

BOOK OF ABSTRACTS

**Workshop on Modelling of Thin Film Solar Cells
Wednesday 28 March – Friday 30 March 2007, Gent – Belgium**

Program Workshop on Modelling of Thin Film Solar Cells

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Conference site: "Het Pand", Onderbergen 1, Gent, nr. 37 on Gent map

Wednesday 28 March 2007

12h30 – 14h15: Lunch available for early arrivers

14h15 – 14h30: Welcome and Opening

14h30 – 15h50: Tutorial Session 1

- 14h30: Optical modelling of thin film solar cells and structures, Marko Topič, University of Ljubljana, Faculty of Electrical Engineering
- 15h10: Electrical modelling of thin film solar cells, Marc Burgelman, University of Gent, ELIS

15h50 – 16h10: Coffee break

16h10 – 17h30: Tutorial Session 2

- 16h10: Numerical simulation of nanoelectronic devices, Hans Kosina, Technische Universität Wien, Austria
- 16h50: Novel concepts in photovoltaics, Antonio Martí Vega, Universidad Politécnica de Madrid, Instituto de Energía Solar – ETSIT

17h30 – 18h15: Pre-presentation of the posters

Thursday 29 March 2007

9h00 – 10h50: Session 1a: Optical modelling

- 9h00: Quantum efficiency of thin film solar cells - optical modeling of short circuit current density and its spectral dependence, Aleš Poruba, J. Springer, J. Holovský, A. Purkrt, M. Vaněček, Institute of Physics, Academy of Sciences of the Czech republic
- 9h30: Optical optimisation of Ag/ZnO back reflector for NIP solar cell, Thomas Söderström, F.-J. Haug, V. Terrazoni-Daudrix, X. Niquille, S. Perregaux, C. Ballif
- 9h50: Anti-reflection layer at the TCO/Si interface for high efficiency thin-film solar cells deposited on rough LP-CVD front ZnO, Peter Buehlmann, A. Billet, J. Bailat, D. Domine, S. Faÿ, C. Ballif
- 10h10: Design of novel concepts of light management in thin-film silicon solar cell using optical simulations, Janez Krč, M. Zeman, A. Čampa, M. Topič
- 10h30: Modelling the current density increase due to "light-trapping" effect in conjugated polymer/fullerene-based bulk heterojunction solar cells, Adam Purkrt, J. Springer, A. Poruba, M. Vaněček, L. Goris, J. Manca

10h50 – 11h10: Coffee break

11h10 – 12h10: Session 1b: Optical modelling, materials oriented

- 11h10: Recombination through amphoteric states at the amorphous/crystalline silicon interface: modeling and experiment, Sara Olibet, E. Vallat-Sauvain, C. Ballif
- 11h30: Optical characterization of transparent tin oxide films deposited by CVD, Nazia Kesri, K. Sedda
- 11h50: Modeling of the near infrared reflectance spectra of LP-CVD ZnO, Jérôme Steinhauser

12h20 – 13h50: Lunch

13h50 – 15h40: Session 2a: Electrical modelling

- 13h50: Specific issues in modeling of thin-film silicon solar cells, Miro Zeman, Delft University of Technology – ECTM/DIMES
- 14h20: Design rules for surface conditioning of widegap chalcopyrite absorbers, David Fuertes Marrón, R. Klenk
- 14h40: Modelling of the effect of a buried pn-junction on cell performance in chalcopyrite thin film solar cells, Paul Pistor, R. Klenk
- 15h00: AFORS-HET 3.0: Development of a two-dimensional simulation mode, Torsten Geipel, M. Kriegel, R. Stangl, K. Lips
- 15h20: Modelling the effects of electronic parameters on the efficiency of amorphous silicon solar cells under AM1.5G spectrum, Christos Monokroussos, A. Al Tarabsheh, R. Gottschalg, A.N. Tiwari

15h40 – 16h00: Coffee break

16h00 – 17h00: Session 2b: Electrical modelling, materials oriented

- 16h00: Lifetime investigation of silicon thin film solar cells a simulation study using AFORS-HET 2.2, Eveline Rudigier, R. Stangl, M. Schmid
- 16h20: SCAPS simulations of capacitance profiles in the Cu(In,Ga)Se₂ solar cells, Michał Ćwil, P. Zabierowski, M. Igalson
- 16h40: Simulations of electrical characteristics of Cu(In,Ga)Se₂ based solar cells with Zn(O,S) and (Zn,Mg)O buffers: metastability issues, Paweł Zabierowski

19h00 – 22h00: Social Event: guided town walk with dinner, start at “Vrijdagsmarkt” (= nr. 33 on Gent map). We leave at 19h00 sharp!!!

Friday 30 March 2007

9h20 – 10h00: Session 3, Empirical I-V modelling

- 9h20: Applicability of the bilinear I-V curve translation method for indoor characterization of thin film devices, Artur Skoczek, M. Nikoaeva-Dimitrova, E.D. Dunlop
- 9h40: Empirical J-V modelling of CIGS solar cells, Jonas Marlein, M. Burgelman

10h00 – 10h30: Coffee break

10h30 – 12h20: Poster session

12h20 – 13h50: Lunch

13h50 – 17h00: Practicum and Demonstrations

- 13h50: Introduction
- 14h00: Demonstrations
- 15h00: Practicum

17h00: Meeting Summary, Closing and Adjourn

Poster presentations

- Influence of phosphorus doping on the structural and optoelectronic performance of (mc-Si:H) thin films, Gullanar M. Hadi
- Numerical simulation of diffraction gratings and their potential for implementation in thin-film silicon solar cells, Andrej Čampa, J. Krč, F. Smole, M. Topič
- Separation of signals from amorphous and microcrystalline part of a tandem thin film silicon solar cell in Fourier Transform Photocurrent Spectroscopy results, Jakub Holovský, A. Poruba, J. Bailat, M. Vaněček
- Calculation of Cu(In,Ga)(S,Se)₂ based solar cells parameters from their spectral photoresponse at various stages of preparation, Mikhail Tivanov, E. Zaratskaya, Valery Gremenok, V. Zaleskii, A. Mazanik, N. Drozdov, A. Fedotov, S. Zukotynski, K. Bente
- CIGS-based thin film solar cells with graded band gap and nanostructured contacts, Valery Gremenok, V. Zaleskii, S. Sergyjenja, A. Khodin, K. Bente, S. Zukotynski
- HIT Solar cell simulations with ASPIN2, Marko Nerat, F. Smole, M. Topič
- AFORS-HET, Version 2.2, Simulation of thin film solar cells and measurements, Rolf Stangl, M. Krieger, T. Geipel
- Deep level transient spectroscopy measurements on Cu(In,Ga)(S,Se)₂-thin film solar cells, Martin Knipper, J. Parisi
- Impurity Photovoltaic Effect in GaAs solar cell with two deep impurity levels, Khelifi Samira, J. Verschraegen, M. Burgelman, A. Belghachi
- Bifacial a-Si:H solar cells: Origin of the asymmetry between front and back illumination, Nicolas Wyrsh, C. Ballif
- Investigation of the electronic properties of the recombination- heterointerface in CGS / recombination- heterointerface / CIGS monolithic tandem solar cell, Gregor Černivec, F. Smolel, M. Topič, M. Burgelman
- Material and device characterization of thin-film polycrystalline-Si solar cells based on aluminum-induced crystallization and epitaxial growth as a first step towards modelling, Dries Van Gestel, I. Gordon, L. Carnel, G. Beaucarne, J. Poortmans
- Modelling MEH-PPV:PCBM (1:4) bulk heterojunction solar cells, Ben Minnaert, M. Burgelman
- Relation between luminescence, quasi-Fermi levels and voltage in semiconductor diodes, Rudi Brüggemann
- Efficient single and multijunction n-i-p solar cells with high quality hot-wire microcrystalline silicon simulated using AMPS, Robert L. Stolk, F.A. Rubinelli, H. Li, R.H. Franken, J.K. Rath and R.E.I. Schropp

Optical modeling and simulations of thin-film solar cells

Marko Topič

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Abstract:

Numerous research laboratories and R&D groups in industry use numerical simulators as a tool to better understand and to improve properties of their products. Optical modeling is along with electrical modeling an inevitable tool to develop self-consistent simulators in area of optoelectronics, photonics or photovoltaics. Accuracy of simulation results does not only depend on the models applied, but often it is limited by the quality of input parameters.

A brief overview of the available approaches in optical modeling and simulations of thin film solar cells is given. In detail, an advanced one-dimensional semi-coherent approach will be presented. It allows in-depth investigation, analysis and optimisation of thin-film multi-layer structures with flat and/or rough interfaces. Powerfulness of simulations will be discussed on examples of thin-film silicon and polycrystalline CIS structures.

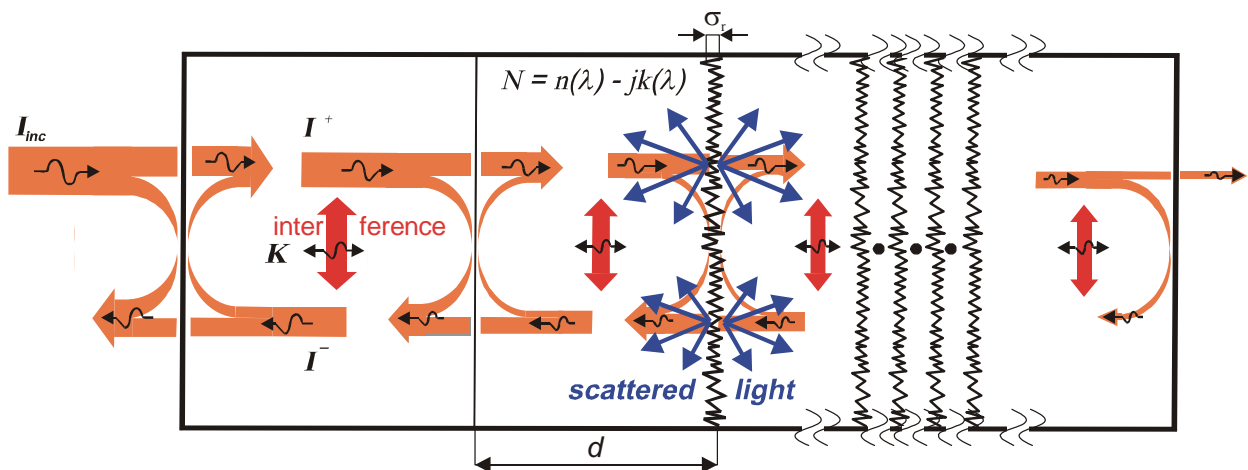


Figure 1: Light propagation in a multi-layer thin-film structure with flat and rough interfaces.

Electrical modelling of thin film solar cells

Marc Burgelman

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Abstract:

Numerical simulation is a powerful tool in understanding the working principles and limitations of thin film solar cells. The principles of modelling semiconductor devices in general and thin film polycrystalline solar cells in particular are introduced: the 'semiconductor equations', their numerical implementation and solution, physical phenomena to be included to simulate thin film cells (band alignment, recombination in bulk, at interfaces, at contacts, current mechanisms), solar cell measurements to be simulated (I-V, C-V, C-f, QE(λ), ...), and finally the limitations of numerical modelling (what it can do and what it can't do).

A main limitation is the large number of parameters involved. This calls for extended characterisation, where as many as possible measurements are performed on materials, substructures and complete cells. Also, the interpretation of these measurements can be greatly facilitated by using analytical or numerical 'sub-models', which only involve one measurement type and a few parameters each. This will be illustrated on several cases from CdTe and CIGS thin film solar cell research.

Numerical simulation of nanoelectronic devices

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Abstract:

Modeling of electronic transport in nano-scale devices requires a theory describing open, quantum-statistical systems driven far from thermodynamic equilibrium. Especially when the electronic device is operated at room temperature, electron-phonon interaction can significantly affect the electrical device characteristics.

A brief overview of the available quantum transport formalisms able to describe this mixed coherent/dissipative transport regime is given. The application of Wigner distributions and non-equilibrium Green's functions in numerical device simulation is discussed in more detail. For realistic device simulations comprehensive scattering models are required. Recently developed Monte Carlo methods are capable of solving the Wigner equation including realistic scattering mechanisms. At present scattering is treated semi-classically by means of a Boltzmann scattering operator. Results for single barrier and resonant double barrier structures are discussed. In the non-equilibrium Green's function formalism, on the other hand, coupling of the electron system to the metal contacts and to the heat bath is modeled by self-energy terms. Models for phonon modes specific to carbon nano-tubes (CNTs) have been implemented. The simulator is used to study various configurations of CNT field effect transistors.

Novel concepts in photovoltaics

Antonio Martí Vega

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Abstract:

To define what a “novel” concept in any area of research is not easy since, by definition, it ceases of being novel in the moment you heard about it for the first time. Anyway, by “novel” concept in photovoltaics we mean those concepts conceived to exceed the limiting efficiency of single gap solar cells and that still have not entered into the market. Under this definition, multi-junction solar cells would not be a novel concept (they are already in the market for space applications and expected to be in the market for terrestrial applications in the next years) while hot carrier solar cells, for example, would. Besides, some of these novel concepts are still, to our knowledge, purely conceptual while for others, some experimental proof supporting their principles of operation has already been provided.

It is relatively easy to propose a novel concept. What is less easy is that this novel concept you propose complies with the laws of thermodynamics. Hence, in the first part of the tutorial will teach the essential related to the application of thermodynamics to photovoltaics and, in particular, to what refers to the fulfilment of its second law.

In the second part we will describe some of these novel concepts, to know: the hot carrier solar cells (solar cells conceived to extract the photogenerated carriers faster than they recombine); the impact ionization solar cells (solar cells in which one photon generates more than one electron–hole pair); the intermediate band solar cells (cells proposed to convert below bandgap energy photons without degradation of the output voltage) and thermophotonics (systems in which the sun heats a light emitting diode that is used to illuminate a solar cell).

Quantum efficiency of thin film solar cells - optical modeling of short circuit current density and its spectral dependence

Aleš Poruba, J. Springer, J. Holovský, A. Purkrt and M. Vaněček

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Abstract:

To calculate an absorption enhancement and the spectral response of nano-textured thin film solar cells simple geometrical optics cannot be used; therefore, usual ray tracing programs cannot be applied. On the other hand, a rigorous treatment using Maxwell electromagnetic theory (being available only for a periodically repeating surface features) is very complicated and time-consuming. Hence, recently we have developed a simple Monte Carlo model [1] based on scalar scattering theory, which takes into account the part of the light scattered at each interface/surface as well as the coherent part of the non-scattered light at each layer. Either idealized Lambertian distribution of the scattered light or directly measured scattering distribution function is included in our model. Using this method, external or internal quantum efficiency of a single-junction or multi-junction cells can be easily calculated.

Furthermore, in our diagnostic lab we measure all optical parameters of each layer of the cells investigated. This is especially important for new and enhanced materials, as for microcrystalline silicon with various crystalline fraction, for doped silicon layers where the optical absorption coefficient and the refractive index depend on the doping level and finally for evaluation of optical properties of transparent conductive oxides (TCO) and back reflectors. In this contribution we are going to present our approaches for the precise evaluation of optical parameters using standard transmission / reflection spectroscopy (T/R), Photothermal Deflection Spectroscopy (PDS) and Fourier Transform Photocurrent Spectroscopy (FTPS).

Our model, thus, has no free parameter, since all input data are determined experimentally. It gives as a result the ultimate performance of nanotextured thin film solar cell in terms of maximum achievable short circuit current (total carrier collection within the active layers) for a given thickness of all layers and the light scattering parameters of layers and interfaces. It enables to analyze and identify the losses due to each parameter. Model gives the results within a few minutes on standard PC.

[1] J. Springer, A. Poruba, M. Vaněček, *J. Appl. Phys.* 96 (2004) 5329

[2] M. Vaněček and A. Poruba, *Appl. Phys. Lett.* 80 (2002) 719

Optical optimisation of Ag/ZnO back reflector for NIP solar cell

Thomas Söderström, F.-J. Haug, V. Terrazzoni-Daudrix, X. Niquille, S. Perregaux, C. Ballif
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Abstract:

Amorphous silicon solar cells were deposited in the nip configuration, which allows the use of cheap substrates such as plastic or stainless steel. We consider processes compatible with low cost plastic such as poly-ethylene-naphthalate (PEN) or poly-ethylene-teraphtalate (PET). These plastics have a cost advantage of three to four times compared to the glass substrates used in pin solar cells. The substrates are covered with sputtered Cr-Ag-ZnO stacks, which serve as back reflector and electrical contact. The silicon films are deposited by plasma enhanced chemical vapour deposition, at very high excitation frequencies (VHF-PECVD, 40-150 MHz) on PEN on glass. The top transparent conductive oxide (TCO) is indium tin oxide ITO, which works as antireflection coating.

The ZnO layer of the back reflector is of particular interest because it acts as a diffusion barrier between Ag and silicon layer and it enhances the current inside a nip solar cell. We optimise the thickness of the layer on flat PEN and found in accordance with optical simulation (SunShine, optical simulation program from university of Ljubljana). On flat reflectors the current does not depend on the ZnO layer thickness.

We then performed a similar optimisation on textured substrates, which are compulsory to lower the cell thickness and thus the degradation of an amorphous solar cell. The silver was deposited at high temperature in order to promote a roughness at its surface. This textured substrate leads to strong current enhancement compare to flat silver. However, the rough silver ZnO interface leads to absorption loss due to interband transitions and plasmon excitations. The optimisation of the ZnO thickness becomes important on textured substrates because the absorption losses can be reduced by interference effects. The losses inside the back reflector can be minimized and the efficiencies of the solar cell enhanced. We deposited amorphous silicon solar cells with initial efficiencies of 8.3 % on the textured substrate.

Anti-reflection layer at the TCO/Si interface for high efficiency thin-film solar cells deposited on rough LP-CVD front ZnO

Peter Buehlmann, A. Billet, J. Bailat, D. Domine, S. Faÿ, C. Ballif

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Abstract:

To decrease the reflection of incident light on thin film p-i-n solar cells, we introduce a TiO₂-ZnO bi-layer as an anti-reflection coating (ARC) between the rough front transparent conducting oxide (TCO) and the p-layer. As front TCO we use a ZnO produced by low pressure chemical vapor deposition (LP-CVD). On the rough ZnO, we deposit the TiO₂ layer by reactive rf-sputtering of a Ti target with H₂O/Ar gas mixture containing less than 10 % H₂O. The roughness of the ZnO already significantly reduces the reflection at the ZnO/Si interface, due to the refractive index grading over the depth of the roughness, as described by the effective medium approximation (EMA). But the typical roughness used for our microcrystalline silicon (μ c-Si:H) solar cells is not sufficient to fully remove the reflection.

With a TiO₂ ARC of ~65 nm, having a refractive index of ~2.5 at 500 nm we decrease the reflectance of a typical μ c-Si:H solar cell at 600 nm from 9 % to 6 %, which leads to an increase of 2.5 % in the current density.

With a plasma surface treatment of the ZnO we can modify the roughness/morphology of the interface without changing the bulk properties of the TCO. We will therefore study the effectiveness of the TiO₂ ARC on ZnO/Si interfaces of different roughness. With numerical simulations and experimental results of μ c-Si:H solar cells we will try to predict the optical performance of the solar cell depending on the roughness of the ZnO/Si interface and the use of a TiO₂ ARC.

Design of novel concepts of light management in thin-film silicon solar cell using optical simulations

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Abstract:

In thin-film (TF) solar cells light management is of great importance. High absorptance in thin absorber layers is essential to achieve high photocurrent of the solar cells. In TF silicon solar cells there still exists a great potential to improve light trapping in the structure, especially of the long-wavelength light, and to minimise optical losses in the supporting non-active layers. However, novel concepts of the light management in TF solar cells are needed. For the design and optimisation of novel optical solutions, numerical modelling and simulation are required.

In this work, one-dimensional photonic-crystal (PC) like structures are used as a novel optical concept in TF solar cells. The PC structures (periodic repetition of two different layers) present an option for realisation of special ‘optical interfaces’ with wavelength-selective (high) optical reflection or transmission properties. Different materials (SiO_x, TiO_x, ZnO and a-Si:H) are used for the layers in our PC structures. By means of optical simulations we design the PC structures that have a potential to be used as a highly reflective (> 99 %) back reflector in TF silicon solar cells. In this way, optical losses which are present in metal reflectors (related to plasmon absorption) can be avoided. Further on, a PC structure is designed for a wavelength-selective intermediate reflector (interlayer) in tandem (micromorph) silicon solar cells, with a high reflectance for the short-wavelength and a high transmission for the long-wavelength light. Based on simulation results, the design rules for the PC structures used in TF silicon solar cells (e.g. as a back or intermediate reflector) are established.

Modelling the current density increase due to "light-trapping" effect in conjugated polymer/fullerene-based bulk heterojunction solar cells

Adam Purkrt¹, J. Springer¹, A. Poruba¹, M. Vaněček¹, L. Goris² and J. Manca²

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Abstract:

Efficient light scattering has great importance for any thin film solar cell. Enhancing the absorption length within the absorber layer of very thin solar cells by introducing nano-roughness on the back reflector proved to substantially increase the efficiency of the cells. In recent past, the general optical model CELL has been successfully used to estimate this increase of efficiency in thin film silicon structures [1].

For organic solar cells, however, attempts to conceive a substantial increase in efficiency are mostly focused on improving the materials properties towards a better matched absorption spectrum, higher charge carrier collection and an optimized morphology. Here we want to demonstrate that a good optical design of the solar cell architecture could also yield a tremendous improvement.

We have modeled bulk-heterojunction organic solar cells with active layer of MDMO-PPV:PCBM (1:4 wt.) mixture with nano-rough surfaces/interfaces using the model CELL. First, we tried to compare our model with independent model presented in [2], which concerns organic solar cells with smooth interfaces, and our model gave exactly the same results.

We then tried to model optical properties of a cell with a nano-rough back reflector. For a 100 nm thick active layer, our results predict the increase of short circuit current density from 6.3 mA/cm² to 9.2 mA/cm², when increasing the back reflector random nano-roughness from 0 to 30 nm (root-mean-square value of roughness). The increase of current can be attributed to the "light-trapping" effect (confinement of photons inside the active layer due to repeated total reflection), which has been experimentally observed in thin film silicon solar cell. Introducing the roughness elsewhere in the cell did not lead to any substantial improvement.

This predicted substantial increase should be supported by extensive experimental study.

[1] J. Springer, A. Poruba, M. Vaněček, S. Fay, L. Feitknecht, N. Wyrsh, J. Meier, A. Shah, T. Repmann, O. Kluth, H. Stiebig, B. Rech: Improved optical model for thin film silicon solar cells, Proc. 17th European Photovoltaic Solar Energy Conf., Munich

Recombination through amphoteric states at the amorphous/crystalline silicon interface: modeling and experiment

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Abstract:

The performance of high-efficient crystalline silicon (c-Si) based solar cells is limited by the recombination losses on both c-Si surfaces. Dangling bonds at the c-Si surface are the defects governing interface recombination irrespective of the overlaying passivation layer (i.e. SiO₂, Si₃N₄, a-Si:H). Dangling bonds are also the predominant defects governing recombination in bulk hydrogenated amorphous silicon (a-Si:H). Considering the amphoteric nature of these defects (i.e. different charge states when singly, doubly or not occupied), a closed-form expression exists for recombination in bulk a-Si:H. The application of this dangling bond recombination formalism to c-Si surface dangling bond recombination in the otherwise classical approach allows us to reproduce the injection-level dependence of the surface recombination velocity S_{eff} , deduced from quasi-steady state photoconductivity (QSSPC) measurements on symmetrically passivated c-Si wafers. Thus we can quantify the respective contribution of the two fundamental mechanisms of surface passivation: the interface defect (dangling bond) density and the image charge density in the c-Si induced by the charged defects in the a-Si:H passivation layer. With a single set of four capture cross sections we can reasonably fit our experimental data that contains a large variety of configurations of c-Si/a-Si:H layers. c-Si wafers are of different doping level and doping type (including intrinsic) and the average charge state of the amphoteric recombination centers in the passivating intrinsic a-Si:H layers is varied by microdoping or by capping the passivation layers with doped layers. The good interface passivation properties of a-Si:H layers are exploited in the heterojunction solar cell: Sanyo is able to achieve efficiencies higher than 20 % with open-circuit voltages (V_{oc}) higher than 700 mV. We are achieving so far a best device efficiency of 19 % (with a V_{oc} of 680 mV and a fill factor (FF) of 82 %) and a best V_{oc} of 705 mV (with 17.5 % efficiency and a FF of 78 %) both on small area cells 5×5mm² n-type (1 Ωcm) FZ wafers. An implementation of our simple a-Si:H/c-Si interface recombination model in a numerical simulation tool for solar cells could for example link these observed trade-offs between V_{oc} and FF to the injection-level dependence of S_{eff} . The V_{oc} corresponds to a rather high injection-level whereas the maximum power point (MPP) corresponds to a rather low injection-level.

Optical characterization of transparent tin oxide films deposited by CVD

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Abstract:

In the field of solar energy conversion, thin films of transparent conductive oxides (TCO) are being used more and more in a large variety of photovoltaic devices: they are deposited on different absorbing materials as monocrystalline silicon, porous silicon, CdTe and CuInSe₂ thin films... . Among TCO materials, transparent tin oxide is extensively used owing to its appropriate optical and electrical properties and to its high chemical and mechanical stabilities. It is well known that the physical properties depend largely on a deviation from stoichiometry in the material composition and on the presence of impurities in the films. In our laboratory, we have deposited SnO₂ thin films on glass and silicon substrate by chemical vapour deposition (CVD). We have optimised their structural, morphological, electrical and optical properties by optimisation of deposition parameters and of post-deposition treatment like thermal annealing. We have measured directly the optical constants (refractive index n and extinction coefficient k) by ellipsometry technique for films deposited on silicon and analysed optical transmittance (T) and reflection (R) spectra of films deposited on glass substrates. SnO₂ is known to be a transparent semiconductor in the visible region which is suitable for solar cells. The optical constants were evaluated from transmittance and reflection data and from the analytical expressions for the dependencies of R and T on the real and imaginary parts of the refractive index (n and k respectively), the wavelength λ , the thickness d and the refractive index of the substrate n_s . From the variation of the square of the absorption coefficient α with photon energy we get the value of the optical direct gap which is about 4 eV for SnO₂. Indirect gap of tin oxide is about 3.2 eV. We deduced thickness of the layers.

Modeling of the near infrared reflectance spectra of LP-CVD ZnO

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Abstract:

Polycrystalline boron-doped zinc oxide deposited by low pressure chemical vapor deposition (LP-CVD) is used as transparent conducting oxide (TCO) in silicon thin film solar cells. These layers exhibit high conductivity and high transmittance. In addition to these characteristics, they also scatter the light at the TCO-cell interface, which leads to an increase of the effective absorption of light within the active layer of the cell.

The LP-CVD ZnO films have an absorbance close to zero in the visible range. In the near infrared region, the reflectance abruptly increases. Important physical parameters such as the optical carrier density and optical mobility can be extracted from the reflectance spectra. This is done by fitting these spectra using a model of the dielectric function with a set of parameters. These parameters are varied in order to get the best match between the measured and calculated data points.

A home developed Labview software is used for the modeling of the reflectance spectra. We assume that the optical properties of the studied material are determined by the complex dielectric function. The classical Drude model is taken as dielectric function. Furthermore, alternative models (Lorentz oscillator, Drude model with non constant damping term) have also been implemented. We use the Fresnel equations, taking into account the multiple reflections, the roughness, and the substrate layer, to calculate the theoretical reflectance curve.

Experimental reflectance spectra of ZnO layers with different doping levels are then measured and fitted with the software. A good convergence of the fitted curves is obtained in the range of validity of the Drude model. The optical carrier density and optical mobility extracted from these fitting curves are compared with the carrier density and mobility measured with the Hall effect method. This comparison allows us to identify the different mechanisms which limit the electrical conductivity of the LP-CVD ZnO films, and at which doping levels these mechanisms play a significant role.

Specific issues in modeling of thin-film silicon solar cells

Miro Zeman

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Abstract:

Modeling of thin-film silicon devices requires to take the electronic structure of a-Si:H and $\mu\text{-Si:H}$ into account. The spatial disorder in the atomic structure of a-Si:H results in a continuous density of states (DOS) in the band gap. When considering the transport properties of charge carriers we have to distinguish between the extended states and the localized states in the DOS distribution. The localized states within the mobility gap strongly influence the trapping and recombination processes and therefore the trapped charge in the localized states cannot be ignored as is often the case in modeling of crystalline semiconductor devices. The localized states in the mobility gap of a-Si:H are represented by the conduction-band and valence-band tail states and the defect states. These states are different in nature. The different nature of the localized states in a-Si:H requires different approaches for the calculation of recombination-generation (R-G) statistics through these states. The models that are commonly used to describe the localized states in a-Si:H and their corresponding R-G statistics will be presented. The experimental techniques, such as deep-level transient spectroscopy, that are used to extract the DOS distribution from a-Si:H will be presented.

For obtaining high conversion efficiencies both the efficient use of the solar spectrum and the light management inside a solar cell plays an important role. The efficient use of solar spectrum has resulted in the multi-junction concept for thin-film silicon solar cells. The tunneling assisted recombination at the interface between two adjoining junctions is responsible for charge-carrier transfer through a multi-junction solar cell. Modeling of such device has pushed for the development of the models that could describe the tunnel-recombination processes at the interface between the component solar cells. This interface is described as the tunnel-recombination junction (TRJ) in literature. There are two approaches that are used to model TRJ. The Delft approach is based on the trap-assisted tunnelling model and enhanced carrier transport in the high-field region of the TRJ and the Pennsylvania approach is based on the introduction of a highly defective layer with strongly reduced bandgap at the n/p interface and grading of the mobility gap of the n-layer and p-layer in the regions adjacent to the defective layer.

In summary, the following models should be included in a thin-film silicon solar cell simulator:

- (i) description of density of state distribution in amorphous and microcrystalline semiconductors with the proper recombination-generation statistics,
- (ii) an optical model that takes both coherent (specular) and incoherent (scattered) light propagation into account,
- (iii) a model for the TRJ that enables to simulate multi-junction solar cells.

Simulation results of a tandem micromorph a-Si:H/ $\mu\text{-Si:H}$ will demonstrate the use of the above mentioned models.

Design rules for surface conditioning of widegap chalcopyrite absorbers

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Abstract:

Photovoltaic devices based on widegap chalcopyrite absorbers, like CuInS₂, Cu(In,Ga)S₂, and CuGaSe₂, should theoretically deliver high voltage outputs well above 1 Volt. However, experimental devices perform below the expectations. Extensive analyses of the electronic transport in such devices have systematically identified the heterointerface formed between the absorber and buffer layers as the critical location limiting the performance. Among the proposed strategies aiming at optimising absorber/buffer interfaces, we have explored the potential impact that surface conditioning of the absorber film prior to buffer deposition can have on relevant PV parameters. The idea behind this approach is to try to make the surface of widegap absorbers, routinely leading to interface limitations in device performance, to resemble the surface of lowgap counterparts, which in turn do not suffer from such interface limitations.

In this contribution we present some guidelines for the design of modified surfaces of widegap chalcopyrites based on numerical calculations realized with SCAPS. The working model consists of a lossy CuGaSe₂ absorber, with a thin overlayer of a material characterised by having similar bulk properties as the absorber underneath, but which now governs the heterojunction properties with the CdS buffer. The idea of transferring the working interface from the widegap absorber to the modified intermediate layer provides an additional degree of freedom in order to engineer the junction, provided that

- i) the intra-absorber junction between the widegap absorber and the intermediate layer does not act as drain for minority carrier recombination, and
- ii) that the new junction between the modified layer and the buffer fulfils certain conditions on proper amount and sign of stored charge, band alignment, and band gap.

The impact of these factors on the final device performance will be analysed separately and summarised in a few design rules.

Modelling of the effect of a buried pn-junction on cell performance in chalcopyrite thin film solar cells

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Abstract:

In view of a hypothesis often found in literature, that chalcopyrite solar cells with a buried pn-junction outperform cells with a regular heterojunction, theoretical models have been implemented and evaluated with the SCAPS software . Numerical calculations were performed concerning the influence of a n-doped surface-near absorber region leading to a pn-junction that is buried within the absorber.

Starting point was a standard chalcopyrite solar cell consisting of a Mo back contact, CIGSe absorber layer (thickness 3 μm , bandgap energy $E_g = 1.2$ eV), CdS buffer layer (50 nm, $E_g = 2.4$ eV) and a ZnO window layer (300 nm, $E_g = 3.3$ eV). At the absorber / buffer interface, the model included a small spike in the conduction band, a high density of neutral defects leading to a high recombination rate and the Fermi level was pinned close to the conduction band by charged defects. An electron reflector was introduced to eliminate recombination at the back contact. In order to implement the buried pn-junction, the surface near region of the p-type absorber was doped with donors. Cell performance and internal quantum were evaluated for different depths of the buried pn-junction (0.1-1 μm) and were compared to those of the standard solar cell with a regular heterojunction. Subsequently, absorber parameters such as absorption coefficient, diffusion length and doping concentration were varied in order to assert that the results are generally applicable.

We find minor or no increase in cell performance (especially with regard to the open-circuit voltage). On the contrary, for some particular parameter sets, the efficiency actually significantly decreases for buried junctions due to the low quantum efficiency for shorter wavelengths of the incident photons.

AFORS-HET 3.0: Development of a two-dimensional simulation mode

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Abstract:

There are a variety of thin film solar cell design concepts, in which the current flow takes place in an essential two dimensional way, i.e. single side contacted thin film solar cells. As an example, we model the thin film poly-Silicon solar cell on glass [1], see Fig.a. Here the absorber layer is contacted with a mesa etched contact grid (stripe contacts).

In order to simulate such solar cells, there is an urgent need to perform at least two dimensional device simulations. We are currently developing a two-dimensional calculation mode within AFORS-HET, a numerical computer simulation program for modelling thin film solar cells together with some common solar cell characterization methods. We describe the development of 2D simulation modes within AFORS-HET.

Progress has been made towards AFORS-HET 3.0 [2], to solve the semiconductor equations (Poisson's equation and the transport equations of electrons and holes) in two dimensions under equilibrium and steady-state conditions. Within an arbitrarily rectangular shaped space region, consisting of different semiconductors, like for example the symmetry element of Fig. b, these equations are solved in order to yield the local potentials and electron and hole concentrations. Radiative band to band recombination, Auger recombination and Shockley Read Hall recombination are considered. Interface currents can be modelled to be driven either by drift diffusion or by thermionic emission. The boundaries of the space region can be modelled as metallic Schottky or Schottky-Bardeen boundaries, as insulator boundaries, as metal/insulator boundaries or as symmetric boundaries.

Moreover, a simplified modelling approach will be included using a two-dimensional network simulation of electronic devices, see Fig c. The problem is reduced to calculate the potentials at the nodes in the network for a given external potential. The bulk of the solar cell is modelled with transport resistances, metallic contacts with contact resistances and the p/n junction is modelled with a one-diode-model.

Treating the simulation of a thin film poly-Si solar cell on glass, the two different modelling approaches are compared, the actual stage of the AFORS-HET development is demonstrated and future developments are sketched.

[1] Gall, S., J. Schneider, et al. (2006). "Large-grained polycrystalline silicon on glass for thin-film solar cells." *Thin Solid Films* 511-512: 7-14.

[2] AFORS-HET, Version 3.0, is planned to be launched free of charge at the 22nd EPVSEC conference in Milan, Sept. 2007. For Version 2.2, see www.hmi.de/bereiche/SE/SE1/projects/aSicSi/AFORS-HET

Modelling the effects of electronic parameters on the efficiency of amorphous silicon solar cells under AM1.5G spectrum

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Abstract:

The purpose of this paper is to model the performance of thin film amorphous silicon cells under realistic spectral conditions. A numerical model for the investigation of thin film amorphous silicon p-i-n cells was developed in Matlab. The light absorption of the device is simulated using a ray tracing approach, which also allows to use spectral ensembles to be investigated. Based on the absorption profile, continuity and current density equations are solved numerically, which is necessary to determine the current flowing through the device. This allows the calculation of the quantum efficiency of the device. One property of p-i-n junctions is that the quantum efficiency has a significant voltage dependence, due to the disproportionate effects of field strength on collection probability. The voltage dependence of the quantum efficiency as well as the current-voltage characteristic under AM1.5G spectral irradiance are calculated. The model is being validated against measurement on an a-Si test cell of known configuration and I-V characteristics. Then the established model is used to investigate the effects of i-layer thickness, surface recombination and electron and hole mobilities, under AM1.5G spectral irradiance, on the efficiency of a-Si thin film solar cells. The key parameters in optimising this type of a-Si cell are then reviewed.

Lifetime investigation of silicon thin film solar cells a simulation study using AFORS-HET 2.2

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Abstract:

Thin film concepts in photovoltaic industry offer an interesting alternative to conventional technologies, as their potential is high for low-cost, large-area and high-efficient energy conversion. During the last years the improvement in this research area has been enormous.

Here, solar cells based on silicon thin films are a promising approach. One major step towards high efficiency is the improvement of the electrical properties of the absorber layer. For this purpose, the identification of electrical loss mechanisms (e.g. recombination) in the layers and at the interfaces is crucial. A measure for the electrical quality of the layer is the lifetime of the minority charge carriers, which is limited by recombination. For silicon wafers the measurement of the lifetime is well established and interface and bulk recombination can be separated. However, for thin films the experimental result is ambiguous and the determined lifetime is an effective lifetime including both interface and bulk properties. Promising candidates to apply to lifetime measurements on silicon thin films are quasi-steady-state-photoconductance (QSSPC) and surface-photovoltage (SPV), as verified experimentally. For the latter the influence of recombination on the steady-state values, i.e. the change of the band bending under illumination, and on the decay behaviour of the excess carriers can be investigated. In this paper we are focused on steady-state value analysis.

Simulation studies are suitable means to interpret the experimental results. The simulation study in this work has been performed using the open-source software AFORS-HET 2.2. As ideal test vehicle for the simulation a silicon layer has been designed with realistic electrical properties of silicon wafers commonly used for solar cell devices. Simulations with varying the layer thickness (from 1 to 500 μm) and the defect density of the interface and the bulk have been carried out for both, QSSPC and SPV. The comparison of the simulated change of the photoconductance (QSSPC) and change of the band bending (SPV) under illumination, combined with a thickness dependence for an ideal case arise that QSSPC is mainly dominated by interface recombination while SPV is sensitive for bulk and interface recombination. In order to reflect realistic silicon thin films, the defect density of the bulk and the interface has been varied. These simulations proof the potential of QSSPC and SPV to investigate lifetimes in those films and enables a discussion of thin film lifetimes.

To overcome the ambiguous interpretation of measured thin film lifetimes, intense simulation studies have been performed. The results are a first step towards the separation of the surface recombination velocity and bulk recombination in thin films, which is important for the identification of the dominant recombination mechanism. The simulated variation of device properties reflects the capability of QSSPC and SPV as characterization tools for silicon thin films.

SCAPS simulations of capacitance profiles in the Cu(In,Ga)Se₂ solar cells

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Abstract:

The electrical properties of Cu(In,Ga)Se₂ (CIGS) solar cells depend on deep defects in the bulk or/and on interface charges, which can distort doping profiles. Thus their contribution to the capacitance often results in overestimation of shallow level concentration in the absorber. The nature of so-called N1 level observed in admittance spectra is not yet fully understood and its interpretation associated even with type of their electric activity is ambiguous and a subject of controversies.

In this work we will show the SCAPS simulations of capacitance profiling in the CIGS solar cells. The aim of this study is to show the input of bulk and interface levels to the capacitance and non-uniformity of measured profiles. We will try to interpret their influence on the shallow acceptor concentrations in the CIGS absorbers of various Ga content: Cu(In,Ga)Se₂ (Ga=20 %), CuInSe₂ and CuGaSe₂. The redistribution of acceptor concentration in metastable states of CIGS devices induced by reverse bias of the cell or/and by illumination will be discussed.

The SCAPS simulation show which of the features of the doping profiles might be attributed to the N1 level, and which are rather due to traps in the bulk of absorber. The numerical calculations confirm that the N1 level is donor-type trap located at the interface or close to the interface, and that it can not be responsible for observed non-uniformities of the capacitance profiles. Acceptor traps situated continuously in the lower half of the bandgap of CIGS absorber affect the shape of the doping profiles. The redistribution of acceptor type centers in the absorber after reverse-bias stress results in characteristic increase of the net doping level in the region close to the junction. These metastable changes fit well into the model of relaxing negative-U defects belonging to VSe-VCu complexes proposed by Lany and Zunger.

Simulations of electrical characteristics of Cu(In,Ga)Se₂ based solar cells with Zn(O,S) and (Zn,Mg)O buffers: metastability issues

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Abstract:

(Zn,Mg)O and Zn(O,S) are promising materials that can replace CdS as a buffer in CIGSe-based solar cells. The best reported devices with these alternative buffers have the efficiencies of 16.1 % and 18.5 %, respectively. It is well known that illumination of ZnO/CdS/CIGSe improves the cell performance in two ways: ‘red’ photons absorbed in the bulk CIGSe increase the open circuit voltage (V_{oc}) whereas the gain in the fill factor (FF) is due to the ‘blue’ light absorbed in CdS. On the other hand reverse biasing the junction leads to a loss in both FF and V_{oc} . However the influence of light and reverse bias on CIGSe-based devices with (Zn,Mg)O and Zn(O,S) is in many aspects different:

- i) a light soaking under short circuit conditions may lead to a deterioration of the FF,
- ii) illumination under open circuit improves the efficiency (mainly the FF) but the time scale of these processes is longer than for standard devices,
- iii) the impact of illumination depends significantly on the temperature at which it is performed as well as the state of the sample prior to the exposure to light (freshly made or stored for a few months in dark – ‘degraded’), and
- iv) reverse bias soaking does not change the device performance. In this contribution we present simulations of electrical characteristics of CIGSe-based solar cells (dark and light current-voltage, quantum efficiency, capacitance-voltage and capacitance-frequency) with alternative buffers.

We discuss the abovementioned differences in metastable phenomena referring to a recently proposed Se-Cu divacancy model in which the state of the junction, and thus the cell parameters, are controlled by the different charge states of the (VSe-VCu) complex.

Applicability of the bilinear I-V curve translation method for indoor characterization of thin film devices

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Abstract:

The paper presents an application of bilinear interpolation/extrapolation I-V curve translation method for reconstruction of indoor temperature and irradiance matrixes of thin film devices. A full PV device matrix is routinely measured at the ESTI laboratory in a broad range of temperatures (from 25 °C to 60 °C) and irradiances (from 50 W/m² to 1000 W/m²) allowing to obtain performance surface of given PV device. The advantage of the bilinear curve translation method is a possibility of estimation of all basic electrical parameters of the device. The accuracy of the method was investigated for both interpolated and extrapolated curves at different values of temperature and irradiance. In order to improve quality of translation procedure additional temperature correction was applied to the I_{sc}. The results indicate good accuracy of the translation procedure not only for interpolated but also for extrapolated curves of different thin film devices if the initial values of irradiance and temperature are distinctly separated

Empirical J-V modelling of CIGS solar cells

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Abstract:

Chalcopyrite based solar modules combine the advantages of thin film module technology with the stability of crystalline silicon cells. Therefore chalcopyrite based modules can take up a large part of the PV market. Today the efficiency of lab scale devices is close to 20 %, comparable to the best multicrystalline silicon cells. Physical insight in the electronic device structure is essential to develop devices with even higher efficiencies.

To analyse the cells we measure I-V curves, both dark and light (different light intensities), Isc-Voc curves, spectral response measurements $QE(\lambda)$ and capacitance measurements. The diode parameters (saturation current J_0 , ideality factor n , series resistance R_s and shunt conductance G_{sh}) are extracted from the dark J-V, light J-V and Isc-Voc curves.

In Gent we investigated the light dependence of these parameters at room temperature for different CIGS cells. At the workshop we will introduce new interpretation schemes: a comparison of the shape of the J-V curves measured over 4 decades of illumination intensity with simulations based on a one diode model, and a study of the fill factor loss (calculated ideal FF_0 minus measured FF) as a function of J_{sc}/V_{oc} or V_{oc}/J_{sc} , obtained by varying the illumination intensity. The interpretations proposed here can help solar cell developers in finding causes for a too low fill factor FF .

Methods to obtain band gap energy in CIGS solar cells

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Abstract:

In the paper results of fitting and numerical simulations of current-voltage (I-V) curves acquired in a wide range of irradiances and temperatures with use of equivalent either single (SEM) or double (DEM) diode model applied for commercial thin-film photovoltaic (PV) module CIGS (CuInGaSe₂) are presented. It shows the differences between the values of band gap energy E_g obtained from Arrhenius plots and in other ways. For that purpose I-V curves systematically acquired in the outdoor monitoring system have been used.

Influence of phosphorus doping on the structural and optoelectronic performance of (mc-Si:H) thin films

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Abstract:

For thin film solar cells based on microcrystalline silicon (nc-Si:H), the structural properties of phosphorus doped (p-doped) nc-Si:H thin films were investigated by means of micro-Raman scattering and conductivity measurements. The strong confinement model alone is unable to completely describe the Raman spectra. By taking into account both the phonon confinement effect and the strain effect, good fitting of Raman spectra were obtained. The derived strain values are found to decrease with the increase of doping concentration, indicating that phosphorus doping is an effective way to relax the strain in nc-Si:H thin films and the structure of the doped sample is more ordered. With a MatLab program, the comparison study of grain size distribution in both the doped and intrinsic nc-Si:H thin films demonstrates that the grains are in similar size, but the thin film is more homogenous in the P-doped samples. The observation of Coulomb-blockade effect, the increase of conductivity and the decrease of activation energy with the increase of doping concentration further support the conclusion from optical measurements.

Numerical simulation of diffraction gratings and their potential for implementation in thin-film silicon solar cells

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Abstract:

In thin-film (TF) silicon solar cells novel approaches of light management are important in order to further improve light confinement. High level of light scattering into large scattering angle(s) above the angle of the total reflection is one of the key challenges in the design. In this respect, diffraction gratings could be a viable solution. To design and optimise the gratings for their implementation at a specific interface in TF solar cells, detailed optical analysis inside the solar cell by means of numerical simulation is required.

In this work optical simulations based on finite element method are used to study diffraction gratings for their implementation as a metal back reflector (BR) in microcrystalline silicon (uc-Si:H) TF solar cells. Scattering at gratings with rectangular perturbation shape and with different sizes are examined. Besides the ability of scattering of long-wavelength light into large angles inside the solar cell, the effect of increased metal (Ag) absorption related to grating textures is analysed. Highest scattering abilities are indicated for small periods P with maximum at $P=1$ - and 2 -times effective wavelength (λ_{eff}) in the absorber. High heights (h) of the perturbations (a few odd multiples of $\lambda_{\text{eff}}/4$) are desired. However, at small P and high h , increased absorption in Ag is observed as well. All results will be presented for TE and TM polarization separately. The differences in results for TE and TM polarizations will be presented and discussed.

Separation of signals from amorphous and microcrystalline part of a tandem thin film silicon solar cell in Fourier Transform Photocurrent Spectroscopy results

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Abstract:

The thin film silicon technology is now already mastered and become one of the most promising branches in present photovoltaic industry. The concern of researchers is now focusing on more sophisticated structures like amorphous – microcrystalline silicon tandem cell that is also hot candidate for successful transfer to industrial production.

Recently we have introduced the fast and highly sensitive method for the evaluation of the optical absorption coefficient of photoconductive thin films [1] and later also for the quality assessment of thin film silicon solar cells [2]. High accuracy of this method, Fourier Transform Photocurrent Spectroscopy (FTPS), has also been demonstrated by interpreting the measured FTPS spectra of solar cells (single or tandem) as the external quantum efficiency data [3].

It is well known that properties of thin films deposited by different methods depend on the substrate parameters such as its conductivity and morphology. Therefore it is necessary to study optical, electrical and structural behavior of (at least) absorbers when incorporated in the whole cell structure. But in this case the measured spectra are influenced by light scattering, light trapping and absorption in other layers of the multilayer structure. The key issue of tandem structure diagnostics referred in this contribution is thus a separation of FTPS signals from amorphous and microcrystalline part of a stacked structure and their correct interpretation.

We utilize similar approach as for the tandem quantum efficiency measurement with various LED light biasing to make one of the cells more conductive so that the photocurrent is limited by the not-light-biased part of the cell. The successful retrieval of separate cell characteristics however requires removing of the optical influence of the second cell. It may act either as an optical filter in the front of the studied cell or as a photon trap behind the studied cell. Mainly the measured spectra of amorphous silicon top cell differ from that one can expect when characterizing the single cell structure. For an appropriate simulation of the light propagation within the structure and confirmation of our measuring approach we use the computer model CELL [3]. Moreover, the correctness of the separation process is checked by comparing the evaluated spectra with the spectra of two single cells (amorphous and microcrystalline) co-deposited with the each part of the tandem structure.

[1] M. Vaněček and A. Poruba, *Appl. Phys. Lett.* 80 (2002) 719

[2] A. Poruba, J. Springer, L. Mullerova, M. Vaněček, T. Repmann, B. Rech, J. Kuendig, N. Wyrsh and A. Shah, *Proc. 3rd WCPEC, Osaka, Japan (2003)* pp. 1827-1830

[3] A. Poruba, L. Hodakova, A. Purkrt, J. Holovský and M. Vaněček, *4th WCPEC Hawaii, USA (2006)*

[4] J. Springer, A. Poruba, M. Vaněček, *J. Appl. Phys.* 96 (2004) 5329

Calculation of Cu(In,Ga)(S,Se)₂ based solar cells parameters from their spectral photoresponse at various stages of preparation

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Abstract:

The development of non-destructive methods to control solar cells (SCs) physical parameters at all stages of their preparation is required for the optimization of the process technology and the improvement of the conformity between SCs photosensitivity and solar spectrum. A simple method for the calculation of Cu(In,Ga)(S,Se)₂-based SCs parameters (space-charge region width and diffusion length of minority charge carriers in Cu(In,Ga)(S,Se)₂ absorber) at various stages of the preparation from the analysis of their spectral photoresponse is proposed.

The method is based on the change of in-depth distribution of the photogenerated carriers in the SC and, hence, on the change of its photoresponse with the wave-length variation. In our work, the one-dimensional model of SC is used. The following assumptions are accepted: the reflection of charge carriers from a back contact and the «drawing» field in the quasi-neutral area of the absorber layers are absent, window and buffer layers are transparent for the analyzed part of photoresponse spectrum, the injection level of minority charge carriers is low, the recombination losses on the metallurgical p-n-junction interface of the studied photosensitive structure linearly depend on the photocurrent density.

For the calculation it is necessary to obtain a following set of the experimental dates: the spectral density of incident radiation, the spectral dependence of photocurrent or photovoltage for the studied photosensitive structure, the spectral dependences of optical absorption index and reflectance.

Acknowledgements: This work has been financed by ISTC project #B1029 and also supported Byelorussian Republican Fund for Fundamental State programmes 'Energy safety' and 'Crystalline and molecular structures'.

CIGS-based thin film solar cells with graded band gap and nanostructured contacts

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Abstract:

The ZnO/CdS/Cu(In,Ga)Se₂ thin film solar cells with graded bandgap of the absorber layer have been modeled. The cells modeled are designed to be fabricated on flexible substrates (dielectric and metal), so, additional requirements and restrictions to metal contacts and interlayers mechanical and electronic properties should be taken into account. The aim of the program under development is to calculate parameters of CuInGaSe₂-based (CIGS) heterostructure solar cells, taking into account the buffer layer effect, zone bending and recombination at grain boundaries and another defects, and to introduce the band gap gradient in the absorber layer.

The model has been developed to optimize the semiconductor layers parameters depending on the band gap profile. The model was based on one-dimensional drift-diffusion approach using Poisson equation and continuity equations for electrons and holes. The modeling for various bandgap gradient profiles have been performed positive (from 1.08 to 1.5 eV), zero (1.21 eV), and inverted (from 1.5 to 1.08 eV) profiles for CIGS layer. The output parameters of the cells (spectral response, efficiency, output voltage and current) have been calculated. It has been shown that the positive gradient structure has the highest current density and the lowest open-circuit voltage due to enhanced charge carriers collection efficiency and optimized recombination profile. The reverse gradient structure has the maximum overall efficiency and open-circuit voltage due to higher potential barrier at the heterointerface, but the lowest current density.

The nanostructured back contact of the solar cells formed on a substrate with porous anodic alumina was considered taking into account recombination processes at grain boundaries and nano-ordered back contact. Charge carriers accumulation at the interfaces leads to local effective bandgap narrowings at the interfaces reducing the efficiency. Reduction of recombination velocity at the grain boundaries near the substrate could be provided due to the built-in charges in alumina.

HIT Solar cell simulations with ASPIN2

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Abstract:

Recent studies on amorphous-crystalline silicon heterojunctions have evidenced the potential of these materials to realize low-cost and high-efficient solar cells. Obviously, one of the perspective structure for manufacturing is HIT solar cell.

There have been many researches made why structure using n-doped crystalline substrate is favourable in comparison with p-doped substrate, but it is still not completely clear. So we tried to find out the answer with computer aided simulations.

We employed two different structures of HIT cells, one with n-type and another with p-type c-Si base, for our simulation. The first one was made in the following configuration: Al grid/ITO/p a-Si(C):H/i a-Si(C):H/n c-Si/i a-Si(C):H/n a-Si(C):H/ITO/ Al grid, and the second: grid/ITO/n a-Si(C):H/i a-Si(C):H/p c-Si/i a-Si(C):H/p a-Si(C):H/ ITO/Al grid. In both cases we assumed all the same material properties and dimensions (thickness) of the layers, except the doping concentration in crystalline layer was just inverted from ND in the first case to NA in the second case. Absolute doping concentration remained the same.

We studied band gap alignment in thermal equilibrium, electron and hole concentration, J-V curve, quantum efficiency and AM1.5g efficiency at room temperature and 100 mW/cm² illumination. The computer simulations showed that the first cell has 0.2 % higher efficiency in absolute figures in comparison with the second cell due to favourable energy band alignment. We explain this the holes generated in n-doped crystalline absorber need to overcome lower barrier in the valence band, so the current density start to decrease at higher output voltage, which contributes to higher Voc , fill factor and efficiency. There is also higher barrier for electrons in conductive band. This is very good because the electrons are reflected away from pn-heterojunction and thus there is less possibility they recombine with holes. On the other side of the cell the situation is just the opposite: electrons have to overcome lower barrier in the conduction band and the holes are reflected away from back np-heterojunction.

The computer simulations predicted advantages using structure p-i-N-i-n instead of n-i-P-i-p, which are acceptable from a theoretic point of view. We demonstrated some typical characteristics of HIT solar cells. It would be interesting to investigate properties of heterojunctions in more detail.

AFORS-HET, Version 2.2, Simulation of thin film solar cells and measurements

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Abstract:

We describe AFORS-HET, a numerical (open source on demand) computer program for modelling thin film solar cells and some common solar cell characterization methods.

Thin film solar cells will become increasingly important within the photovoltaic market due to their high potential of cost reduction, i.e. energy and material cost, compared to wafer based technologies. However, a profound understanding of thin film layer-, heterostructure-, and device-characterisation is at a comparatively early stage of development. In order to support the interpretation of such measurements, we developed a numerical computer simulation tool, AFORS-HET (automat for simulation of heterostructures). AFORS-HET not only simulates multi-layer heterojunction solar cells, but also the observables of a variety of corresponding measurement techniques.

The current version 2.2 of AFORS-HET solves the one dimensional semiconductor equations (Poisson's equation and the transport equation for electrons and holes) with the help of finite differences under different conditions, i.e.: (a) equilibrium mode (b) steady state mode, (c) steady state mode with small additional sinusoidal perturbations, (d) simple transient mode, that is switching external quantities instantaneously on/off, (e) general transient mode, that is allowing for an arbitrary change of external quantities. The generation of electron/hole pairs can be described by simple Lambert-Beer absorption or by taking incoherent/coherent internal multiple reflections into account. Radiative band to band recombination, Auger recombination and Shockley-Read-Hall recombination can be considered and super-bandgap and sub-bandgap generation/recombination can be treated. Interface currents are modelled to be driven either by drift diffusion or by thermionic emission. The metallic contacts can be modelled as Schottky or Schottky-Bardeen metal/semiconductor contacts or as MIS metal/insulator/semiconductor contacts.

Thus, the internal cell characteristics, such as band diagrams, local generation/recombination rates, carrier densities, cell currents and phase shifts can be calculated. Furthermore, a variety of solar cell characterisation methods can be simulated, i.e.: current voltage, quantum efficiency, transient or quasi-steady-state photo conductance, transient or quasi steady-state surface photovoltage, spectral resolved steady-state or transient photo- and electroluminescence, impedance/admittance, capacitance voltage, capacitance-temperature and capacitance-frequency spectroscopy and electrical detected magnetic resonance.

The simulation principles of AFORS-HET will be described and demonstrated, showing selected results on the simulation of amorphous/crystalline silicon heterojunction solar cells.

AFORS-HET, version 2.2, is distributed free of charge and can be downloaded via internet: www.hmi.de/bereiche/SE/SE1/projects/aSicSi/AFORS-HET

Deep level transient spectroscopy measurements on Cu(In,Ga)(S,Se)₂-thin film solar cells

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Abstract:

Thin film solar cells made of Cu(In,Ga)(S,Se)₂ are ready for volume production because of their favorable attributes, e.g. high absorbing capacity. We characterize these solar cells with deep level transient spectroscopy (DLTS) to get a better understanding of bulk-effects and defects. Measuring the transient capacity at different temperatures from 25 K up to 320 K allows us to determine the activation energy and the concentration of electron traps. An energetic profile of the defects was identified by varying the level and time of the reverse voltage. Furthermore the effect of the bulk-defects onto the solar cells parameters, especially the performance of the solar cell, is evaluated.

Impurity Photovoltaic Effect in GaAs solar cell with two deep impurity levels

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Abstract:

Single junction solar cell energy conversion efficiencies are typically less than 30 % because, for any given material the sun's spectrum contains photons with both too much and too little energy for optimal conversion.

Impurity photovoltaic effect was proposed to improve solar cell performance by utilizing low energy photons. This can be possible by incorporating impurities with energy levels somewhere in between the valence and conduction bands of a semiconductor, which can provide additional photons process via the intermediate state.

For larger band gap materials, the IPV effect is more attractive for solar cells improvement. However one of the most interesting factors to improve solar cell efficiency by the use of the IPV effect is the use of the suitable impurity, with the suitable characteristics: position of the energy level, concentration of the impurity and optical and thermal cross sections of electrons and holes. In addition, theoretical works suggested that the efficiency may be improve even more by introducing more than one impurity level.

In previous works, we have investigated the IPV in Si solar cells with indium acceptor impurity level. The calculations were carried out using a new version of scaps software, which was extended to include the IPV effect.

In this work, we investigate the IPV effect in a wide band gap material such as GaAs with two deep acceptor copper impurity levels. Cells with varying defect density, as well as light trapping are treated. The occupation probability of the deep levels was calculated for the two levels to show the effect of the concentration and the level position on the solar cell performances.

Also quantum efficiency and current-voltage simulation of the IPV effect in GaAs solar cells were carried out to show the long wavelength absorption improvement due to the IPV effect.

Bifacial a-Si:H solar cells: Origin of the asymmetry between front and back illumination

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Abstract:

a-Si:H cells are designed in such a way to have illumination of the active layer of the device through the p-layer. This design rule permits generation of the light as close to the p-layer as possible to minimize the length holes have to travel to be collected. As a matter of fact, experiments show that bifacial a-Si:H cells exhibit reduced performance when illuminated through the n-layer.

For some uncommon applications of cells deposited on metallic substrates (e.g. solar cells deposited on dials for watches), the use of a p-i-n configuration is required in order to have the positive contact on the substrate. It is therefore necessary to understand the intrinsic limitations of such devices and to get indications for their optimization.

In this paper, the asymmetry in performance between front and back illumination of a single-junction bifacial a-Si:H cell is analyzed by numerical simulation using the ASA software and compared to experimental results. It is found that both the difference in the band mobility of electron and the one of holes, as well as the difference in the band tail characteristic energy values are responsible for the asymmetry. The latter is characterized by a reduction in the cell current and FF for an illumination through the n-layer due. The magnitude of this reduction, due to a deficient collection of holes, increases with increasing cell thickness.

Investigation of the electronic properties of the recombination- heterointerface in CGS / recombination- heterointerface / CIGS monolithic tandem solar cell

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Abstract:

The idea of thin film tandem solar cells on II-VI compounds has occurred more than two decades ago [1]. Logical evolution of the great success of the single junction CIGSS thin film solar cell is the two-junction mechanically stacked tandem solar cell. A lot of experimental and theoretical research has been done on these 4-terminal devices where main goals still remains development of the top cell with the AM1.5g efficiency above 17 %, preferably CGS structure with the transparent back contact. 4-terminal devices elegantly surmount the problem of the recombination heterointerface, but the final goal is the development of the monolithic CGS top cell/ CIGS bottom cell tandem structure. With optimized top cell the main obstacle is a formation of an efficient and transparent recombination heterointerface.

With the use of the advanced numerical simulator ASPIN2 we will study the physics of the recombination heterointerface in the monolithic tandem solar cell. P-type TCO forms ohmic contact with the top CGS layer but rectifying recombination junction with the bottom cell's TCO. Although it still has not been successfully used in PV applications we will investigate its potential as the back contact. If heavily doped (technological, physical obstacle?) the recombination might be enhanced by tunneling. N-type TCO forms a rectifying recombination junction with the top CGS layer but if the barrier height is below 0.4 eV the recombination current still flows. When thin enough the recombination current might be enhanced by the thermally activated hole tunneling. Since there exist some potential candidates in P-type materials (ZnTe:Cu, Cu_xSe_2) [2] and several N-type materials (SnO₂:F, ITO, ZnO:Al/MoSe₂), with poor rectifying character in heterointerface with CGS which have already been successfully used in semitransparent and bifacial devices [3], we will try to identify the optimal material properties for the recombination (tunneling recombination) heterointerfacial layer (layers)- from the electrical point of view (doping, band gap, electron affinity, recombination centers) and from the optical point of view with its thickness.

We will use the optimal recombination or tunneling recombination layer (layers) in the monolithic ZnO:Al/ZnO/CdS/CGS/TCO(p, n, p⁺, n⁺)/ZnO:Al/ZnO/CdS/CIGS structure and search for the optimal thicknesses of the top CGS and the bottom CIGS absorbers with real optical and electrical parameters. Preliminary optimization results show that the recombination heterointerface transmission with the bottom cell absorption limit the short circuit current of the monolithic tandem solar cell, fill factor is limited by the thickness of the top cell and the open circuit voltage depends on the quality of the recombination junction.

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Material and device characterization of thin-film polycrystalline-Si solar cells based on aluminum-induced crystallization and epitaxial growth as a first step towards modeling

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Abstract:

We recently showed promising solar cells (efficiencies of 8 %) made from polycrystalline-silicon (pc-Si) layers obtained by aluminum-induced crystallization (AIC) of amorphous silicon in combination with thermal chemical vapor deposition (CVD). To obtain highly efficient pc-Si solar cells however, the material quality has to be further optimized and different cell processes have to be developed. A better understanding of the material and device under investigation by means of characterization and modeling could therefore be of great value. In this paper we present characterization results of our pc-Si layers which might be used in future modeling of these layers. For each result we also formulate some interesting modeling questions from device fabrication point of view.

Our layers were formed by epitaxial growth on a 200 nm thick pc-Si layer made by AIC. The AIC process consists roughly of the deposition of double layers of Al and a-Si and an annealing step. During this annealing layer exchange together with crystallization of the a-Si layer takes place. Electron backscattered diffraction (EBSD) measurements of the pc-Si seed layers showed a preferential orientation and a grain size distribution (typically with grains within the range of 1 to 50 μm). Secondary crystallites are formed on top of the pc-Si layer. Interesting modeling questions are: What is the origin of the preferential orientation, to which extent is the performance limited by the smallest grains, what is the mechanism behind secondary crystallite formation, ... Some simple models already exist but there is still a need for more advanced models.

Recently we also showed by defect etching, photoluminescence and room temperature electron beam induced current (EBIC) measurements the presence of $\sim 10^9 \text{ cm}^{-2}$ electrically active intragrain defects (IGD) in the epitaxial thickened layer. These defects clearly limit the solar cell performance. The influence of these IGD's and the ratio between the negative contribution of this defects and the grain boundaries is a nice modeling question as well as the interaction of the IGD with impurities and the reduction of the IGD by annealing.

After epitaxial growth an emitter was formed either by phosphorus diffusion (homojunction) or by deposition of thin double layers of undoped and P-doped a-Si layers (heterojunction). Solar cells with a heterojunction emitter typically have 70 mV higher V_{oc} values than homojunction based solar cells. Can this be modeled by only using a difference in hydrogenation and preferential diffusion, or are there other mechanisms necessary to model the trend?

Finally we will present some light coupling related results. Thinning of the BSF layer and texturisation of the front surface are important steps and can be monitored by e.g. absorption and reflection measurements. A model for optimal BSF and absorber layer thickness based on optical measurements would be of great help.

Modelling MEH-PPV:PCBM (1:4) bulk heterojunction solar cells

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Abstract:

Modelling of organic bulk-heterojunction solar cells is difficult because of the complicated geometry and because of the microscopic scale of the internal mechanisms. Two methods to model the I-V curves of nano-structured solar cells were worked out. The first is a network model in which the microscopic unit cells are represented by diodes, and the transport through the nano-structured blend is represented by resistors. The second model is an effective medium model in which the whole p-n nanostructure is represented by one single effective semiconductor layer, which then is fed into a standard solar cell device simulator, e.g. scaps. Basic solar cell characteristics were examined in an organic bulk heterojunction device. The active layer is a spin-coated organic blend of a p-material (MEH-PPV) and an n-material (the fullerene derivative PCBM), sandwiched between a transparent ITO-PEDOT/PSS electrode and an Al/LiF back-contact. We carried out light and dark I-V and spectral response measurements and measured the transparency of the active layer. We applied both models to this organic bulk heterojunction. First, a parameter set was built up that simulates the measured characteristics of the MEH-PPV / PCBM blend cells. The dark and illuminated I-V, and the spectral response measurements are fitted fairly well. A parameter set for the effective medium model was sought and found that describes (with qualitative agreement) the measured I-V curves. This parameter was then used for a numerical parameter study. Critical issues for cell performance were identified, and their influence quantified (based on the actual parameter set for MEH-PPV:PCBM cells). First, the cell performance is sensitive to the electron and hole mobilities in the materials: the efficiency increases monotonously with increasing mobility, over many decades. The sensitivity is about 25 % relative efficiency gain for an order of magnitude of increase of the mobilities. Second, the poor absorption of the solar illumination is a cause of weak performance. We investigated the influence on cell thickness, and of the absorption characteristic.

Relation between luminescence, quasi-Fermi levels and voltage in semiconductor diodes

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Abstract:

Luminescence from a semiconductor diode or solar cell is determined by the splitting of the quasi-Fermi levels of electrons and holes and the absorptivity according to Kirchhoff's Generalised Law. The determination of the quasi-Fermi level splitting from the photoluminescence yield is particularly useful for solar cells: under certain assumptions the open circuit voltage can be deduced in a contact-less mode. The ideal-diode concept goes beyond the open-circuit operating point and provides a simple relation between quasi-Fermi level splitting and applied voltage, namely that the quasi-Fermi level splitting is homogeneous and equals the applied voltage times elementary charge.

In this paper we provide evidence that this ideal-diode concept cannot be applied to semiconductor pn and pin diodes constructed from realistic semiconductors. We apply the basic analytic theory to the ideal Shockley pn diode from which we calculate the excess carrier profile, the resulting current and photoluminescence yield at different operating points. For example, in short circuit one may find a small but substantial photoluminescence yield. This is in clear contrast to the ideal-diode model which assumes zero quasi-Fermi level splitting in short circuit.

We present complementary simulation results with the simulation programme SC-Simul, developed by M. Rösch at Oldenburg University, on the voltage dependence of the photoluminescence and electroluminescence of a-Si:H/c-Si heterojunction diodes which are in good agreement with the straightforward Shockley-diode approach. The simulation results for thin-film pin diodes show that the quasi-Fermi level splitting in the i-layer is higher than expected from the applied voltage. The above-mentioned correlation of the photoluminescence yield with the open-circuit voltage is thus not straightforward for these devices.

Efficient single and multi-junction n-i-p solar cells with high quality hot-wire microcrystalline silicon simulated using AMPS

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Abstract:

At the Utrecht Solar Energy Laboratory (USEL) we conduct a research program on thin film silicon solar cells. For tandem solar cells that were current-limited by the microcrystalline ($\mu\text{-Si:H}$) bottom cell, we observed that the FF-value of 0.75-0.77 was substantially higher than the value of 0.70 we obtain for single junction $\mu\text{-Si:H}$ cells with a similar absorber layer thickness. Experiments and calculations identified the red-shifted, attenuated illumination of the bottom cell and the higher operational voltage of tandem cells as causes for the high tandem cell FF values.

We performed computer simulations using the D-AMPS computer code to obtain a deeper insight into tandem cell operation. We varied the thickness of the $\mu\text{-Si:H}$ i-layer of the bottom cell while keeping the top cell absorber layer unchanged, and calculated the illuminated J-V parameters. It was found that the tandem cell FF increases with an increasing mismatch of the subcell currents. Additionally, we calculated the charge carrier recombination profiles. With respect to the current-matched case, we found that for a bottom cell limited case the recombination rate in the top cell increases, while it decreases in the bottom cell. The difference with the matched case becomes increasingly pronounced with an increasing current mismatch. From the simulation results it is clear that a current mismatch positively influences the FF of the limiting cell and, thereby, the tandem cell FF.