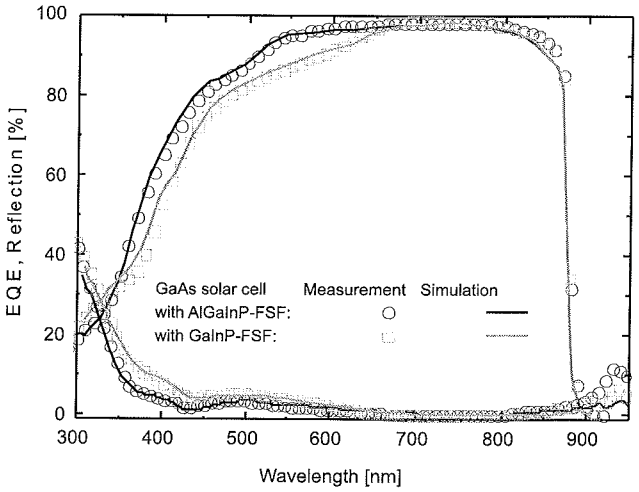

Fig. 2: Comparison between measured and simulated EQE and reflection for two GaAs solar cells with different window (FSF) layer material.

The good agreement between measurement and simulation proves the validity of the numerical model. The GaInP window layer leads to significant absorption in the short wavelength range between 300 - 650 nm and therefore reduces the EQE. This underlines the importance of a high band gap material for the window layer. After setting the material to high band gap $Al_{0.35}Ga_{0.16}In_{0.49}P$, the next task is to find the optimal window thickness and doping. Figure 3 shows based on the results of the high band gap $Al_{0.35}Ga_{0.16}In_{0.49}P$ window layer, how the efficiency of the investigated GaAs solar cell varies for different thicknesses and doping levels of the window layer. Two trends influence the optimum configuration: The window should lead to low absorption, but should also serve as a good passivation layer. The first demand favours thin window layers, whereas the second demand sets a lower boundary to the minimum thickness which is necessary for a sufficient passivation. Additionally the passivation properties are favouring high doping levels in the window material. Thus, the optimum configuration lies at high doping levels > $2x10^{18}$ cm^{-3} and a thin window layer around 20 nm.

Following a one-layer-at-a-time optimization approach, the next layer to be analyzed is the emitter. The efficiency contour plot (Figure 4) shows a plateau with quite stable efficiency values ranging from very thin but highly doped configurations to rather thick, but low doped values. The strong drop in efficiency for configurations in the upper right corner is caused by the decrease of the short-circuit current due to low diffusion lengths of the minority carriers. In contrast the drop in the lower left corner is caused by the increasing lateral sheet resistance of the emitter.

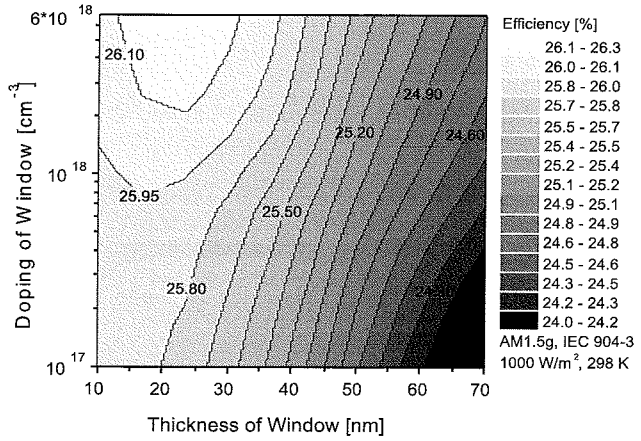

Fig. 3: Efficiency contour of a GaAs solar cell as a function of the thickness and doping level of the $Al_{0.35}Ga_{0.16}In_{0.49}P$ window layer.

These two trends are commonly observed for emitter variations. Yet, their individual strength strongly depends on the particular material parameters. The shape of the plateau is also influenced by the voltage, which shows a strong dependence on material parameters, especially on the carrier lifetime. Usually, the voltage increases with higher doping levels and lower thicknesses. However, for solar cells with very high SRH lifetime in the emitter the influence of the doping level on the open-circuit voltage can be inverted due to the increase of radiative and Auger recombination with higher doping.

It is important to note that the results of the optimization strongly depend on the material parameters of the individual cell. Of particular importance are the Shockley-Read-Hall lifetimes and the interface recombination velocities, which can vary significantly with the doping level and the growth conditions. Therefore, the results of this study are only valid for the material parameters obtained for our grown layers. It should also be mentioned that the analysis presented here uses the approach of optimizing one-layer-at-a-time, which will not necessarily lead to the global optimum for the device structure.

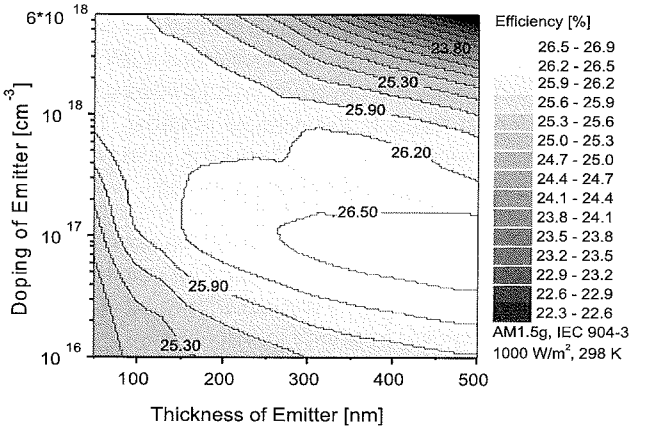

Fig. 4: Efficiency contour of a GaAs single-junction solar cell as a function of the thickness and doping level of the emitter layer.

2.2.3 Results for dual-junction solar cells

The modelling of multi-junction solar cells poses additional challenges. First, a proper and numerically stable model for the tunnel diode, which connects the subcells in series, is required. Second, the numerical complexity is highly increased due to the simultaneous computation of two or more subcells. Only few research groups have presented results on the modelling of III-V multi-junction solar cells within semiconductor simulation environments /5-8,24,25/. Recently, we presented a numerical model of a $Ga_{0.51}In_{0.49}P$-GaAs dual-junction solar cell taking into account the necessary material parameters and physical processes /8/. The theoretical modelling results were shown to be in good agreement with measurements. Figure 5 shows a comparison of the measured and simulated EQE and reflection for the investigated dual-junction solar cell.

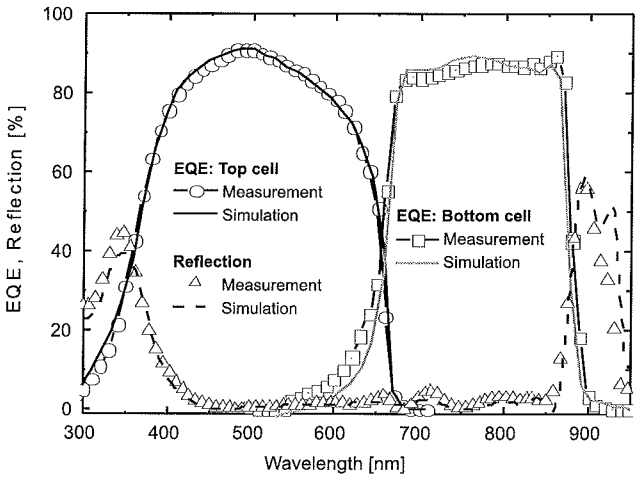

Fig. 5: Simulated and measured EQE and reflection of the investigated $Ga_{0.51}In_{0.49}P$-GaAs dual-junction solar cell agree well (after Ref. /8/).

Based on the effect of current-limitation in a series interconnected multi-junction solar cell, a special calculation method was developed to compute the quantum efficiencies of the subcells. This method follows the measurement procedure for the EQE in which appropriate bias light conditions are chosen to determine the EQE of the current limiting subcell. With the developed simulation tools specific aspects of the device behaviour can now be theoretically predicted and understood. An example is the optimization of the top and bottom cell thickness as shown in Ref. /8,25/.

2.3 Optimization of the front contact grid

As shown above, the semiconductor layer structure can be very well modelled with a two-dimensional symmetry element. Yet, for the optimization of the front contact grid such a model is not sufficient. In principle it would be possible to model and simulate a complete solar cell in all three dimensions within the Sentaurus TCAD simulation environment. However, due to the high number of mesh points necessary for a realistic model, the computational effort

would be enormous, leading to intolerable computing time of weeks or even months. Therefore, we optimize the front contact separately with an electrical network model, which will be discussed in this section.

2.3.1 Modelling approach

The IV-characteristic of a solar cell is often described with the two diode model. The lack of this model is the missing spatial distribution, thus neglecting the influence of the distributed series resistance and the perimeter effects at the solar cell surrounding. The two diode model can be enhanced by dividing the solar cell in elementary cells consisting of diodes, resistances and current sources to model the saturation currents and the photo generated current. The elementary cells are connected in parallel through ohmic resistances representing e.g. the lateral conducting emitter layer or the metal fingers. Thereby a network of electrical components is created, which describes the whole solar cell. The IV-characteristic is calculated with the circuit simulator LTSpice, which uses a SPICE (Simulation Program with Integrated Circuit Engineering) approach. More details about our network model can be found in Ref. /26/.

Compared to the modelling approach described in Section 2.2 a network model requires more integral parameters such as the short-circuit current density, the resistances of emitter and base layers, the dark current density as well as the parallel resistance. This has the advantage that most of these values can be measured or fitted directly from existing solar cell samples. Of course the obtained results are strongly connected to the particular epitaxial structure as well as to the technological processing and may differ significantly for other solar cell structures.

2.3.2 Exemplary results

The network model was validated through a comparison of measured and simulated data. The measured data was gained by a flash-lamp based system described in /27/. For the validation GaAs single-junction solar cells with the same epitaxial structure as in Section 2.2.2 were used. Figure 6 shows a good match between simulation and measurement for a concentration ratio of up to 1000 suns. The increase of efficiency caused by the increase in open-circuit voltage and fill factor is well reproduced by the simulation as well as the drop caused by the losses through series resistances. The optimum efficiency for this specific GaAs solar cell is reached at about 100 suns.

The network simulation now enables the prediction of device parameters for variations in the front contact metallization. This makes it a suitable tool for the grid optimization. Figure 7 shows the calculated dependency between efficiency and grid finger distance for the same GaAs solar cell under a concentration ratio of 100 suns. The best finger spacing turns out to be about 260 µm. For this configuration Figure 8 presents a variation of the grid finger length and an optimum is found at 760 µm.

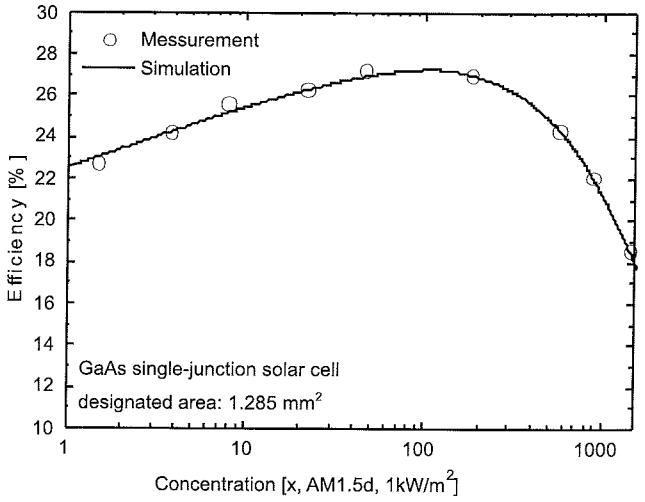

Fig. 6: Correlation between efficiency and concentration of a GaAs single-junction solar cell with an $Al_{0.35}Ga_{0.16}In_{0.49}P$ window layer.

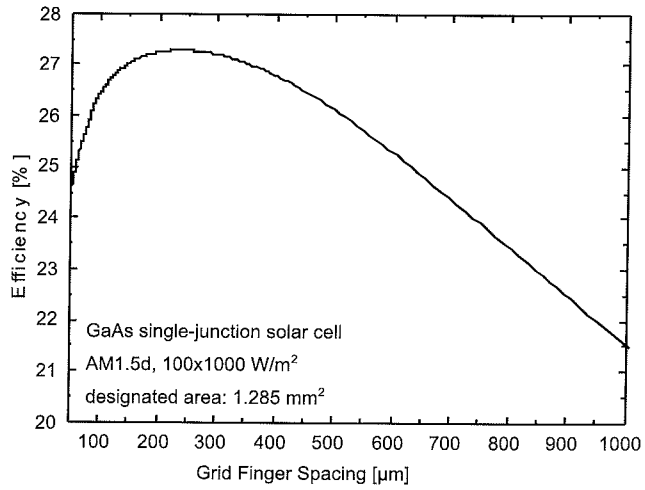

Fig. 7: Calculated GaAs solar cell efficiency as a function of the grid finger spacing.

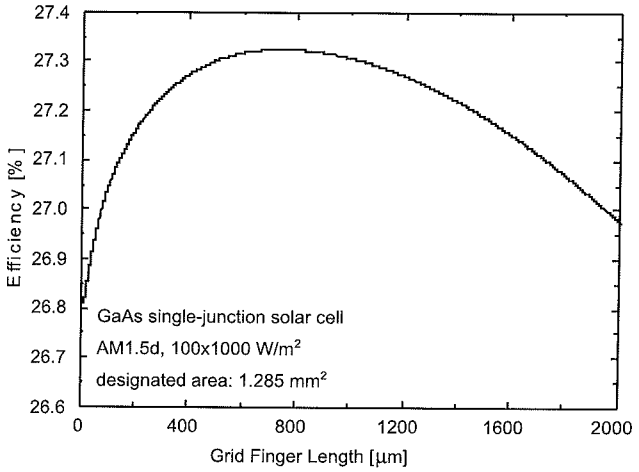

Fig. 8: Calculated efficiency as a function of the grid finger length for a GaAs solar cell.

3 Experimental realisation

After showing the current status of our modelling activities, this section focuses on the experimental realization. Although many different cell concepts are under investigation and show promising results, we are concentrating on a metamorphic triple-junction solar cell, which recently achieved an efficiency of 41.1% at 454 suns /1,2/. The fill factor and efficiency versus concentration ratio are shown in Figure 9. In the following a short description of the improvements that were made to achieve this record efficiency is given. More details about this topic were presented in Ref. /1/.

One of the key factors for the success of the metamorphic triple-junction solar cell is its nearly optimal band gap combination as indicated by the ideal efficiency calculations (Figure 1). Starting from the lattice-matched configuration (LM), the indium content in the top and middle subcells were gradually increased leading to the metamorphic configuration (MM2). In this configuration the $Ga_{0.35}In_{0.65}P$ and the $Ga_{0.83}In_{0.17}As$ subcells are grown lattice-matched to each other, but mismatched to the Ge substrate. Hence, the calculation of ideal efficiencies provided a valuable guidance during the strategical decisions of which configuration to head for.

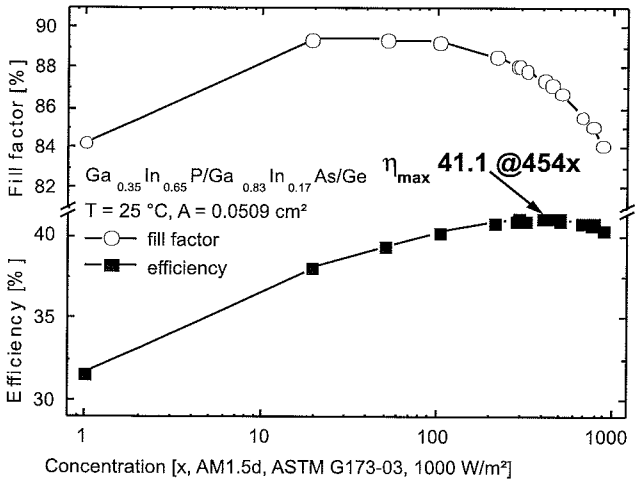

Fig. 9: Progress of fill factor and efficiency of a metamorphic $Ga_{0.35}In_{0.65}P/Ga_{0.83}In_{0.17}As/Ge$ triple-junction solar cell versus concentration level (after Ref. /1/).

However, the main assumption for the calculation of ideal efficiencies is that perfect solar cells are realised with none but the physically inevitable losses. Of particular importance is a perfect material quality, which makes it possible to neglect non-radiative recombination. Obviously in reality this assumption is rather difficult to be met. This is particularly true for metamorphic concepts as the lattice-mismatch between the subcells usually induces a high number of defects in the active solar cell layers. We overcame this limitation through the development of a novel buffer layer structure consisting of seven GaInAs layers with stepwise increasing indium content. Misfit dislocations are confined into this structural element leading to dislocation densities in the active layers of the solar cell below 10^6 cm^{-2}.

Another important factor is the optimal structure, in particular the thicknesses and doping levels of its semiconductor layers. As described above in Section 2.2 the determination of the optimal design could be facilitated through the use of semiconductor simulation environments. Although the numerical models are available the predictive capabilities of the simulation are still particularly limited for metamorphic structures due to the lack of material data. This is caused by the fact that many experimental methods for the measurement of important material data, like spectral ellipsometry or Hall measurements, require simple sample structures. Yet, such samples are difficult to realise for metamorphic materials due to the necessity of a metamorphic buffer structure. Thus, the model-based optimization of the semiconductor layers of metamorphic structures is – in contrast to lattice-matched structures – still limited to rather rough guidelines. The structure of the metamorphic triple-junction solar cell discussed here was hence optimized in a long-term experimental procedure and is certainly not ideal.

Concerning the semiconductor layer structure one of the key factors for the high performance of our metamorphic triple-junction solar cell is the tunnel diode, which achieves very high maximum tunnel current densities in the range of 15 to 25 A/cm^2. It consists of a p-doped AlGaInAs layer and an n-doped GaInP layer. Due to optimized lattice-match to the surrounding layers the generation of dislocations is avoided /1,28/.

Finally, another key factor for the structure was the optimal grid layout, which was optimized with the network model described in Section 2.3. A central factor for the grid design is the intended concentration ratio. As current concentrator systems use different concentration ratios several grids were designed and processed. Such a fine optimization and adjustment of the complex grid structure is hardly possible with only experimental investigation. This example shows that an optimised interaction between theoretical and experimental efforts is absolutely essential for the development and the realization of highest efficient solar cells.

3 Conclusions

In this work the current status and the newest results of the modelling activities for III-V multi-junction solar cells at Fraunhofer ISE are presented. It is shown that ideal efficiency calculations give a valuable guideline for the decision on which band gap combinations to realize. For triple-junction solar cells the band gap configuration of the metamorphic $Ga_{0.35}In_{0.65}P/Ga_{0.83}In_{0.17}As/Ge$ structure comes close to the global optimum. The analysis and optimization of the semiconductor layer structure can be greatly enhanced through simulations with semiconductor simulation

environments. Good modelling results have been achieved for lattice-matched single- and dual-junction solar cell structures. However, the capabilities for metamorphic structures are limited due to the lack of suitable material parameters. The third modelling approach described is network simulation for the optimization of the grid layout. This approach is highly predictive and is successfully applied for the design of contact grids for different cell structures and various illumination conditions. Concerning the experimental realization, the key factors leading to the design of a metamorphic triple-junction solar cell with an efficiency of 41.1 % at 454-fold concentration are highlighted. It is shown that numerical modelling techniques are now well established and supporting the design process of multi-junction solar cells.

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