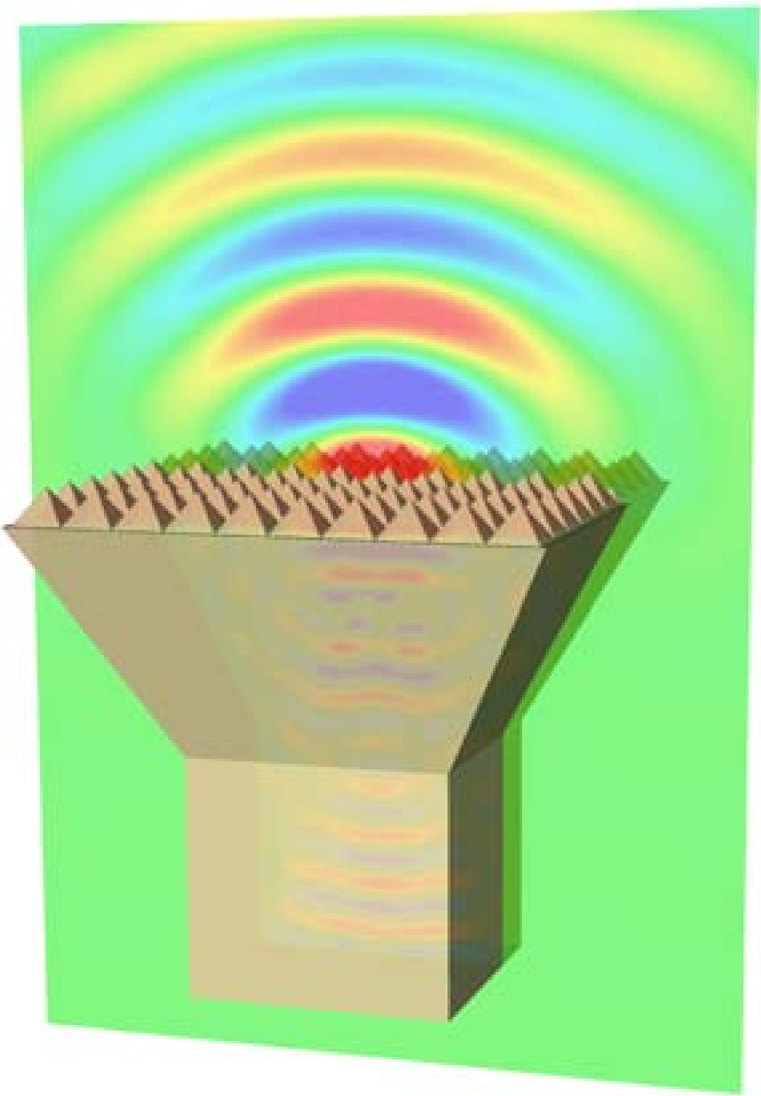
Zürcher Hochschule
für Angewandte Wissenschaften

School of
Engineering

ICP Institute of
Computational Physics

# Research Report 2009



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Das Titelbild zeigt eine dreidimensionale optische Finite-Elemente Simulation einer Leuchtdiode mit strukturierter Oberfläche, die ihr Licht in den freien Raum abstrahlt. Mit Hilfe von detaillierten numerischen Simulationen untersucht das ICP, zu welchem Grade sich Abstrahlcharakteristik und Effizienz von Leuchtdioden durch den Einsatz von mikroskopischen Oberflächenstrukturen, beispielsweise Pyramiden, verbessern lassen.

The title graphic shows a three-dimensional finite element optical simulation of a light-emitting diode with a textured surface radiating into free space. Based on full-wave numerical simulations the ICP investigates to which extent the radiation characteristics and optical efficiency of such devices can be improved by applying various surface textures such as micro-pyramids.

# Contents

# Kapitel 1

# Einleitung

Im Jahr 2009 wurden wir am Institute of Computational Physics unserem Namen erneut gerecht. Wir bearbeiteten verschiedenste Forschungsprojekte im Bereich der numerischen Modellierung von Multiphysik-Systemen und durften in unserer Forschungstätigkeit viele spannende Herausforderungen zusammen mit unseren Industrie- und Hochschulpartnern meistern. Wie Sie diesem Bericht entnehmen können, haben wir im Jahr 2009 in 16 Projekten mit nicht weniger als 37 externen Forschungspartnern zusammengearbeitet.
An der Schnittstelle zwischen akademischer und angewandter Forschung sehen wir uns täglich neuen Herausforderungen gegenüber. Wie können wir mit unseren Modellen und Simulationen für unsere Forschungspartner einen Mehrwert schaffen? Die Antwort ist vielschichtig. Zum einen müssen wir das Vertrauen unseres Partners gewinnen und zeigen, dass wir mit unseren Berechnungen Erkenntnisse erzielen, welche allein durch experimentelle Untersuchungen nur schwierig zu erreichen sind. Andererseits müssen wir auch überzeugend darlegen, dass wir numerische Simulationen nicht nur unserem Handwerk zuliebe durchführen, sondern im Sinne der Projektziele optimal einsetzen. Eine Zusammenarbeit beginnt denn typischerweise auch mit einer umfangreichen Analyse des vorhandenen Problems und der Bedürfnisse des Partners. Oft ist es dann während der Zusammenarbeit zentral aufzuzeigen, wie unsere Simulationsresultate mit der Realität verknüpft sind. Dies erfolgt, indem wir z.B. mit Hilfe des Vergleichs zwischen Experiment und Simulation, Parameter bestimmen oder mit Simulationen Wege zur Verbesserung der Systemeigenschaften aufzeigen. Auch wenn die Verfügbarkeit von schnellen Rechnern und benutzerfreundlicher Simulationssoftware weiter steigt, stellen wir fest, dass dies alleine z.B. einem Industrieingenieur nicht genügt um eigenhändig mit Multiphysiksimulationen Fortschritte zu erzielen. In der Regel ist einschlägige Erfahrung in der Beschreibung physikalischer Phänomene auf verschiedenen Längenskalen unabdingbar. Es gibt zu viele Beispiele, bei denen in der Industrie oder an anderen Hochschulen Simulationssoftware beschafft wird, welche dann aufgrund von Schwierigkeiten in der Einarbeitung kaum weiter genutzt wird. Es gibt also viele Anzeichen dafür, dass wir auch in Zukunft als Partner attraktiv bleiben. Die Opportunitätskosten für den Fall, dass man der Simulation als Entwicklungsmethode fern bleibt, steigen weiter an.
Um diesen Leistungsauftrag zu erfüllen, dürfen wir auf finanzielle Unterstützung von verschiedenen Förderagenturen und Forschungsstiftungen zählen. Letztlich sind für unsere Arbeit aber auch die Mitarbeiterinnen und Mitarbeiter zentral. Leider ist in der zweiten Hälfte des vergangenen Jahres unser Kollege und ICP Pionier Hansueli Schwarzenbach schwer erkrankt. Dies hat uns erschüttert. Wir bewundern seine Offenheit gegenüber diesem Schicksal und wünschen ihm und seiner Familie viel Kraft.
Im Jahr 2009 begrüssten wir mehrere neue Mitarbeiter am ICP, welche unsere Kompetenzen verstärken. Mit Thomas Lanz ist erneut ein diplomierter ETH Physiker zu uns gestossen, welcher an unserem Institut eine Doktorarbeit absolviert. Unser Umfeld mit internationalen Forschungspartnern und -Themen und der Status als wissenschaftliche Assistenten macht eine Dissertation an der ZHAW attraktiv. Wir schätzen diesbezüglich auch die Offenheit und Unterstützung der involvierten ETH Professoren. Mit Dr. Rebekka Axthelm, Beat Odermatt und Dr. Martin Loeser sind zudem drei wissenschaftliche Mitarbeiter zu uns gestossen. Es freut uns auch, dass wir im vergangen Jahr gleich drei frisch diplomierte Bachelor of Science in Systems Engineering (Mechatronik) von

unserer Schule aufnehmen konnten. Es sind dies Kai Brossi, Martin Neukom und Adrian Gentsch. Die Attraktivität einer Tätigkeit an unserer Schule bzw. unserem Institut wurde auch erhöht mit dem im Herbst 2008 lancierten Masterprogramm MSE (Master of Science in Engineering), das es den Master-Studenten ermöglicht, neben dem Unterrichtspensum in aktuellen Forschungsprojekten mitzuarbeiten. Mit Benjamin Perucco schloss im Dezember 2009 der erste Master Student unseres Instituts aber auch unserer Schule das MSE Studium ab.
Im Bachelor Unterricht waren Dozenten unseres Instituts in Grundlagenmodulen zur Physik und Mathematik in verschiedenen Studiengängen sowie in mehreren höhersemestrigen Modulen der Studiengänge Mechatronik und Maschinentechnik tätig. Wir betreuten im vergangenen Jahr insgesamt knapp zehn Studentenprojekte und nahmen auch erstmals einen IAESTE Studenten aus Belgien für ein Praktikum auf.
Unsere Sichtbarkeit als Institut in der Schweiz haben wir im Jahr 2009 auch mit verschiedenen Teilnahmen an Messen und Tagungen gepflegt, so zum Beispiel auf nationaler Ebene an den zwei Tagungen zu Nanotechnologie und Organischer Elektronik, welche wir in Zusammenarbeit mit dem Verband Electrosuisse an der ZHAW organisierten. Am lokalen Anlass zum nationalen Tag der Technik mit dem Thema erneuerbare Energien sprach ich zum Thema Forschung an Solarzellen der nächsten Generation und an der Nacht der Technik referierte Nils Reinke über Lichtquellen der Zukunft. International trugen wir letztjährig an Tagungen in Spanien, Italien, Österreich und Deutschland bei. Eine ausführliche Liste von Vorträgen, Publikationen etc. im vergangenen Jahr entnehmen Sie dem Anhang.
Nennenswert ist auch der weitere Ausbau des Mess- und Validierungslabors am ICP (kurz ”OLAB”) unter der Leitung von Nils Reinke. Es wird in neu bezogenen Räumlichkeiten im benachbarten Laborgebäude weitergeführt. Dank diesem Labor können wir vermehrt eigene Messungen zur Validierung von Simulationsresultaten ausführen oder sogar einen Beitrag in der Entwicklung von Messtechnik und Sensorik allgemein leisten. Letztlich ist dieses Labor auch bestens geeignet um Studentenarbeiten auf Stufe Bachelor und Master im Bereich Mechatronik, Elektrotechnik und Informatik auszuführen.
An dieser Stelle möchte ich im Namen des ICP Teams der School of Engineering der ZHAW sowie dem Kanton Zürich für die Unterstützung und insbesondere unseren Förderagenturen für die erfolgreiche Zusammenarbeit danken. Ich freue mich, die eingangs genannten Herausforderungen gemeinsam im ICP Team anzupacken und möchte mich bei jedem einzelnen ICP Mitglied für den persönlichen Einsatz im vergangenen Jahr bedanken.

Nun wünsche ich Ihnen eine spannende Lektüre.

Beat Ruhstaller
Institutsleiter

# Chapter 2

# Introduction

In 2009 the Institute of Computational Physics again lived up to its name: We carried out numerous research projects in the field of numerical modeling of multiphysics systems and enjoyed tackling many challenges in our R&D activities together with academic and industrial partners. As you can read in the following, we collaborated with some 16 projects and as many as 37 external research partners.

At the boundary between academic and applied research we are facing many challenges on a daily basis. How can we generate value to our research partners with our numerical models and simulations? The answer is not straightforward. On the one hand we must earn the trust of our partners and demonstrate that our calculations indeed help gaining insights which could hardly be obtained by experimental means. On the other hand we must explain convincingly, that we do not perform numerical simulations just for the fun of it but rather because they are the most efficient way of achieving the objectives. Thus a collaboration typically starts with an analysis of the problems at hand and the needs of the partners. Generally it is crucial to demonstrate how the simulation results are connected to reality. This happens with the help of comparisons between experiment and simulation, parameter extraction or by formulating possible ways of improvement of the system properties. Although the availability of fast computers and user-friendly simulation software is further advancing, we can state that this alone won't allow an engineer to get up to speed with multiphysics simulations. In general, appropriate experience is indispensable. There exist too many examples of simulation software purchases in industry and at universities, in which the software is hardly used any longer after initial training difficulties. Thus there are numerous signs that we will remain attractive partners also in the future. The opportunity cost for the case in which simulation software is not taken advantage of is large.

In order to fulfill our mission we count on financial support of various research funding agencies. But after all, our staff members are crucial. Unfortunately, our colleague and ICP pioneer Hansueli Schwarzenbach is suffering a severe illness since the end of last summer. We are very sad about this but admire his way of facing this destiny and wish him and his family all the best.

In 2009 we welcomed several new staff members which strengthen our competences. Thomas Lanz is a physics graduate from ETH that joined us and is writing a Ph.D. thesis at our institute. Our work environment with international research partners and topics and the status as scientific assistant makes a Ph.D. thesis at the ZHAW attractive. We are grateful for the openness and support of the involved ETH professors. In addition, three research associates, namely Dr. Rebekka Axthelm, Beat Odermatt and Dr. Martin Loeser joined the ICP. We are happy that we recruited three Bachelors of Science in Systems Engineering (Mechatronics) from our own school of engineering. Their names are Kai Brossi, Martin Neukom and Adrian Gentsch. The attractivity of the working environment at our school and institute was increased also with the launch of the Master of Science in Engineering (MSE) program in Fall 2008. It allows the students to get practical training in research projects besides attending classes. Benjamin Perucco in December 2009 was the first MSE master student of our institute and our school (!) to graduate with an MSE Master of Science degree.

At bachelor level our lecturers of the ICP were teaching entry-level courses in physics and mathematics in several degree programs as well as higher-level courses in in mechatronics and me-

chanical engineering. We coached a total of almost ten student projects last year and for the first time welcomed an IAESTE student from Belgium.
The visibility of our institute was maintained with the attendance of various conferences and symposia in 2009. For instance at national level we organized the two conferences on Nanotechnology and Organic Electronics in collaboratoin with the Electrosuisse association. At the local event of the national day of technology with its focus on renewable energy I gave a presentation on research on next generation solar cells. Nils Reinke spoke about light sources of the future at the "Nacht der Technik" event of our School of Engineering. Internationally, we contributed to conferences in Spain, Italy, Austria and Germany. A detailed list of talks, publications etc. is provided in the appendix.
Please note the further extension of our laboratory for measurement and validation lead by Nils Reinke. It moved to a new location in the neighboring laboratory building. Thanks to this laboratory we are able to carry out some of the measurements for validation of the simulation results on our own. We may even contribute to the development of suitable measurement techniques and sensors in general. This laboratory is also ideally suited for student thesis projects at bachelor and master level in the fields of mechatronics, electrical engineering and computational science.
On behalf of the ICP team I would like to express our gratitute to the School of Engineering and the Canton of Zurich for supporting us and the research funding agencies for the successful collaboration. I am looking forward to tackle the above-mentioned challenges together with our team and would like to thank each ICP team member for her/his commitment in 2009.

Enjoy reading this report!

Beat Ruhstaller
Head of the institute

# Chapter 3

# Sensors and Actuators

## 3.1 Numerical modeling of anisotropic plastic deep-drawing

Contributors: Guido Sartoris

Partners: Alcan Technology and Management AG
Funding: Commission for Technology and Innovation (CTI)
Duration: 2008–2009

Modern laminates for the production of pharmaceutical blisters have a complex inner structure. Several layers of different plastic and alumina sheets of thickness between $5 - 100\ \mu m$ are packed, stacked and glued together with the intent to provide the best environmental protection from external agents. When forming the blisters by deep-drawing, the overall functional role of the layers in the original laminate should be preserved and no holes, cracks or layer delamination are allowed to evolve during deformation. One may try to get physical insight on the disruptive processes of the sandwiched layers by running complex, time-consuming experiments, but they do not necessarily yield ultimate and correct answers on the causes of failure. Therefore a numerical approach to laminate deep-drawing is almost a necessity and numerical modeling is expected to provide a better and more detailed insight of the deformation processes with respect to a solely experimental approach.
From the numerical point of view, the major concern is the correct description of the anisotropic elasto-plastic behavior at large strains. The theory of anisotropic plasticity at finite strain has not yet reached full acceptance and an ultimate model is not yet established. This is in opposition to the isotropic case, where valid numerical models are available and ready to be used. For our case of orthotropic plasticity, we have chosen to use the more physically sounded multiplicative approach of plasticity instead of the additive one, which, however, is numerically more expensive. In general, by requiring fully spatial covariance of the material laws, one just derives isotropic laws, so that to handle anisotropic effects, one needs to add some tensorial dependencies representing privileged crystal directions. The problem is for a given physical situation to identify these structural tensors, but then we can apply well known theorems on the representation of isotropic tensor functions to derive anisotropic material laws depending on a limited number of scalar invariants. For orthotropy which is assumed here, the structural tensor is known to be a symmetric 2nd order tensor. With some additional assumptions on the physical processes involved, e.g. incompressibility condition of the plastic flow, one can shown the dependency of the elastic law to be from nine invariants and that of the yield function to be from seven ones. These invariants must be combined together to form functions depending on constant material parameters which need to be fitted from experimental data.
In general, it is not a simple task to fit these material parameters since we can have quite some parameters and a large sensitivity. One may think to proceed automatically with some optimization algorithms, however, because of the large sensitivity, these functionals may have a lot of local minima and the optimum or even an acceptable solution can be hard to find. Therefore, for the initial phase, we have opted for a three steps manual approach with a low number of material parameters. As first one fits the elastic behavior, then the yield function at the onset of plasticity and as least the hardening function during plastic flow. In general, there is a low sensitivity with respect to the elastic coefficients and a high one for the plastic ones.
The next figure shows uniaxial stress-strain relations for an *OPA* specimen in a logarithmic scale together with fitted curves. Several strips have been cut at increasing angles of $15$ degrees. One clearly can observe sharp transitions between elastic and plastic behavior, the orthotropic behavior and good fitting characteristics.

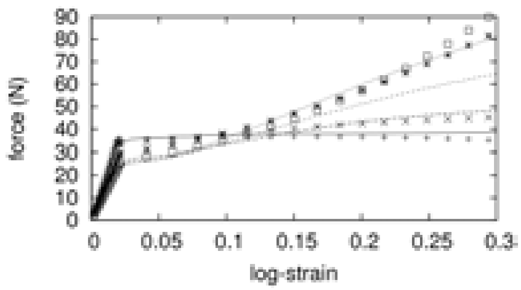



Fig.1 Fitted stress-strain relations for an *OPA* specimen.

## 3.2 Berührungslose Schichtcharakterisierung durch Hochgeschwindigkeits-Infrarotsensorik

Contributors: Nils A. Reinke, Kai A. Brossi, Remo Ritzmann, Andor Bariska (IDP)

Partners: Flo-IR und weitere 5 Industriepartner
Funding: Kommission für Technologie und Innovation (KTI)
Duration: 2007 – 2009

Die berührungs- und zerstörungsfreie Charakterisierung von Schichtsystemen auf nichtmetallischen Substraten wie Kunststoffen und Keramiken ist ein kaum gelöstes Messproblem der Industrie. Die School of Engineering (SoE) der Zürcher Hochschule für Angewandte Wissenschaften (ZHAW) und die Firma Flo-IR entwickeln ein Messverfahren, welches die Charakterisierung von Mehrschichtsystemen durch Hochgeschwindigkeits-Infrarotsensorik erlaubt. Dazu gehören die Bestimmung von Schichtdicken, thermophysikalischer Parameter, chemischen Zusammensetzungen der Schichten sowie das Erkennen von Haftungsproblemen.

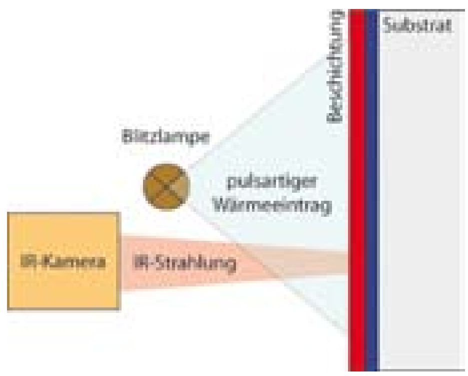



Fig. 1 Messprinzip

Im vorgestellten Messverfahren wird die untersuchte Probe pulsartig durch einen Lichtblitz aufgeheizt und das zeitliche Verhalten der Oberflächentemperatur mit einem Hochgeschwindigkeits-Infrarotsensor gemessen. Das zeitliche Verhalten der Oberflächentemperatur wird durch die Filmdicke, die Absorptivität sowie die Wärmeleitfähigkeit der einzelnen Schichten dominiert. Das Absorptionsverhalten und das thermische Verhalten des gesamten Schichtsystems werden mathematisch beschrieben. Aus dem ermittelten Verlauf der Oberflächentemperatur werden numerisch die physikalischen Parameter des zugrunde liegenden Schichtsystems bestimmt.

Fig. 2 Prototyp I

Das vorgestellte Messsystem bestimmt Schichtdicken in vier nebeneinanderliegenden Punkten von je vier Quadratmillimetern Grösse. Es lassen sich Schichtdicken im Bereich von 5 $\mu$m bis hin zu einigen 1000 $\mu$m bestimmen. Die Messqualität ist unempfindlich gegenüber Verkippung und eignet sich damit auch für unförmige Messobjekte. Die Messdauer beträgt je nach Art der Beschichtung etwa 40 ms bis 400 ms. Die Genauigkeit der Messung verbessert sich mit zunehmendem Kontrast zwischen den thermophysikalischen Parametern der einzelnen Schichten des Messobjekts. Das Messverfahren wurde bereits erfolgreich für unterschiedliche Lack- und Pulverbeschichtungen auf Kunststoff-, Metall- und Holzsubstraten getestet.

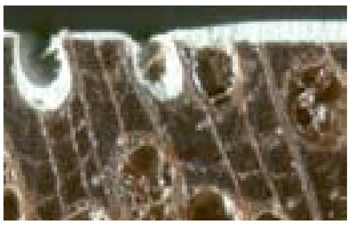


Fig. 3 Beschichtete Holzprobe

An der School of Engineering arbeiten das Institute of Computational Physics (ICP) und das Institut für Datenanalyse und Prozessdesign (IDP) gemeinsam an der Entwicklung des Messprototypen und der statistischen Signalanalyse.

## 3.3 Velocimetry in railcars by a run-time measurement of thermal markers

Contributors: Nils A. Reinke, Beat Odermatt, Andor Bariska

Partners: Siemens Transportation Systems
Funding: Commission for Technology and Innovation (CTI)
Duration: 2008 – 2009

State-of-the-art velocimetry for transportation systems using the Doppler method, dynamic image analysis and global positioning systems suffers from unreliabilities to a greater or lesser extent. This disaffection arises from a liability to interference towards environmental influences. Leaves, snowfall, rainfall and artificial lighting (light pollution) may lead to severe distortions in the measured velocity.
This feasibility project verifies a patent pending velocimetry technique which is based on a run-time measurement of thermal markers. The thermal-marker is applied from the railcar by optical excitation and subsequently photothermally detectation by an infrared sensor. The velocity of the railcar can be determined by measuring the run-time from excitation to detection and the spatial distance between excitation and detection setup.

Fig. 1: Corroded steel disc spinning behind the germanium zoom lens of the infrared detector

In recent years significant progress has been made in developing powerful, compact and inexpensive solid-state lasers. Nowadays, solid-state lasers replace traditional gas-lasers due to their higher reliability and low maintenance cost. At the same time, fast and inexpensive sensors for the mid-infrared regime (MIR) become more and more available. Improvements in laser technique and MIR sensors enable this innovative velocimetry technique.
This project includes three sequential steps:

- Computational modeling for estimating the amount of light necessary to deposit the thermal marker with different optical excitation sources (Laser, LED, flashlamps). The optical deposition of the thermal marker leads to a transient temperature distribution inside the rail. In order to detect the deposited thermal marker by the infra-red sensor, the amplitude of this temperature distribution has to be sufficiently high.
- An experimental setup has to be developed from scratch. This experimental setup has to reflect conditions close to reality, e.g. the optical and thermal properties of the rail. Computational modeling will help to specify the individual components used in this experiment. The experimental setup will be controlled and data acquired by LabView.
- In a final step of the project test measurements will be performed and analyzed to verify results from computational simulations and to proof the concept of the pending patent.

A prototype experimental setup comprising a fixture for a spinning steel disc and an infra-red detector is shown in fig. 1. Results of this feasibility project will be further investigated in a field test, if the third step turns out to be successful.

## 3.4 Automatic mesh generation based on geometrical and mathematical algorithms

Contributors: M. Robbiani, H. Schwarzenbach, G. Sartoris, M. Roos

Partners: ZAMP, Numerical Modeling GmbH
Funding: Gebert Ruef Stiftung
Duration: 2009–2010

A key element of the numerical solution of partial differential equations (PDE) by the finite element method in a multidimensional domain is the generation of the computational grid. Since the characteristics of the grid crucially influences the quality and the efficiency of the numerical solution, the success of modeling physical processes is closely linked to the development procedures for generating suitable grids. It is therefore not surprising that grid generation is a rapidly growing autonomously mathematical discipline of applied mathematics. Generally the development of techniques for mesh generation lags behind the techniques for discretizing the PDEs and so is often the lack of experience in constructing the grid which prevents the optimal numerical solution of PDEs. When solving a system of three-dimensional nonlinear PDEs on a domain of complex geometry - a frequent task in today's engineering life - the effort necessary to construct the computational grid, can by far dominate the remaining task of computing the numerical solution. The starting position becomes even more demanding if the geometry of the computational domain changes dynamically during the simulation. As techniques for flexible, robust and efficient dynamic grid generation are still missing, an effort in the engineering community is underway to overcome these difficulties. For the FE-simulation of e.g. thermo-, electro- or fluid-dynamic processes there are two main approaches for grid generation: geometry import from CAD tools, with subsequent automatic mesh generation or algebraic and functional grid construction from simple domains mapped and combined together to form the real geometry. The simplicity of the first apporach allows the treatment of complex geometries with little user interaction but it is counterbalanced by the fact that unnecessarily large grids are created. The second approach is time consuming and requires quite a bit of skills to discover appropriate maps but has an inherent mathematical description enabling easy variations of the geometry and a better control of the numerical error. The AutoGrid project aims to develop new methods for algebraic automatic grid generation which are relevant to practical applications. The actual practical limitations of the algebraic approach should be explored and new theoretical methods investigated, validated and implemented in efficient algorithms ready to be used in real engineering problems. Likewise an open-source version of the project for the 2D case should be made available to a wider audience. AutoGrid is a project of the newly founded Center of Mathematics and Physics (ZAMP) in collaboration with the Institute of Computational Physics (ICP) and the industrial partner Numerical Modeling GmbH.

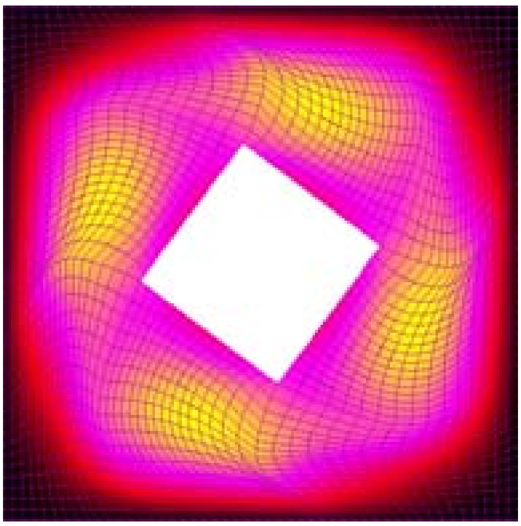


Fig. 1 Algebraic mesh adaption.

# Chapter 4

# Electrochemical Cells and Energy Systems

## 4.1 Status of model based investigation of PEM fuel cell performance

Contributors: Yasser Safa, Jürgen O. Schumacher, Felix N. Büchi

Partners: Paul Scherrer Institute PSI (Villigen, Switzerland)
Funding: Swiss Federal Office of Energy SFOE
Duration: 2007-2010

The principle of Proton Exchange Membrane Fuel Cell (PEMFC) as an energy producer is based on the electro-chemical reaction between an anodic fuel (mainly hydrogen) and a cathodic gas containing oxygen. This gives rise to a vapor condensation phenomenon where liquid water may affect the transport properties in the porous Gas Diffusion Layer (GDL) of the PEMFC. An accurate numerical prediction of the water distribution is thus of great importance in order to provide a guideline design of a reliable PEMFC.

Our ICP's contribution to the ongoing efforts in this technology is the advanced study of the two phase flow in the porous GDL with focus on modelling, numerical code programing and industrial test cases simulations. The so called Multi-Phase Mixture Model ($M^2$) is adopted to describe the two-phase flow. An important feature of $M^2$ is its usability in the domain where single and double-phase zones coexist.

In order to account for the momentum evolution caused by the water phase changing we suggest a new approach for an advanced use of the $M^2$ concept without violating the momentum conservation (Fig. 1). We have to find the global velocity, the global pressure, and the liquid water saturation $(u, p, s_\ell)$ such that

$$u = -\kappa\,\lambda\nabla p,$$
$$\nabla\cdot u = \tfrac{f_a}{\rho_a} + \tfrac{f_\ell}{\rho_\ell},$$
$$\phi\tfrac{\partial s_\ell}{\partial t} + \nabla\cdot\left(\hat{q}_\ell\,\tilde{G}(u,\nabla p_c) + \kappa\lambda_a\check{q}_\ell\nabla p_c\right) = \tfrac{f_\ell}{\rho_\ell},$$

[1] where $\tilde{G}(u,\nabla p_c)$ is a corrected global velocity, and $\hat{q}_\ell$ and $\check{q}_\ell$ are corrected fractional flow rates of water. This correction reflects the momentum exchange between the two phases of water. Material parameters of the GDL are the absolute permeability $\kappa$, the global mobility of water $\lambda(s_\ell)$, and the porosity $\phi$. Here, $\lambda_a(s_\ell)$ is the mobility of the air phase. $f_a$ and $f_\ell$ are source terms that are determined by the evaporation and condensation rates of water.

The numerical methods used for solving the system of equations were implemented in Mathematica. A degeneracy in the transport problem is treated by perturbating the diffusive coefficient to obtain a non-degenerate problem. The saturation equation is solved by a stabilized Galerkin approximation (SUPG) and the Darcy problem is solved by a stabilized mixed finite element method (GLS). The time discretization is achieved by a semi-implicit scheme. Since the time-scale of the total flow is longer than that of the water saturation evolution, a multi-time step discretization is introduced.

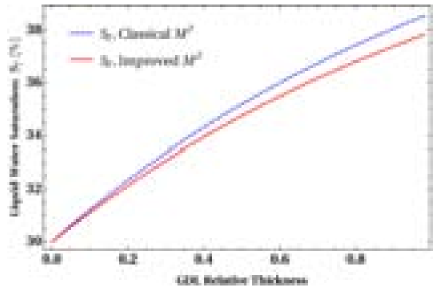


Fig. 1 Simulations with relatively high Evaporation-Condensation Rates and relatively high permeability

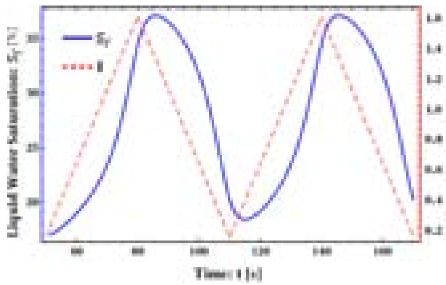


Fig. 2 Dynamic simulation result for the GDL.

A dynamic simulation result for the GDL material "E-Tek Cloth A" is shown in Fig. 2. A linear time-sweeping of the electrical current density $(0.05\frac{A}{cm^2\,s})$ was used as simulation input. An asymmetric profile of the average liquid water saturation is observed that is due to a transport limitation of the water through the porous GDL. Liquid water saturation profiles of different GDL material types are investigated in this study, both, as a function of time and space.

[1] Incompressible liquid phase has been assumed. The terms $\frac{\partial p}{\partial t}$ and $u_a.\nabla\rho_a$ have been neglected

## 4.2 Development and application of a electrode micromodel to optimize performance and to predict degradation phenomena in mixed conductors Ni-YSZ anodes

Contributors: Thomas Hocker

Partners: Boris Iwanschitz, Andreas Mai, Hexis AG and several Swiss partners.
Funding: SOF-CH, SwissElectric Research, Swiss Federal Office of Energy
Duration: 2008 – 2010

The development of a FE-based electrode model that mimics the real 3D microstructure of mixed conducting electrodes has been finished. It is especially suited for investigating the impact of microstructure on electrode performance and degradation. For example, it allows one to assess the effect of experimentally obtained single degradation phenomena such as particle coarsening and electrode poisoning on the electrode performance. Since the electrode model is directly linked with a repeat unit model (a complete cell plus current collectors on both sides) it predicts the impact of electrode degradation on the repeat unit performance.

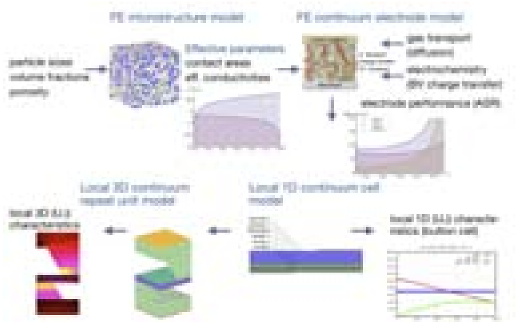


Fig. 1 FE-based microstructure model of a mixed-conducting Ni/YSZ-anode. The electrode model is linked to local cell as well as repeat unit models.

To mimic realistic solid-phase networks, up to eight different particle sizes can now be specified for each solid phase. Furthermore, the limiting effect of sinter necks on the ion and electron transport is taken into account via contact resistances between neighboring particles. When compared with literature data, the electrode model exhibits all main observations known from experimental analyses. Comparisons have been made with common electrode characteristics discussed in the following review-article: S. Sunde, "Simulations of Composite Electrodes in Fuel Cells", *Journal of Electroceramics*, **5**, pp. 153-–182, 2000. The model has been validated against conductivity- and EIS-data at Hexis.

Fig. 1 gives an overview about the developed modeling framework that spans from a finite element model to resolve the microstructure of an electrode up to a continuum model for a repeat unit, i. e. a complete cell with nonhomogeneous electrical current collection. Fig. 2 shows results of a finite-element model of two adjacent electrode particles, both of cylindrical shape. Due to the sintering process, the two particles are deformed and form a more or less narrow sinter neck. During this process the particle volumes are preserved. This "two-particle model" investigates limitations in the charge transport for different sintering scenarios. With narrow sinter necks (see right picture in Fig. 2), the drop of the electrical potential happens over a short distance in the vicinity of the sinter neck. Under those conditions the sinter neck becomes limiting for the overall charge transport.
The model allows one to calculate effective conductivities that account for limited charge transport by sinter necks. These effective conductivities are then used in the microstructure model of a complete electrode, see Fig. 1.

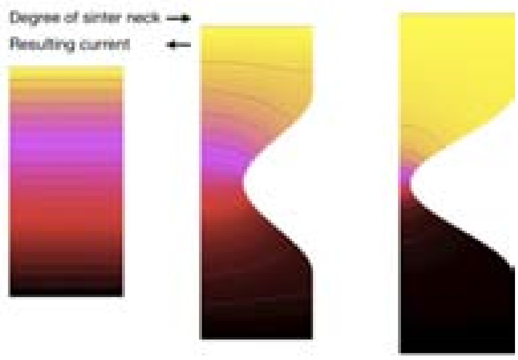



Fig. 2 Rotational-symmetric FE-model of two adjacent particles of cylindrical shape to investigate the limitation of sinter necks on the charge transport. The colors indicate electrical potentials that go from high (yellow) to low (black) values.

## 4.3 Status of numerical simulation for the development of a SOFC system

Contributors: Yasser Safa, Thomas Hocker

Partners: Hexis AG (Winterthur), EPFL (Industrial Energy Systems Laboratory)
Funding: Swiss Federal Office of Energy SFOE, SwissElectric Research
Duration: 2007–2010

The concept of SOFC heater "Galileo System", established by Hexis AG, is devoted to cover the essential power and heat requirement for a representative Central European single-family home. In this project we develop an advanced computational reactive flow model of the coupled transport phenomena in SOFC. The physical model that we study is governed by a system of nonlinear partial differential equations describing the conservation law for mass, charge, energy and species. The fluid flow in the porous media is described by Darcy Law. To reduce the computing time without losing consistency certain geometric restrictions are assumed. For example a low aspect ratio exists between the thickness and the cross-section of the cell. Therefore, the cell is treated in one dimension only and is coupled with the flow inside the gas channels. A slip boundary condition appears on the surface which constitutes the contour of a porous body through which the fluid flow also takes place. In several known approaches the slip velocity is taken as a a priori known quantity and it usually serves as a boundary condition to solve the momentum conservation equation like Navier-Stokes. The limitation of those approaches is that slip conditions are most frequently estimated in an empirical way and do not necessarily correspond to all real situations. A simultaneous solution of the equations describing the flow in both media is carried out. At the interface the slip velocity is considered as an arbitrary quantity not known a priory and which can be determined by matching the shear stresses on the porous wall of the channel. As presented in Fig. 1 we start solving the 1D Channel problem on the center level. The boundary values are used to update those on the boundary of the channel-electrode interface. Then we solve the 1D Channel problem at the porous wall level and the obtained value is used as Dirichlet boundary condition for the 1D Cell problem.

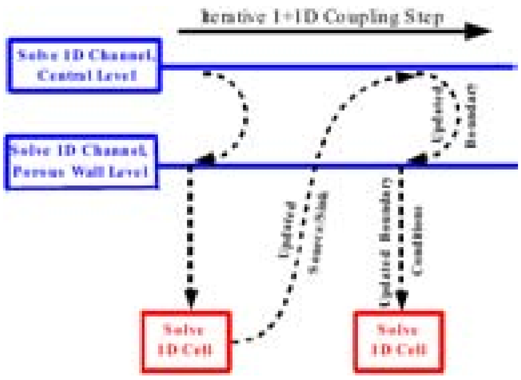



Fig. 1: Iterative solving 1+1D cell-channels moddel

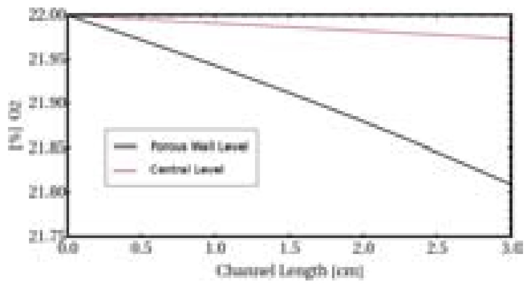



Fig. 2: Oxygen Concentration in the Air Channel

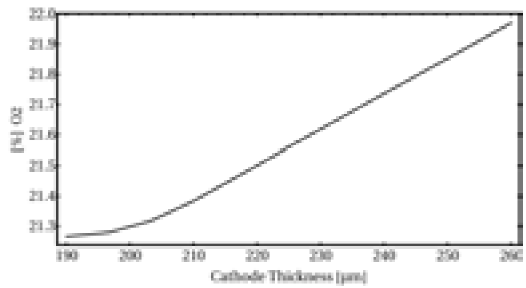



Fig. 3: Oxygen Concentration in the Cathod

In a new iterative step, we solve the cell problem and the outer species flux is applied as a source term for the 1D Channel on the central level. Note that in each step the species flows are computed in both the anodic and the cathodic gas channels.

## 4.4 Feasibility of a portable SOFC for Hilti's mobile machine tools

Contributors: Roman Gmür, Christoph Meier, Thomas Hocker

Partners: ETH Gauckler group, Hilti Corporation, Schaan.
Funding: Direct funding by Hilti Corporation
Duration: 2008 – 2010

Solid oxide fuel cell (SOFC) systems operate at temperatures between 700 °C and 900 °C. They are typically designed for stationary combined heat and power (CHP) applications in the small to medium power ranges, i. e. from about 1 kW up to several MWs. However, due to their potential for high power densities and their tolerance for different hydrocarbon fuels, SOFC systems were recently proposed for portable applications with electrical outputs from about 20 W to 250 W. The fabrication of the SOFC membranes used in these systems is usually based on classical thick film processing such as tape casting or screen printing which results in membrane thicknesses of several tenths of a millimeter. Driven by the progress in thin film technology, micro-fabrication and micro-packaging, the concept of a so-called micro-SOFC ($\mu$-SOFC) has been recently investigated. In contrast to conventional SOFCs, $\mu$-SOFCs are characterized by membrane thicknesses of only a few micrometers and operation temperatures as low as 500 °C. Feasibility studies of such systems suggest electrical power outputs as low as 1 W. $\mu$-SOFCs could be employed in combination with or as replacement of batteries to power small electronic devices, such as laptop computers, portable digital assistants, camcorders, or industrial scanners. Compared to state-of-the-art energy storage devices such as Li-ion and NiMH batteries, up to ten times higher energy densities (per volume or weight) were anticipated.

The development of $\mu$-SOFCs still is in research status. To assess the potential of such membranes for commercial applications already at an early stage, simple, yet physically sound modeling tools are required. Such tools need to incorporate all relevant system parameters including operation conditions, material properties as well as basic features of the layouts of the various system components. We developed such a model and subsequently applied it to different application scenarios. The model employs the global conservation principles for the species masses, the electrical charges and the energy for each system component. It allows one to calculate the efficiency of the overall system, its dimensions and weight. A schematic overview of the ONEBAT® $\mu$-SOFC system is given in Fig. 1 and 2. Shown are the mass and energy flows entering and leaving the system as well as the internal heat sources. The core of the ONEBAT® $\mu$-SOFC system is the so-called "hot module" which consists of the gas processing unit (GPU), the SOFC stack (Cells) and the post combustion unit (PCU).

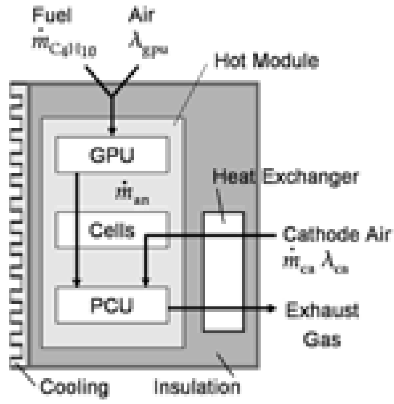



Fig. 1 Schematic of ONEBAT® $\mu$SOFC with entering and leaving mass flows.

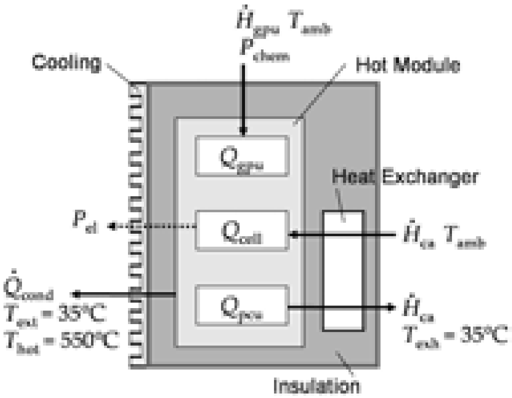


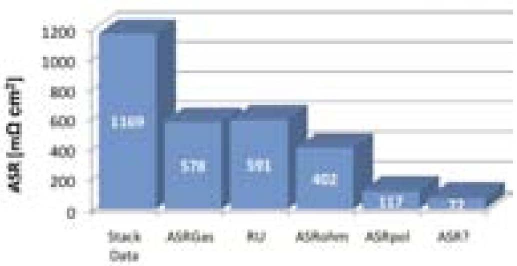

Fig. 2 Schematic of ONEBAT® $\mu$SOFC with entering and leaving energy flows and internal heat sources.

## 4.5 Time-dependent analysis of Hexis 5-cell stack (U,i)-data to predict degradation behavior on the stack level and for natural gas as fuel

Contributors: Markus Linder, Thomas Hocker

Partners: Roland Denzler, Andreas Mai, Hexis AG and several Swiss and EU-partners.
Funding: AccelenT, Swiss Federal Office of Energy
Duration: 2009 – 2011

A simplified, Mathematica-based model to analyze the current-voltage characteristics of SOFC-stacks has been developed and is in regular use at Hexis. The model predicts the starting performance for a large number of current-voltage stack data without the need for any fitting parameters. It has been used to study the sensitivity of various input parameters such as changes in mass-flows, fuel composition, temperature, and humidity. For the remaining project year it shall be extended to the Hexis Galileo system to perform model-based analysis of field tests. Here the goal is to explain unusual system behavior that, for example, could result from composition changes in the natural gas supply, and to assess long-term degradation from the field test results. Furthermore, we plan to implement a statistics tool to automatically discriminate between reproducible and unreproducible data. The prior will be used to assess long-term performances, the latter to investigate phenomena not yet well understood. The model development is shared between the SOF-CH and the AccelenT-projects. The latter focuses on methods to accelerate the testing of SOFC stack performances and related degradation phenomena.




$$\mathrm{ASR_{tot}} = \mathrm{ASR_{gas}} + \underbrace{\mathrm{ASR_{ohm}} + \mathrm{ASR_{pol}} + \mathrm{ASR?}}_{\mathrm{ASR_{RU}}}$$

Fig. 1 Typical area specific resistances as obtained with the Uj-Analyzer.

Fig. 1 shows a model-based analysis of ASR-values (ASR = Area-Specific Resistance) for a five-cell Hexis stack that runs on natural gas. The total resistance (ASRstack) has been obtained from five current-voltage curves. The simplified system model has been used to subdivide the total resistance into a gas contribution that accounts for the details of the reforming process and possible fuel leakages. The remaining losses are denoted as ASR RU they represent the sum of the resistances of the repeat unit. They can be further subdivided into the ohmic losses of the electrolyte and the polarization losses of the anode and cathode.

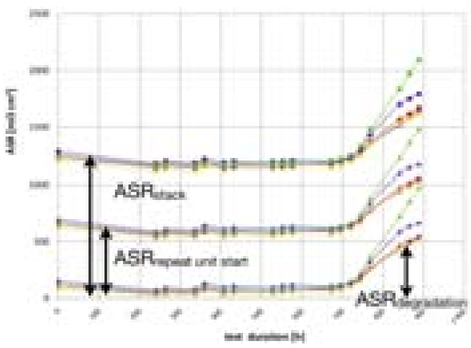



Fig. 2 Time-dependent area-specific resistances as obtained with the Uj-Analyzer.

The difference between the repeat unit losses and the sum of ASRohm and ASRpol is denoted as ASR?. ASR? specifies all contributions that are not explicitly accounted for by the model. One sees from Fig. 2 that for the first 700 hours of operation, ASR? remains constant and is rather small. However, after 700 hours, one or more degradation processes commence to significantly reduce the stack performance. Note also that two cells show a degradation rate that is different from that of the other three cells. This could be a temperature-effect, since even small differences in the operation temperature (say around 20°C) have a rather large impact on the stack performance.

# 4.6 Modeling of fixed-bed wood gasifiers for combined heat and power applications

Contributors: Thomas Hocker, Christoph Meier

Partners: ITFE Institut für Thermo- und Fluid-Engineering
Funding: GEBERT RÜF STIFTUNG
Duration: 2009–2011

Wood gasification is a thermo-chemical conversion of wood into a combustible gas. Due to their simple design, fixed-bed reactors are often the technology of choice for small range applications up to 5 MWth. Several CHP pilot plants with wood gas driven internal combustion engines went on grid throughout Europe during the last decade. Since carbon monoxide and hydrogen are the main contributors to the wood gas caloric value (typically 4 - 6 MJ/m$^3$), and as the gasification takes place between 600 and 1000°C, solid oxide fuel cells are a potential alternative to combustion engines, promising remarkable high efficiencies for micro-CHP with a renewable fuel. The aim of our project is to develop a toolbox of flexible, application-oriented models to design and optimize fixed-bed gasifiers by combining known approaches with observations from plant operators and own experiments. Key issues are the minimization of tars in the produced gas and more flexibility towards wood modality. However, until now model based design only plays a minor role for plant developers and operators. To validate models and to identify different gasification mechanisms a laboratory gasifier was built, suited to a wide range of operation conditions and fuels. Gas composition, temperature and pressure distribution are measured on-line. Experiments with single particles are conducted as well. Several types of gasification models are under development, as shown in Figure 1. Combining thermal equilibrium calculations with energy and mass balances, an overall model predicts the output gas species for a given input composition. This concatenates e.g. wood moisture and stoichiometric combustion coefficient $\lambda$ with the process efficiency. But since equilibrium achievement depends on the reactor design and operation conditions, the usability of this approach as predictive model is rather limited. Introducing reaction kinetics and single particle sub-models leads to more comprehensive results. Thus, stage models can predict e.g. the required dimensions for pyrolysis and char gasification zones considering particle shape and size distribution. Further developments are planned toward continuous, transient multiphase models.

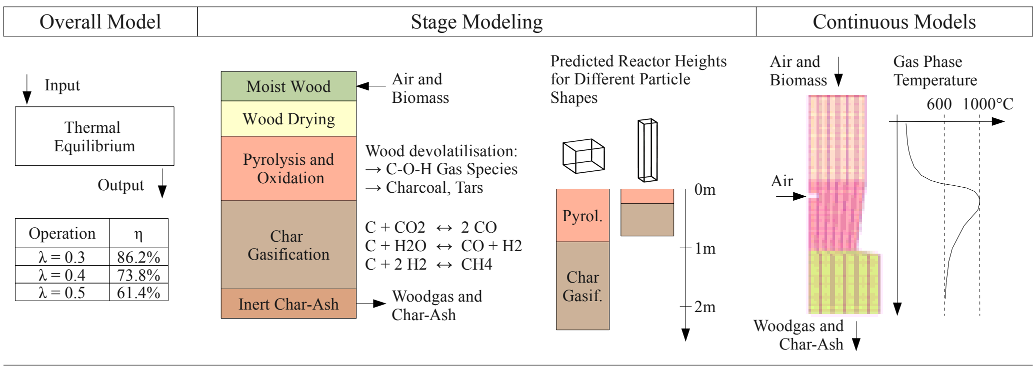



Fig. 1: Model Development and Process Overview.

## Chapter 5

# Organic Electronics and Photovoltaics

## 5.1 Advanced experimentally validated integrated OLED model

Contributors: Evelyne Knapp, Beat Ruhstaller

Partners: Philips Research Aachen and Eindhoven, Technical University Dresden, University of Cambridge, University of Groningen, Eindhoven University of Technology, Sim4tec, Fluxim
Funding: EU FP7
Duration: 2008 – 2011

Organic Light-Emitting Diodes (OLEDs) are solid-state devices composed of thin films of organic molecules that create light when a voltage is applied. They can be used for displays as well as lighting. OLEDs are energy-efficient and very thin, and in fact can be put on flexible materials (plastic or metal foil) to make bendable displays. The European project AEVIOM aims at a more accurate physical and numerical description of OLEDs. The developed model should be continuously validated with experiments and measurements. This is what AEVIOM - Advanced Experimentally Validated Integrated OLED Model- stands for.
So far, the basic concepts of OLED operation -charge carrier injection, charge transport, exciton formation, radiative decay and light extraction-as shown in Fig. 1 have been refined and integrated in a second generation model.


Fig1.: Fundamental processes in the OLED operation: electrons and holes are injected and transported in the organic material until they form excitons. Then they decay and emit light.

The main difference to the first generation model is that the disordered nature of organic semiconductors is taken into account in terms of a Gaussian density of states. This affects the above mentioned fundamental processes. A new description for the charge injection with barrier lowering, a density-, field- and temperature-dependent mobility (Extended Gaussian Disorder Model), the generalized Einstein relation and traps were obtained within AEVIOM and simulated for disordered semiconductors.
In the second year of the project, the disorder-enhanced physics has been added to the numerical solver of the ZHAW. This simulator solves the semiconductor equations consisting of the Poisson equation and the continuity equations for electrons and holes in a coupled manner for transient and steady-state problems. The results have been cross-checked with other simulation methods developed within the AEVIOM project like the Monte Carlo, Master equation and Bonham-Jarvis approach and experimental data as shown in Fig. 2.

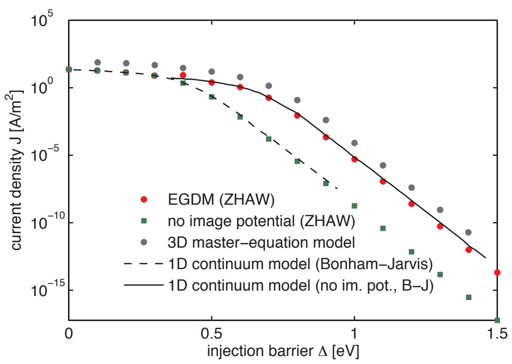



Fig 2.:The current density depending on the injection barrier is shown for different simulation methods. Also the effect of the image charge potential and the electric field on the current density is displayed.

As a further way to validate models and their parameters, the ZHAW has extended its solver to conduct a small-signal analysis. To study the ac response of an OLED under small-signal conditions, the steady-state voltage $V_0$ is modulated with a sinusoidal voltage of amplitude $V^{ac}$ and with angular frequency $\omega$: $V = V_0 + V^{ac}e^{i\omega t}$. The calculated impedance will be validated with measurements.

## 5.2 Efficient areal organic solar cells via printing

Contributors: M. T. Neukom, T. Lanz, N. A. Reinke, B. Ruhstaller

Partners: TU/e Eindhoven University of Technology (NL), University Jaume I (E), CSEM, BASF
Funding: Swiss Federal Office of Energy
Duration: 2008 – 2011

This international research project with universities and industry aims at creating more efficient and stable organic solar cells. The ICP is simulation partner and provides a comprehensive electro-optical model to numerically characterized organic solar cells.
The electron and hole mobilities are essential parameters that influence the cell efficiency. Measuring the mobilities accurately is therefore important. The CELIV and photo-CELIV experiment is a established method to extract mobility values of organic solar cells. The results are usually analysed with a simple analytical model. We use a comprehensive numerical model to investigate the accuracy of this analytical model and show the possibilities of the CELIV method.

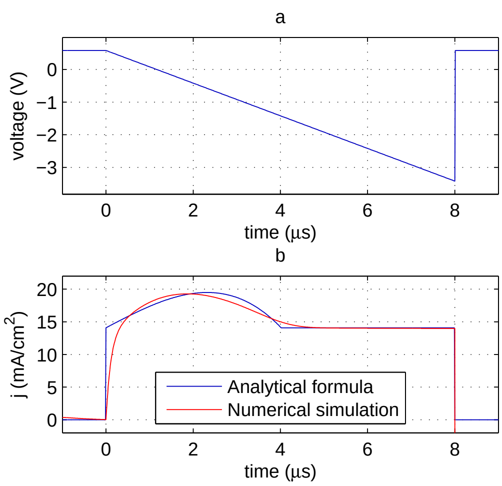



Fig. 1: (a) Applied voltage ramp. (b) Transient current with typical overshoot

In the CELIV technique (charge extraction with linearly increasing voltage) charge carriers inside of a solar cell are extracted with a triangular voltage pulse. The transient current is analysed and the mobility of the faster charge carrier can be calculated with the position of the current peak according to Juska et al.[1] In figure 1 a voltage ramp and the corresponding current of a typical CELIV experiment is shown. Due to the linear increasing voltage a constant displacement offset occurs.

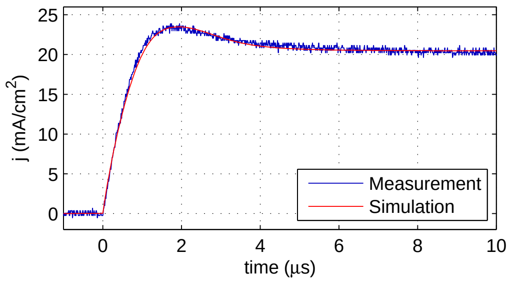



Fig. 2: CELIV measurement and numerical simulation of an organic solar cell

In our numerical model we assume that incoming photons directly generate free charge carriers inside the donor/acceptor blend. With a drift-diffusion model the charge transport inside the cell is simulated. All models used are implemented in the software SETFOS that is developed by the ICP spin-off Fluxim AG[2]. We simulate the CELIV experiment and compare it with measurements as shown in figure 2. With our current model CELIV experiments can be reproduced and device parameter can be extracted.
We can show the accuracy and the limitations of the analytical formulas frequently used to analyse CELIV experiments. Because several effects are neglected in the analytical model only the order of magnitude of the mobility value can be determined. The numerical simulation offers a more accurate mobility determination. By fitting simulation to measured currents we show that CELIV experiments can be reproduced with our numerical model. We also demonstrated the possibility to extract minor and major mobilities.

[1] G. Juska, K. Arlauskas, M. Viliunas, J. Kocka, Phys. Rev. Lett. 84 (2000) 4946
[2] Semiconducting thin film optics simulator (SETFOS) by Fluxim AG, Switzerland (www.fluxim.ch)

## 5.3 Cost efficient thin film photovoltaics for future electricity generation

Contributors: Thomas Lanz, Nils A. Reinke, Beat Ruhstaller

Partners: EPFL, EMPA, PSI, Oerlikon Solar, Greatcell, Solaronix, Flisom
Funding: SwissElectric Research
Duration: 2007 – 2010

The extension of the optical model for arbitrary combinations of coherent and incoherent layers has been completed. This now allows to treat the light propagation in selected layers exclusively using the intensity. The extension is physically motivated by the finite coherence length of the sunlight which is on the order of 1 $\mu$m. Layers with a thickness that exceeds the coherence length may be treated as incoherent, effectively reducing the interference fringes obtained in coherent simulations that are not observable in the experiment.

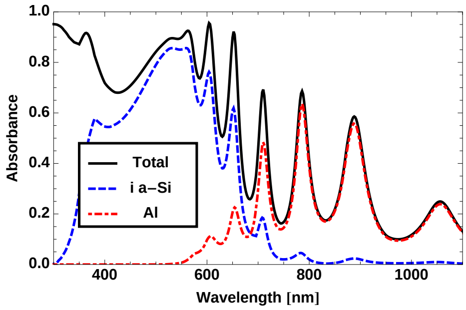



Fig. 1: Layer absorbances for an a-Si:H solar cell calculated with the extended transfer-matrix formalism. The glass and the aluminum layer are treated as incoherent.

Figures 1 and 2 illustrate the use of incoherence in the optical simulation of an a-Si:H solar cell. As the cover glass layer has a thickness of 1 mm it is treated as incoherent in both cases. The interference effects observed in the layer absorbances in Figure 1 in the wavelength rage from 600 to 1000 nm can be attributed to internal reflections in the intrinsic a-Si:H layer. Scattering of the light caused by rough layer interfaces may cause some of the interference effects to average out. Measurements from cells that are built using textured substrates show significantly less interference effects. This may be reproduced by introducing incoherence in the simulation of these devices. Figure 2 illustrates the layer absorbances for the same device as in Figure 1 but with an incoherent intrinsic absorber layer.

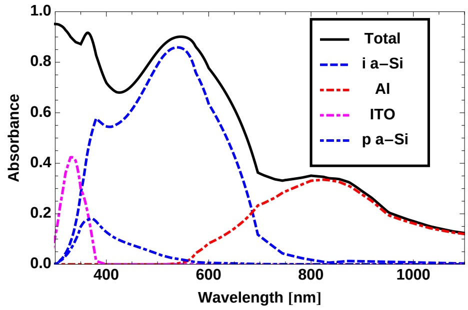



Fig. 2: Layer absorbances for an a-Si:H solar cell calculated with the extended transfer-matrix formalism. The glass, the aluminum and the intrinsic layer are treated as incoherent.

Scattering at rough layer interfaces is employed in thin film silicon solar cells to increase the absorption by prolonging the optical path in the absorbing layers. Even though the suppression of interference effects caused by scattering can be reproduced by incoherence, the increase in absorption can not. For an accurate modeling of solar cells containing rough layer interfaces, scattering needs to be incorporated in the optical model. This is achieved in the net-raditation method. Figure 3 illustrates the layer absorbances of an a-Si:H solar cell containing a rough layer interface that were computed using the net-radiation method.

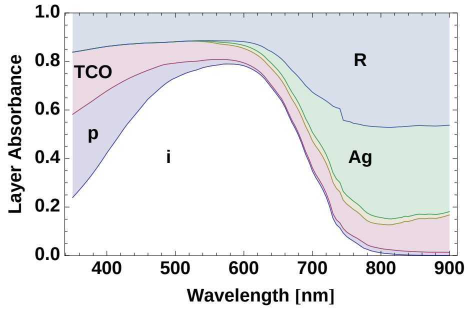



Fig. 3: Layer absorbances for an a-Si:H solar cell calculated with the net-radiation method. The TCO/p interface is rough and scatters the transmitted light.

## 5.4 Three-dimensional full-wave optical simulation of light - emitting diodes

Contributors: Martin Loeser, Beat Ruhstaller

Partners: Osram Opto Semiconductor, Fluxim AG
Funding: ICP
Duration: 2009

Modern light-emitting diodes with material systems optimized for the visible range usually suffer from poor outcoupling efficiencies due to the large refractive index contrast between the semiconductor material and the surrounding air. Taking conventional GaN LEDs as an example, it is well known that internal reflections trap more than 90% of the internally generated light. Many efforts have been made to improve the optical design of such optoelectronic devices, and artificial surface textures are among the most promising approaches for increasing the device efficiency. In general, either random textures such as surface roughening, or systematic textures such as photonic crystals can be applied, and it has already been shown in literature that both approaches can boost the outcupling efficiency.

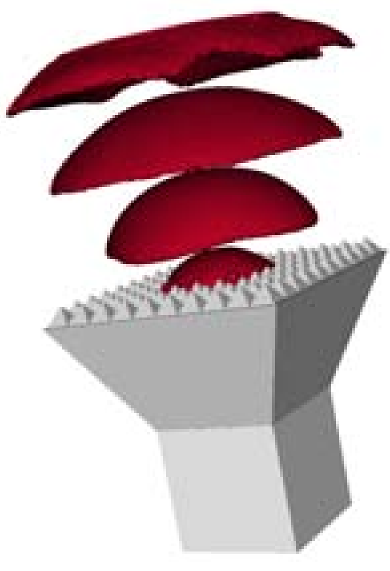


Fig. 1: Light emitted from a device featuring a textured surface.

The design of such surface textures is a challenging task, and to keep development times short numerical simulations are of utmost importance. The lack of particular symmetries in most devices mandates three-dimensional simulations. It is the combination of large simulation domains, inherent for LEDs, and subwavelength structures that makes accurate optical simulations a complicated task. In general, large domains call for approximative ray-optical methods such as ray-tracing whereas small substructures require full-wave methods such as Finite Elements (FEM) or Finite-Difference Time-Domain (FDTD). However, it is well known that for these full-wave methods the computational cost explodes with increasing device size such that so far only small device structures can be efficiently simulated.

This project investigates to which extent a novel and very efficient finite-element based approach—the Ultra-Weak Variational Formulation (UWVF)—can reduce the computational cost when running three-dimensional optical simulations. At present, the ICP is further developing a software, written in C++, that incorporates the UWVF-formalism to solve the optical problem on arbitrary structures.


Fig. 2: Light propagation in a complex structure that has been imported from a CAD tool.

In order to enhance the computational efficiency, the entire software has been parallelized with using the Message Passing Interface. Special care is also taken to guarantee maximum user-friendliness. Thus, the software does not only offer advanced pre- and post-processing features, but also allows to import and simulate arbitrarily complex CAD drawings.

## 5.5 Modeling, simulation and loss analysis of dye-sensitized solar cells

Contributors: Matthias Schmid, Adrian Gentsch, Jürgen O. Schumacher

Partners: EPFL Laboratoire de Photonique et Interfaces (LPI)
Funding: Gebert Rüf Stiftung
Duration: 2008 – 2010

In September 2008 the ICP started a research project for the modeling of dye-sensitized solar cells (DSCs). The objective of this project is to develop validated mathematical models for the DSC. The models aim at describing the coupled optical, electrical and electrochemical processes taking place within the solar cell.
In the past year, we finished the work on the optical part of the model. The optical model allows us to simulate absorption and reflection loss and the spatially resolved sensitizer excited state generation rate. The optical model has been validated by optical reflection and transmission measurements. The generation rate calculated from the optical model serves as an input for the electrical model, which describes the injection of

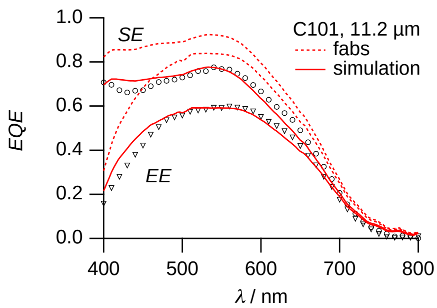



Fig. 1: Measured EQE for illumination from the substrate side (SE, open circles) and the electrolyte side (EE, open triangles) on a $11.2\ \mu m$ thick test cell sensitized with the dye C101. Red bold lines are the simulated EQEs for bothillumination cases. The simulated fraction of absorbed light (dotted red lines) is also shown.

electrons into the $TiO_2$ conduction band and their consequent transport through the nanoporous $TiO_2$ layer. The electrical model takes into account recombination of conduction band electrons with the oxidized electrolyte species (tri-iodide) and trapping of electrons to an exponential distribution of band gap states. Using the coupled optical and electrical model we can calculate the IV characteristics, the external quantum efficiency (EQE) and the spatially resolved concentrations of charged species (electrons and ions) within the DSC. It is also possible to precisely quantify the different loss channels within the DSC. By comparing the measurements of the EQE to our simulations (see Fig. 1), we extracted the relevant model parameters of the stationary model, the electron diffusion length and the electron injection efficiency. The measurements are performed on test DSC cells of different thicknesses sensitized with different dye types and for illumination from both the substrate and the electrolyte sides.
The stationary model has been extended to simulate time-dependent perturbations around the stationary state

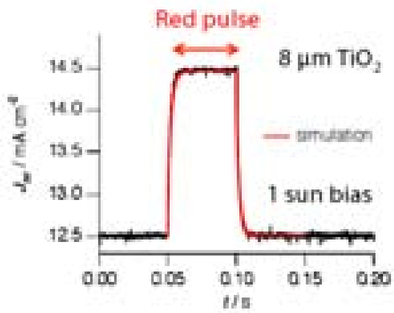



Fig. 2: Simulated (red line) and measured (black line) transient short circuit current density for a small perturbation induced by a red light pulse (642 nm). The DSC was exposed to white bias light from a filtered Xenon lamp.

of the DSC. Comparing the time-dependent measurements to simulations we find the lifetime for conduction band electrons, the effective density of states of trapped electrons and the shape of the (exponential) trap distribution (Fig. 2).
We equipped our simulation software with a graphical user interface (GUI). The GUI allows the user to run the different simulation tools (stationary, transient, impedance spectroscopy) using different sets of parameters. In the forthcoming project year we will further extend our model to incorporate additional physical and electrochemical effects.

## 5.6 Optoelectronic research laboratory

Contributors: Kai Brossi, Martin Neukom, Nils A. Reinke

Partners: Various project partners
Funding: ICP, School of Engineering
Duration: ongoing

True-to-life modeling always is based on accurate input parameters from the real world. The purpose of the optoelectronic research laboratory (O-LAB) is both providing such input parameters and experimentally validating simulation results. Combining advanced computational methods and state-of-the-art experimental methods allows us to develop innovations in measurement engineering.

Fig. 1: Optical microscopy image of an organic photovoltaic cell.

The O-LAB is a consequent expansion of our existing computational toolbox, facilitating the collaboration with experimentally-oriented partners and industry. Our current investigations comprise the following fields of interest:

- Ultra-fast photo-thermal heating and detection
- Thin film optical spectroscopy
- Transient optoelectronic device characterization

Fig. 1 shows an microscopical photography of electrode organic solar cell. An impedance analyzer used for the characterization of organic semiconducting devices is depicted in Fig. 2. Our experimental toolbox comprises fast oscilloscopes, signal generators, impedance analyzers, IR-sources, detectors and cameras, optical flashers and spectrometers covering the spectral range from 0.35 and 14 $\mu$m. A measuring setup for time resolved fluorescence and phosphorescence spectra is currently under construction.

The O-LAB supports industrial needs in the characterization of sensors and actuators and several ICP projects related to thermal labeling, thin-film spectroscopy, organic light emitting devices and photovoltaics. In addition, our laboratory is ideally suited for educational purposes in teaching B.Sc. and M.Sc. students in mechatronics, electronics and informatics. The O-LAB gives young scientists and engineers the possibility of getting in contact with R&D and working on exciting issues in ongoing projects.

Fig. 2: Impedance analysing instruments for organic semiconducting device characterization

## 5.7 Organic electroluminescent pictograms for push-button applications

Contributors: Nils A. Reinke, Roger Häusermann, Beat Ruhstaller

Partners: CSEM, Ciba, EAO
Funding: Commission for Technology and Innovation (CTI)
Duration: 2007 – 2009

The novelty of the envisioned product in this project is the possibility to produce very thin, custom-designed self-luminous pictograms for applications in push-buttons. They combine existing pushbuttons (EAO) with patterned emissive pictograms (CSEM) made from electroluminescent semiconductor materials (Ciba SC). The characterization and optimization of material properties, device and system architecture is supported by computational engineering and simulation software[3] development at ZHAW as illsutrated by prototypes in Fig. 1.

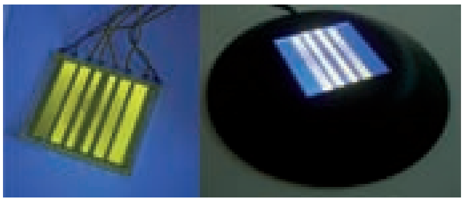


Fig. 1: Transparent PLED (left) and backlighted PLED prototype (right) developed in this project. The combination of blue backlight and yellowish emission from the PLED yields a white color emission.

The numerical simulation activities subdivide into electronic and optical device modeling as well as advanced analysis algorithms. The electronic device model contains charge drift-diffusion and exciton rate equations for modeling organic semiconductor devices including multiple excitons, several charge mobility and injection models and charge doping and trapping. The numerical algorithm delivers charge distribution profiles, transient electroluminescence, as well as current-voltage curves. The optical solver evaluates the angular emission characteristics as well as the substrate, thin-film and plasmon modes. The modes can be visualized and integrated to extract relative mode contributions and position-dependent lifetimes. Key performance figures such as luminous efficacy, CIE, CRI, etc. are calculated. Advanced analysis features allow to extract device parameters, for instance the shape of the emission zone, from experimental data. Our model fits experimental current-voltage curves of PLEDs considering a field dependent charge carrier mobility (cf. Fig. 2).

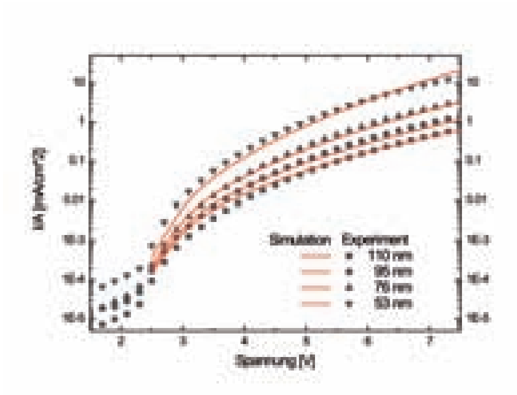



Fig. 2: Experimental and simulated current-voltage curves considering a field dependent mobility.

In large-area OLEDs non-uniformities in the luminance arise from potential drops across a low-conductive electrode. FEM-simulations allow to study such potential drops (cf. Fig. 3).

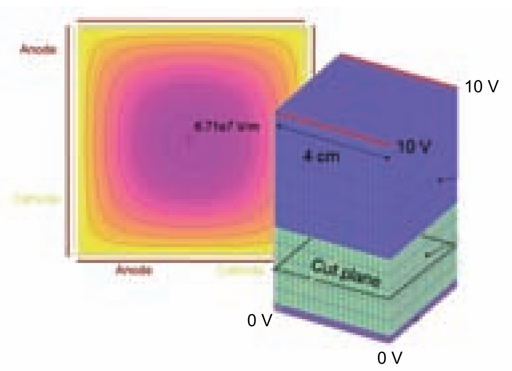



Fig. 3: SESES simulation of the potential drop.

[3] SETFOS Semiconducting Emissive Thin Film Optics Simulator, Fluxim AG, Switzerland, www.fluxim.com.

# Chapter 6

# Student Projects

## 6.1 Characterization of optically pulsed solar cells

Students: Martin T. Neukom

Category: Bachelor thesis
Mentoring: Beat Ruhstaller, Nils A. Reinke
Period: January 2009 – June 2009

Photovoltaic energy conversion is considered as a key technology to secure the worldwide energy need without enforcing climate change. Organic solar cells have the potential of significantly lower costs for solar cells that are flexible, thin and even transparent.

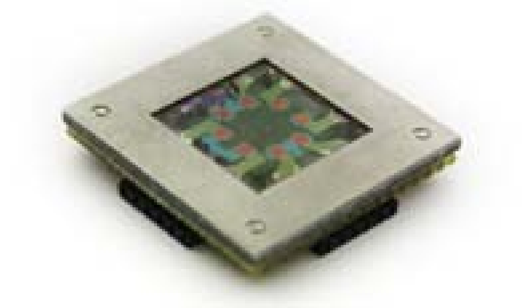


Fig. 1 Sample with 8 Organic Solar Cells

With these possibilities it would be possible to coat the surface of a window with a solar cell or a façade of a building. Despite the flexibility of usage and the huge interest of the industry there is no single product available on the market with this technology. The reason for that is the low power conversion efficiency and the short lifetime. Normally, solar cells are measured with a steady state current voltage characteristic. But this does not allow extracting fundamental physical parameters which are essential to increase the efficiency systematically. A very promising approach is the dynamic measurement. In this thesis a measurement setup was built for pulsed and steady-state measurements on organic solar cells. The recording of IV characteristics was completely automated. Beside established methods in this thesis a new way of measurement has been developed to close the cap between steady state and dynamics. It is based on dynamic measurement after pulsed illumination with variable load resistors. The interpretation of the measured data was done with SETFOS, a simulation software developed by Fluxim AG. With SETFOS organic solar cells can be numerically described. The numerical model includes the light-penetration into the cell as well as the electrical transport of the generated free charge carriers. With simulation the effects that have been measured could be reproduced and quantified. During the Bachelor thesis the cells showed effects of ageing. This effect allowed also elaborating degradation of organic solar cells.

This thesis enables insight into the physical processes of organic solar cells and allows identifying limiting factors for efficiency or lifetime. It contributes to further developments of organic solar cells and to reach market entry of this future technology.

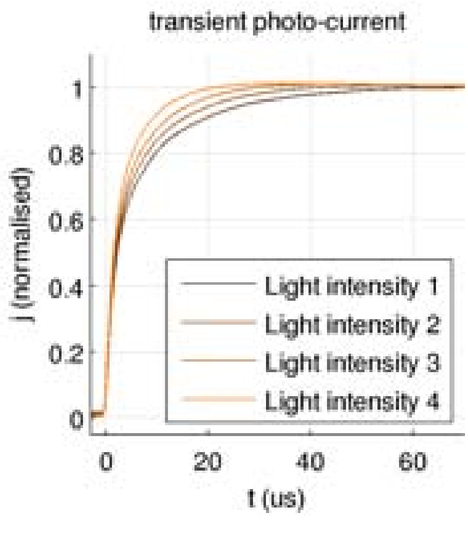



Fig. 2 Transient photo-current with varying light intensity

## 6.2 Transient measurement of electroluminescence in organic light-emitting devices

Students: Kai A. Brossi, Mario Luchsinger

Category: Bachelor thesis
Mentoring: Beat Ruhstaller, Nils A. Reinke
Period: January 2009 – June 2009

The particular attraction of organic light-emitting diodes (OLED) lies in the thin design, the large viewing angle and the high theoretical efficency. Despite these advantages, OLEDs are not widely used on the mass market. Two reasons are the limited efficiency and lifetime. It is widely assumed that those limiting parameters can be identified and quantified by dynamic measurements. The aim of this work is to realize a measurement setup for dynamic characterization of OLEDs.

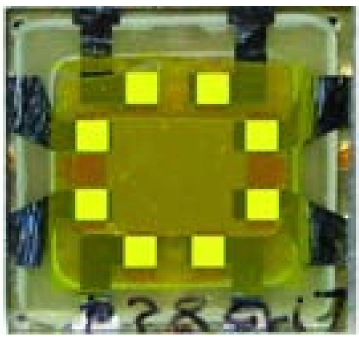


Fig. 1: Sample with eight light-emitting devices.

For the characterization, the applied voltage, the current and the electroluminescence have to be measured. The measurement of electroluminescence makes high requirements concerning sensitivity and response time. To measure the very short rise time and the weak intensity of electroluminescence as exactly as possible, the measurement has been done with a highly sensitive avalanche photodiode (APD) as a detector. The measurement of dark current in unipolar devices gives the feasibility to determine the charge carrier mobility in organic semiconductors. This requires the measurement of a low current in a nanosecond range with high dynamics. To setting up the dark current measurement setup, a new measurement method has been developed, that allows an elegant correction of RC effects. The developed measurement setup gives the possibility to drive 25 OLEDs sequentially. The measured signals can be checked on frequency and voltage dependency by the developed software. The measurement setup has been used to determine the charge carrier mobility in OLEDs. The metrologically determined data has been analyzed with the simulation software SETFOS and compared with the simulated data.

Fig. 2: Measurement box and two compact digital oscilloscopes.

This work has been prepared at the Institute of Computational Physics (ICP) and it helps to validate simulation results obtained by the simulation software SETFOS. The developed measurement setup and methods will be important for the research on OLEDs in the Optical Laboratory at the ICP.

## 6.3 Analysis of the emission profile in organic light-emitting devices

Students: Benjamin Perucco

Category: Master thesis
Mentoring: Beat Ruhstaller, Nils A. Reinke
Period: July 2009 – December 2009

Organic light-emitting devices (OLEDs) are ideal light sources for future display applications, general lighting and chemical sensors for their low power consumption and beneficial emission characterisitics. The outcoupling efficiency of OLEDs is sensitive to the shape of the emission profile. Unfortunately, this shape is typically unknown and the analysis of light extraction is therefore often based on the assumption of a delta-shaped emission profile. The emission profile is determined by the recombination profile and exciton diffusion mechanisms, as well as other electrical and device parameters. Already in the early days, Tang used luminescent sensing layers to estimate the shape of the emission profile. Recently, experimental investigations were performed using a combinatorial method for device fabrication for comprehension of the emission profile and its relation to electrical parameters. In recent years, models have been developed to accurately simulate the optical and electrical behavior of OLEDs. With the help of optical simulation, Roberts illustrated how the shape and location of the emission profile is related to the outcoupling efficiency. There have also been several reports, where simulation results were combined with a fitting method to extract the emission profile. Kuma et al. measured electroluminescence (EL) spectra, which were used for a least-square fit of simulated EL spectra as a function of the emission profile. Generally, a superposition of simulated emission spectra originating from different positions of the emissive dipoles in the light-emitting layer has been used for the determination of the emission profile. Van Mensfoort et al. have presented new aspects of parameter extraction and introduced an asymmetric analytical shape for the description of the emission profile in single-layer polymer LEDs, which goes to zero at the layer boundaries. They studied spectral and angular emission data and estimated the resolution of the method based on the condition number of a related matrix equation. However, I am not aware of any publication where different fitting methods and aspects of parameter extraction (i.e. a linear fitting method vs. a nonlinear fitting method, the incorporation of angular information, multi-emitter OLEDs, noise on the emission spectrum, etc.) have been summarized, evaluated with adequate examples and validated on the basis of consistency checks.

The objective of this study is thus to present and test numerical fitting algorithms for the extraction of the emission profile and source spectrum. This is achieved by an optical model, where a transfer-matrix theory approach for multi-layer systems is used in combination with a dipole emission model. The optical model is implemented in the semiconducting thin film optics simulator (SETFOS). With SETFOS, I simulate the emission spectrum of an OLED based on an assumed emission profile together with a known source spectrum. The fitting methods are then applied to the calculated emission spectra in order to estimate the emission profile and source spectrum. The comparison between the obtained and assumed emission profile and source spectrum is an indication of how successfully the inverse problem can be solved.

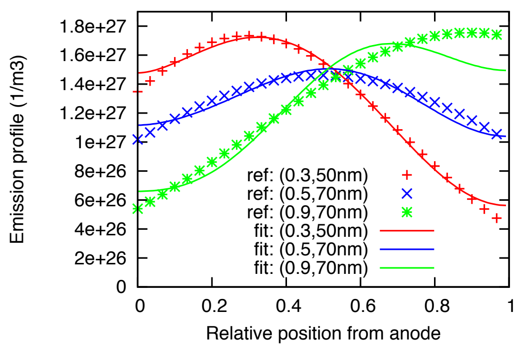



Fig. 1: Comparison between the assumed and extracted emission profiles. A linear method was used here without incorporation of angular information. The values in parenthesis show the combination of parameters used for the assumed emission profile to calculate the emission spectrum. The first value indicates the relative position, the second value stands for the width of the profile.

## 6.4 Benchmarking of optoelectronic device simulations with SETFOS

Students: Michiel Boes

Category: IAESTE internship
Mentoring: Thomas Lanz, Beat Ruhstaller
Period: September 2009

The goal of this internship was to provide an overview of the different fields of research where simulation results can be obtained with the software SETFOS. The topics that were considered are passive optics, light outcoupling in organic light emitting diodes (OLEDs), optical as well as electrical calculations for organic solar cells, fluorescence biosensors and purely electrical simulations for OLEDs. Figure 1 illustrates the result of a reflectance calculation as function of wavelength and incidence angle.

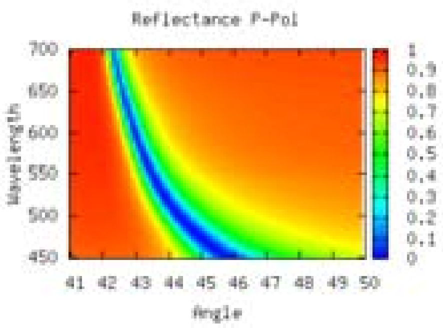



Fig. 1: Dependence of the reflectance on wavelength and incidence angle[1].

One main quantity of interest when optimizing OLEDs is the light outcoupling behavior. SETFOS allows to calculate the emission from such a device as a function of emission angle and wavelength. Figure 2 displays the result of this calculation for a structure based on the materials TPD and Alq [2].

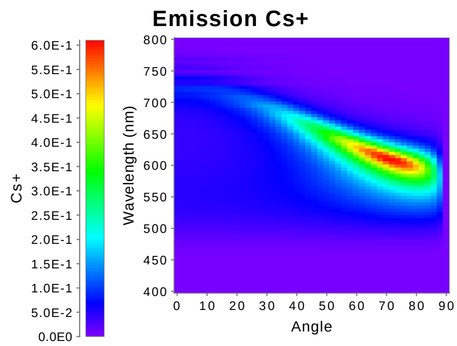



Fig. 2: Study of the outcoupling from an OLED structure as a function of wavelength and outcoupling angle.

One approach to optimize the performance of organic solar cells is to improve the light incoupling into the device by adding a coating layer on the device that minimizes the external reflection [3]. Figure 3 illustrates the effect of a coating layer (cap) on the generation inside an organic solar cell.

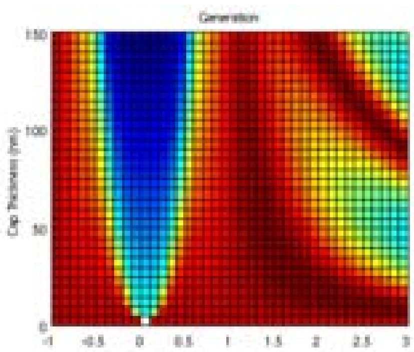



Fig. 3: Influence of the thickness (y-axis) and the index of refraction (x-axis) of a coating layer (cap) on the generation inside an organic solar cell.

[1] Jörg Frischeisen, Christian Mayr, Nils. A. Reinke, Stefan Nowy, Wolfgang Brütting, *Surface plasmon resonance sensor utilizing an integrated organic light emitting diode*, Optics Express 22 (16), 2008

[2] Stefan Nowy, Nils A. Reinke, Jörg Frischeisen, Wolfgang Brütting, *Light extraction and optical loss mechanisms in organic light-emitting diodes*, Experimental Physics IV, University of Augsburg, 86135 Augsburg, Germany

[3] Brendan O'Connor, Kwang H. An, Kevin P. Pipe, Yiying Zhao, Max Shtein, *Enhanced optical field intensity distribution in organic photovoltaic devices using external coatings*, Applied Physics Letters 89 (2006) 233502

## 6.5 High Performance Grating Spectrometer

Students: Martin Neukom, Simon Hübscher

Category: Project Work in Mechatronics
Mentoring: Nils A. Reinke, Christoph Stamm
Period: Oktober 2008 – Januar 2009

In this work a grating spectrometer with a focal length of $30\mathrm{cm}$ is constructed from scratch. The exploded assembly drawing in Fig. 1 shows the external and internal compartments of the device. The spectrometer offers both fixed entrance slits ranging from $20\mu\mathrm{m}$ to $1\mathrm{mm}$ and an adjustable entrance slit. An additional mount allows to connect optical fibers to the device. A holographic grating with 1200 $\mathrm{lines/mm}$ is used as a dispersive element. The concave curvature of the grating defines the focal length of the device making additional optical components needless. The curved grating thus allows a very compact design of the device and reduces optical aberrations and losses. The spectrum is detected with a highly sensitive CCD line sensor comprising 3000 pixels.

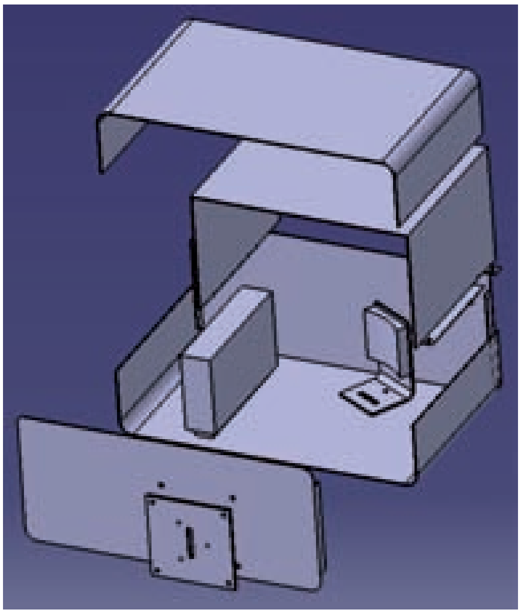


Fig. 1: Exploded assembly drawing of the spectrometer comprising the internal and external body, the mounted holographic grating and the CCD line sensor.

The inner shielding of the device encapsulates the CCD sensor from optical noise. The detectable spectrum ranges from $450\mathrm{nm}$ to $750\mathrm{nm}$ at a maximum spectral resolution of 0.1 nm depending on the width of the entrance slit. The sensor is both powered and controlled by an USB 2.0 interface. The developed LabView software allows calibrating both spectral positions and absolute intensities by a build-in polynomial fitting routine and reading calibration data from a file, respectively. A screenshot of the developed LabView software is displayed in Fig. 2. The software offers the basic functionality of background subtraction and setting the integration time. During long acquisition processes the user is informed about remaining recording time. Transient processes can be recorded at a speed of 300 scans per second which can be accelerated up to 3000 scans per second using an alternative line sensor.

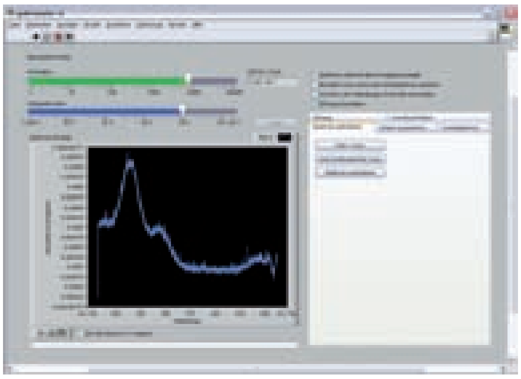


Fig. 2: Spectrometer software developed in LabView.

This high performance spectrometer offers high resolution, high sensitivity and high speed making it competitive with upper-class commercial products. This spectrometer will thus be a valuable tool for prospective projects in the field of thin-film optical spectroscopy and bio-sensing applications.

## 6.6 Reflectometer with algorithm for refractive index extraction

Students: Oliver Kunz, Felix Müller

Category: Bachelor Thesis
Mentoring: Beat Ruhstaller, Nils A. Reinke
Period: February 2009 – June 2009

The task of this bachelor thesis was to develop a reflectometer. A reflectometer is a device to measure reflectance of film systems and is used to determine characteristics such as thickness and refractive index of thin film systems like solar cells and light emitting diodes (LEDs). More precisely, light is coupled into a Y-glass fiber to irradiate the film system. The outer channel of the fiber guides the reflected waves back towards a spectrometer, where the reflected light intensity is measured. Subsequently a mathematical algorithm is used to fit the measured data to the physical model, defined by the user. In this way, unknown and/or variable parameters of the film system can be determined. This thesis is concentrated on building the respective measurement setup and on developing an analysis software. The spectrometer mentioned was developed in a previous student thesis [4].
The user interface and the measuring procedures were implemented using the graphical programming language LabVIEW. The user can enter specifications and estimations of the respective film system and perform the measurement. Due to performance reasons, fitting the physical model to measurement data is implemented using the programming language C. A DLL interface links the two implementations. As a physical model of thin film optics, parts of the software *Setfos* of Fluxim AG were implemented and extended. The challenge of this thesis was the interaction between measuring technique, numerical optimization algorithms and optics. The developed software provides interfaces between user and the various program modules. It is capable of determining refractive index parameters of various models (Cauchy, Tauc-Lorentz oscillator) as well as film thicknesses with nanometer accuracy.

Fig. 1: Measurement setup of the reflectometer. The graphical user interface of reflectometer software is visible on the screen. The measurement setup including spectrometer, light source and sample fixture is shown in the front.

[4] Semester thesis *"High Performance Grating Spectrometer"* by Martin Neukom and Simon Hübscher.

## 6.7 Motorisiertes Reflektometer zur optischen Charakterisierung von Dünnschichtsystemen

Students: Timon Löw, Joel Lehner

Category: Projektarbeit
Mentoring: Nils A. Reinke, Beat Ruhstaller
Period: September 2009 – Januar 2009

Wichtige Parameter für die opto–elektronische Simulation von Solarzellen sind das Streuverhalten, Brechungsindizes, die Absorptivitäten sowie die Dicken ihrer einzelnen Schichten. Die Qualität der durchgeführten Simulationen steigt und fällt mit der Güte dieser Parameter. Eine effiziente Methode zur Bestimmung der genannten Parameter ist die so genannte Reflektometrie, bei welcher das Reflexionsvermögen von einer Probe als Funktion der einfallenden Wellenlänge gemessen wird. In Vorarbeiten wurde ein Reflektometer mit einer Y-Glasfaser, einer Faserlichtquelle und einem Faserspektrometer aufgebaut, welcher die Reflektivität eines Schichtsystems bei einem festen Winkel von 90° misst. Die Messdaten können automatisiert mit einem PC ausgewertet und die Probenparameter Brechungsindex, Absorptivität und Schichtdicke numerisch ermittelt werden.

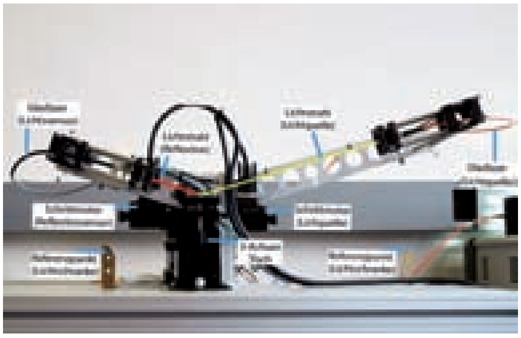


Abb. 1 Aufgebautes Reflektometer mit motorisierten Sende- und Empfangsarm.

In dieser Projektarbeit wurde aufbauend auf bisherigen Vorarbeiten ein motorisiertes Reflektometer konzipiert, welches eine automatisierte Reflexionsmessung unter variablen Einfalls- und Ausfallswinkel erlaubt. Die mit diesem Instrument gewonnenen Messdaten sollen die Extraktion von Brechungsindizes von dünnen Schichten (n,k–Daten) sowie Die Ermittlung von winkelabhängigen Verteilungsfunktionen von Grenzschichten ermöglichen, welche die Lichtstreuung an Grenzflächen innerhalb von Solarzellen beschreiben. Die Arbeit umfasste die folgenden Punkte:

- Konzeption und Aufbau eines Reflektometers mit motorisierten Sende- und Detektorarm
- Konzeption und Aufbau einer Faserlichtquelle
- Ansteuerung des Aufbaus unter LabView und Entwicklung einer graphischen Benutzerschnittstelle

Die Abbildungen 1 und 2 zeigen das aufgebaute motorisierte Reflektometer und die entwickelte graphische Benutzeroberfläche. Das Reflektometer wird in laufenden und zukünftigen Projekten für die Charakterisierung und Optimierung von Solarzellen eingesetzt.

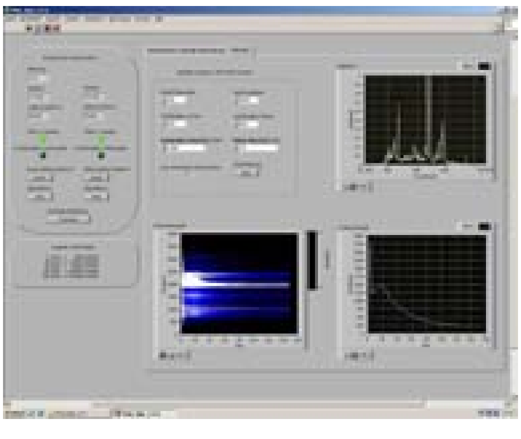


Abb. 2 Graphische Benutzeroberfläche zur Steuerung des motorisierten Reflektometers.

## 6.8 Innovative Schichtcharakterisierung mit Hochgeschwindigkeits-Infrarot-Sensorik

Students: Markus Suter, Nenad Tripic

Category: Praktikumsarbeit
Mentoring: Nils A. Reinke, Andor Bariska
Period: January 2009 – June 2009

Seit Jahren bedient man sich der Infrarot-Technologie, beispielsweise für einfache Anwendungen, wie in Fernbedienungen für elektronische Geräte oder die Beheizung von Raumstationen. Aufgrund des breiten Wellenlängenbereichs deckt die Infrarot-Technologie eine riesige Vielfalt an Anwendungen ab.
In dieser Arbeit werden Teile eines photothermischen Messsystems zur Untersuchung von Beschichtungen untersucht und optimiert. Das photothermische Messsystem ist in Kollaboration zwischen dem ICP und dem IDP entstanden und soll bestehendes Messproblem der Industrie lösen: Die Charakterisierung von Schichtsystemen auf elektrisch nicht leitfähigen Substraten aus Kunststoff oder Keramik.

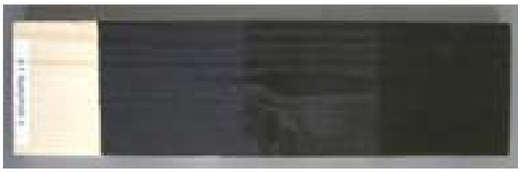


Abb. 1 Testprobe Acryllack auf Naturholzuntergrund.

In Vorarbeiten wurde bereits ein erster Prototyp des Messsystems entwickelt. Dieser beleuchtet die zu untersuchende Materialoberfläche mit einem kurwelligen Xenon–Lichtblitz und erhöht somit für einen kurzen Moment die Oberflächentemperatur. Gleichzeitig misst eine Infrarotkamera die von der Oberfläche ausgehende Wärmestrahlung.
Mit Hilfe der experimentell ermittelten Übertragungsfunktion lassen sich die Parameter des zugrundeliegenden Schichtsystems bestimmen. In dieser Projektarbeit wurden die Limitierungen und das Potential des bestehenden Prototyps anhand von Messungen und Messdatenanalyse ermittelt. Verbesserungen am Prototypen sollen helfen, das Potential dieser innovativen Messmethode voll auszuschöpfen.

Abb. 2 Mikroskopische Aufnahme der Testprobe in Längsschnitt.

Es konnten die folgenden Arbeitspakete erfolgreich ausgeführt werden:

- LabView–Steuerung des Offset-Abgleichs der IR–Kamera
- Aufbau einer Bibliothek aus Testproben
- Messung und Auswertung der Testproben

Bei einer der Testprobe handelt es sich um eine mit einem Acrlyllack mehrfach beschichtete Naturholzplatte (siehe Abb. 1). Wie in der mikroskopischen Aufnahme in Abb. 2 zu erkennen ist, zieht der Acryllack nach der Beschichtung in die Naturholzplatte ein. Neben der photothermischen Schichtcharakterisierung existieren keine zerstörungsfreie Messmethoden, solche Effekte gezielt zu untersuchen.

## 6.9 Aufbau und Inbetriebnahme eines Experimental - Holzvergasers

Students: Claudio Roffler, Fabian Senn, Marcel Weiss

Category: Bachelorarbeiten Maschinentechnik
Mentoring: Thomas Hocker, Christoph Meier, Markus Weber (ITFE)
Period: Juni - August 2009

Unter der Holzvergasung versteht man den verfahrenstechnischen Prozess der Teilverbrennung unter Luftmangel, um aus Holz ein brennbares Gasgemisch zu gewinnen. Im Rahmen zweier Bachelorarbeiten ist ein Holzvergaser aufgebaut und in Betrieb genommen worden. Nebst dem mechanischen Aufbau ist viel Zeit in die umfangreicher Messtechnik investiert worden, da der Vergaser zur Modellvalidierung eingesetzt werden soll.

Abbildung 1: Experimental-Holzvergaser auf dem Dach des Maschinenlabors

Insgesamt wurden zehn Messungen durchgeführt. Mit Ausnahme der eingesetzten Biomasse kann der Prozess ausschliesslich über die zugeführte Luftmenge gesteuert werden. Der auf den Reaktordurchmesser bezogene Luftmassenstrom ist dabei zwischen 35 und 200 g/($m^2$s) variiert worden. Die Luftüberschusszahl $\lambda$ bewegte sich dadurch zwischen 0.23 und 0.95 ($\lambda$ = 1 bedeutet stöchiometrische Verbrennung), die Flammfrontgeschwindigkeit zwischen 0.12 und 0.21 mm/s, der Restkohlenanteil zwischen 2 und 28 Massen-% bezüglich der unvergasten, trockenen Biomasse.

Abbildung 2: Erste Zündung des Vergasers durch Marcel Weiss

Bei drei Versuchen wurde ausserdem die Gaszusammensetzung ermittelt. Die erste Stufe der Messgasaufbereitung besteht aus einer beheizten Gasentnahmesonde und einem Kondensatabscheider. Die Kühlung ist mit einem Abscheiden von Teeren verbunden, da diese als längere Kohlenwasserstoffe bei Raumtemperatur nicht mehr gasförmig vorliegen. Die eigentliche Teerabscheidung erfolgt in Waschflaschen mit Rapsöl, in welchem die entstandenen Teere eine gute Löslichkeit aufweisen. Nach einem Feinfilter werden die Gasspecies $\mathrm{CO}$, $\mathrm{CO_2}$, $\mathrm{CH_4}$ infrarotbasierend und $\mathrm{H_2}$ mittels Wärmeleitfähigkeitssensor gemessen. Die Elementarbilanz für die Elemente C, H, O und N ist befriedigend genau ausgefallen, was auf ein funktionierendes Messkonzept hindeutet. Die Durchführung von Versuchen ist noch störungsanfällig. Auf der Prozessseite soll der kontinuierliche Betrieb des Reaktors die Bilanzierung vereinfachen und die Reproduzierbarkeit der Messungen verbessern. Hierzu sind Vorschläge ausgearbeitet und zum Teil bereits umgesetzt worden.

# 6.10 Optimierung eines Prüfstands für thermomechanische Belastungstests von Hochtemperatur-Brennstoffzellen

Students: Marcio Ferreira dos Santos, Jakob Spillmann

Category: Bachelorarbeit Maschinentechnik
Mentoring: Thomas Hocker sowie Dirk Haberstock und Thomas Gamper (Hexis AG)
Period: 15. Juni bis 17. August 2009

Der Brennstoffzellen-Stapel bildet den Kern der Brennstoffzellen-Heizgeräte der Hexis AG, Winterthur. Die Hexissysteme sind mit ca. 60 Keramik-Brennstoffzellen bestückt. Um Erkenntnisse über das Verhalten der Zellen bei inhomogenen Zellentemperaturen zu erhalten, wurde in vorangegangen Studentenarbeiten ein Prüfstand für thermomechanische Belastungstest entwickelt. Mit diesem Prüfstand werden Versuche durchgeführt, in denen die Brennstoffzellen durch vorgegebene Temperaturgradienten zerstört werden. Die auftretenden Zellenrisse werden über einen Akustiksensor detektiert, siehe Fig. 1

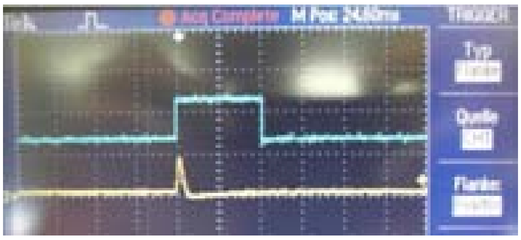



Fig. 1 Akustiksignal aufgrund eines thermisch induzierten Risses der Brennstoffzelle.

In dieser Bachelorarbeit soll dieser Prüfstand optimiert werden. Wichtig sind dabei eine deutliche Verkürzung der Versuchsdauer, das Detektieren des Risszeitpunktes und das Erhöhen der maximal erreichbaren homogenen Temperaturverteilung. Im Prüfstand (siehe Fig. 2) wird die Brennstoffzelle zwischen zwei übereinander angeordneten Stahlplatten eingeklemmt. Die obere Stahlplatte kann durch drei unabhängige Heizungen erhitzt werden. An der unteren Platte sind Temperatursensoren und die Anbindung an einen Akustiksensor, welcher den Zellbruch registriert, angebracht.
Ein typischer Messzyklus läuft wie folgt ab: zuerst wird der Prüfstand homogen auf eine Basistemperatur aufgeheizt, dann wird ein Temperaturgradient induziert und so lange erhöht, bis die Zelle bricht. Anschliessend wird abgekühlt. Mit einer Vielzahl an Verbesserungsmassnahmen wurde der Prüfstand Schritt für Schritt optimiert. Durch den Einsatz einer Isolationsbox, einer verbesserten Regelung und einem Redesign des Prüfstands konnte die Aufheizzeit von 103 min auf 12.5 min verkürzt werden. Das Verwenden einer aktiven Kühlung erbrachte eine Zeitersparnis von weiteren 20 min. Insgesamt wurde die Zykluszeit von 170 min auf 50 min verkürzt.
Eine verbesserte Anbindung des Akustiksensors an den Prüfstand erlaubt nun ein zuverlässiges Erkennen des Zellrisses, solange die Keramikummantelung intakt bleibt. Die maximal erreichbare Basistemperatur konnte von 255°C auf 500°C erhöht werden. Zudem wurde die Regelung optimiert und der Prüfstand beinahe vollständig automatisiert. In FE-Rechnungen wurde die T-Verteilung über der Zelle simuliert, siehe Fig. 3. Das Modell konnte anhand der Messdaten verifiziert werden.

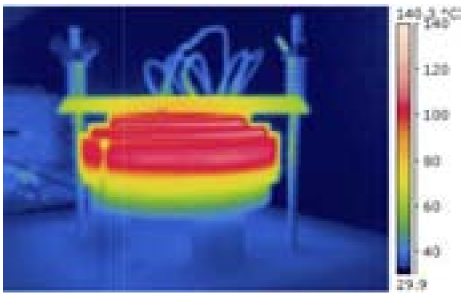



Fig. 2 Wärmebildaufnahme des Prüfstands.

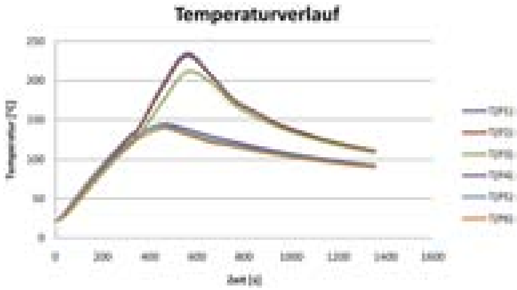



Fig. 3 Seses FE-Rechnungen der T-Verteilung über die Zelle als Funktion der Zeit.

## Chapter 7

# Appendix

## 7.1 Scientific Publications

- J.O. Schumacher, J. Eller, G. Sartoris: *A 2+1D Model of a Proton Exchange Membrane Fuel Cell with Glassy-Carbon Micro-Structures, 6th Vienna International Conference on Mathematical Modelling*, ARGESIM-Publishing House, ARGESIM Report no. 34, Eds. I. Troch and F. Breitenecker, ISBN 978-3-901608-34-6, Vienna, Austria, 2396–2405 (2009).
- S. Wenger, M. Schmid, G. Rothenberger, M. Grätzel, J.O. Schumacher: *Model-based Optical and Electrical Characterization of Dye-Sensitized Solar Cells*, 24th European Photovoltaic Solar Energy Conference EU PVSEC, Hamburg, Germany, 21-25 September 2009 (2009).
- Th. Lanz, B. Perucco, D. Rezzonico, F. Müller, N. A. Reinke, R. Häusermann, B. Ruhstaller: *Optical Simulation of Arbitrary Thin Film Solar Cells with Rough Interfaces*, 24th European Photovoltaic Solar Energy Conference and Exhibition EU PVSEC, Hamburg, Germany, 21-25 September 2009 (2009).
- Y. Safa and T. Hocker: *Numerical Simulation of Reactive Transport Phenomena in the Hexis SOFC Stack*, ECS Transactions, 25 (2) 1221-1230 (2009).
- Y. Safa and J. O. Schumacher: *Numerical Modelling of The Two Phase Transport in a PEM Fuell Cell*, Proceedings of Third European Fuel Cell Technology & Applications Piero Lunghi Conference EFC2009,161–162 (December 15-18, 2009).
- R. Häusermann, E. Knapp, M. Moos, N. A. Reinke, Th. Flatz, and B. Ruhstaller: *Coupled optoelectronic simulation of organic bulk-heterojunction solar cells: Parameter extraction and sensitivity analysis*, J. Appl. Phys. 106, 10450 (2009).
- J. Frischeisen, N. A. Reinke, W. Brütting: *ORGANIC EMITTERS: OLEDs enable integrated surface-plasmon-resonance sensor*, Laser Focus World Art. No. 359812 (2009).

## 7.2 News Articles

- B. Ruhstaller: *Organische Solarzellen eröffnen kostengünstige Möglichkeiten*, energeia Newsletter des Bundesamts für Energie, Ausgabe 6 (November 2009).
- H.U. Schwarzenbach: *Möglichkeiten und Grenzen der Modellbildung*, Innovation (Juni 2009).
- R. Häusermann and B. Ruhstaller: *Organische Solarzellen*, SEV Bulletin (Mai 2009).
- B. Ruhstaller: *Brillante Bilder und leuchtende Wände*, Polyscope (April 2009).

## 7.3 Conferences and Workshops

- B. Ruhstaller: *Optoelectronic simulation of organic semiconductor devices for displays, lighting and photovoltaics*, Case Study Seminar Computational Science and Engineering at ETHZ, Zürich, 26 February (2009).
- J. O. Schumacher and Y. Safa: *Numerical simulation of transport phenomena in PEM fuel cells*, ALGORITMY 2009 Conference on Scientific Computing, Vysoke Tatry, Podbanske March 15-20 (2009).
- E. Knapp, H. Schwarzenbach, R. Häusermann, N. A. Reinke, B. Ruhstaller: *Advanced Simulation Methods for Charge Transport in OLEDs*, Deutsche Physikalische Gesellschaft (DPG) Frühjahrestagung, Symposium Organic Photovoltaics, Dresden, March (2009).
- N. A. Reinke, R. Häusermann, E. Knapp, M. Moos, T. Flatz, B. Ruhstaller: *Fully Coupled Opto-electronic Modelling of Organic Solar Cells*, Deutsche Physikalische Gesellschaft (DPG) Frühjahrestagung, Symposium Organic Photovoltaics, Dresden, March (2009).

- R. Häusermann, N. A. Reinke, E. Knapp, T. Flatz, M. Moos, B. Ruhstaller: *CT-State Dissociation and Charge Carrier Recombination in OPV cells*, Deutsche Physikalische Gesellschaft (DPG) Frühjahrestagung, Symposium Organic Photovoltaics, Dresden, March (2009).
- N.A. Reinke, R. Häusermann, E. Knapp, M. Moos, T. Flatz, B. Ruhstaller: *Fully Coupled Opto-electronic Modelling of Organic Photovoltaic Cells*, Hybrid and Organic Photovoltaics Conference (HOPV), Benidorm, Spain, 10-13 May (2009).
- Häusermann, Reinke, Ruhstaller: *CT-State Dissociation and Charge Recombination in Organic Photovoltaic Cells*, Hybrid and Organic Photovoltaics Conference (HOPV), Benidorm, Spain, 10-13 May (2009).
- B. Ruhstaller: *Organische Halbleiterbauelemente für Bildschirme, Beleuchtung und Photovoltaik: Modellbildung und Simulation*, Electrosuisse Fachtagung "Elektronik der Zukunft", Winterthur, 2. Juli (2009).
- B. Ruhstaller, R. Häusermann, N.A. Reinke: *Comprehensive simulation of organic solar cells*, 2nd International User Workshop 2009, Winterthur, July (2009).
- B. Ruhstaller, E. Knapp: *Advanced simulation of charge transport in OLEDs*, 2nd International User Workshop 2009, Winterthur, July (2009).
- B. Ruhstaller: *Next Generation (Organic) PV: Modeling and Simulation*, 3rd Generation Photovoltaics Meeting of the Swiss Laser Net, CSEM Basel, Switzerland, 19 August (2009).
- S. Wenger, M. Schmid, G. Rothenberger, M. Grätzel and J.O. Schumacher: *Model-based optical and electrical characterization of dye-sensitized solar cells*, 24th European Photovoltaic Solar Energy Conference and Exhibition (EU PVSEC), Hamburg, Germany, September (2009).
- Th. Lanz, B. Perucco, D. Rezzonico, F. Müller, N. A. Reinke, R. Häusermann, B. Ruhstaller: *Optical Simulation of Arbitrary Thin Film Solar Cells with Rough Interfaces*, 24th European Photovoltaic Solar Energy Conference and Exhibition (EU PVSEC), Hamburg, Germany, September (2009).
- B. Ruhstaller: *OLEDs für Beleuchtung*, FutureLight Meeting, ZHAW, Winterthur, 22 October (2009).
- B. Ruhstaller: *Forschung an Solarzellen der nächsten Generation*, Nationaler Tag der Technik an der ZHAW, Winterthur, 10 November (2009).
- Y. Safa, T. Hocker: *Numerical Simulation of Reactive Transport Phenomena in the Hexis SOFC-Stack: Modelling Concept & Numerical Methods*, 216th ECS Meeting and 11th International Symposium on Solid Oxide Fuel Cells (SOFC-XI), Vienna, Austria, October 4-9, (2009).

## 7.4 Prizes and Awards

- Martin Neukom received the *Thales–Preis* for his Bachelor Thesis *Characterisation of optical pulsed solar cells*.

## 7.5 Teaching

### Bachelor of Science

- ”Mathematik für Ingenieure 1” (MAE 1) **- R. Axthelm**
- ”Diskrete und Numerische Mathematik” für Mechatroniker (DNM) **- H. Schwarzenbach**
- ”Signale und Systeme 1” (SiSy 1) **- J.O. Schumacher**
- ”Signale und Systeme 2” (SiSy 2) **- J.O. Schumacher**
- ”Physik 1” für Maschinentechniker (PHMT1) **- M. Schmid**
- ”Physik 1” für Wirtschaftsingenieure (PhWI 1) **- T. Lanz**
- ”Physik 1” für Unternehmensinformatiker (PhUI 1) **- N. A. Reinke**
- ”Physik 2” für Maschinentechniker (PHMT2) **- J.O. Schumacher**
- ”Physik 2” für Wirtschaftsingenieure (PhWI 2) **- M. Roos**
- ”Physik 2” für Unternehmensinformatiker (PhUI 2) **- N. A. Reinke**
- ”Modellbildung und Simulation für Material- und Verfahrenstechniker (MBS)” **- Th. Hocker**
- ”Mensch, Technik, Umwelt” für Maschinentechniker (MTU)**- Th. Hocker**

### Master of Science

- ”Material Properties of Crystals / Tensors for Engineers” (Engineering)**- M. Roos**
- ”Heat and Mass Transfer with Two-Phase Flow” (Engineering) **- Th. Hocker**
- ”Multiphysics Modelling and Simulation” (Engineering) **- J.O. Schumacher**
- ”Applied Photonics” (Mirco and Nano Technolgoy) **- B. Ruhstaller**

## 7.6 ICP Team Members

The ICP team members as of December 2009 are listed below.

| Name | Title | Function |
|---|---|---|
| Axthelm, Rebekka | Dr. rer. nat., Dipl. Math | Research Associate |
| Brossi, Kai | B.Sc. in Systems Engineering | Research Assistant |
| Flatz, Thomas | Dipl. Ing. FH | MSE Student |
| Gentsch, Adrian | B.Sc. in Systems Engineering | Research Assistant |
| Häusermann, Roger | Dipl. Phys. ETH | Research Assistant, PhD student |
| Hocker, Thomas | Prof. Dr. Chem. Eng. | Lecturer |
| Knapp, Evelyne | Dipl. Rech. Wiss. ETH | Research Assistant, PhD Student |
| Lanz, Thomas | M.Sc. Physics ETH | Research Assistant, PhD Student |
| Lindner, Markus | MSc. in Engineering | MSE Student |
| Loeser, Martin | Dr. sc. ETH, Dipl. Ing. TUM | Research Associate |
| Neukom, Martin | B.Sc. in Systems Engineering | Research Assistant |
| Odermatt, Beat | Dipl. Ing. FH | Research Associate |
| Perucco, Benjamin | Dipl. Ing. FH | Research Assistant, MSE Student |
| Reinke, Nils A. | Dr. rer. nat., Dipl.-Phys. | Lecturer |
| Roos, Markus | Prof. Dr., Dipl. Phys. ETH | Lecturer |
| Ruhstaller, Beat | Prof. Dr., Dipl. Phys. ETH, e-MBA | Lecturer, Head of the ICP |
| Safa, Yasser | Dr. ès sc., MSc. | Research Associate |
| Sartoris, Guido | Dr., Dipl. Phys. ETH | Research Associate |
| Schmid, Matthias | Dr. ès sc., Dipl. Phys. ETH | Research Associate |
| Schwarzenbach, Hansueli | Prof. Dr., Dipl. Math. ETH | Lecturer |
| Schumacher, Jürgen | Dr. rer. nat., Dipl.-Phys. | Lecturer |
| Tiefenauer, Andreas | Dipl. Ing. FH | MSE Student |
| Toniolo, Lilian | | Administrative Assistant |

The following visiting scientists were staying at the ICP for some time during 2009:

- Michiel Boes, IAESTE trainee, Ghent University, Belgium: August – September 2009
- Remo Ritzmann, LED Hardware Designer, Pfunzle.ch, Switzerland: May 2009

## 7.7 Location and Contact Info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