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of Applied Sciences

School of Engineering

ICP Institute of Computational Physics

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Research & Development

Beispiel einer virtuell konstruierten Mikrostruktur. Diese wird mit Hilfe eines stochastischen Simulationsansatzes mit kontrollierter Variation der relevanten Transportparameter wie Tortuosität oder Konstriktivität erstellt. Dargestellt mit Visualisierung von Transport-Stromlinien.

Example of a virtual microstructure produced with a stochastic simulation approach with controlled variation of transport relevant parameters as tortuosity or constrictivity together with visualization of transport streamlines.

Contents

Vorwort

Auf welche Energie vertrauen Sie?

«Das Vertrauen in die Kernenergie nimmt zu» titelte 2008 eine Medienmitteilung der «swissnuclear», Fachgruppe Kernenergie der swisselectric.[1] Im Frühling 2011 hätte das Ergebnis der schweizweiten Telefonbefragung wahrscheinlich anders ausgesehen. Die Katastrophe von Fukushima erschütterte auf der ganzen Welt das Vertrauen in die Beherrschbarkeit der Kernenergie.[2]
Setzte die Schweiz in der Vergangenheit hauptsächlich auf die beiden Eckpfeiler Wasserkraft und Kernenergie, so haben Bundes- und Nationalrat mittlerweile den Ausstieg aus der Kernenergie beschlossen.[3] Um Alternativen zu entwickeln, sind neue Konzepte gefragt. Klar ist, dass es keine einfache Lösung geben wird. Die Kernenergie wird nicht durch eine einzige Technologie ersetzt werden können. Anstatt dessen ist ein breiter Mix an Massnahmen in den Bereichen Effizienztechnologie, Elektrizitätsübertragung, Energiespeicherung sowie der Bereitstellung von Elektrizität gefragt.[4] Neben zentralen Grosskraftwerken werden auch dezentrale, auf bestimmte Anwendungen massgeschneiderte, Lösungen eine Rolle spielen.
Die Wissenschaftler des Institute of Computational Physics (ICP) beschäftigen sich schon seit einigen Jahren mit Themen der dezentralen Energieversorgung. Dazu zählen Brennstoffzellen für mobile und stationäre Anwendungen (Kapitel 2) sowie neue Typen von Solarzellen (Kapitel 3). Effiziente Energienutzung ist ein wichtiges Merkmal der Displays und Beleuchtungen auf Basis organischer Halbleiter (OLEDs) in Kapitel 3.
Dass wir bei aller Euphorie über die Mitgestaltung der Energiezukunft nicht die Bodenhaftung verlieren, verdanken wir dem starken Praxisbezug unserer Projekte – nicht nur im Energiebereich, sondern auch in anderen Anwendungsgebieten wie beispielsweise der Thermografie. Zur kontaktlosen Messung von Beschichtungen haben wir zusammen mit unserer Spin-Off-Firma Winterthur Instruments ein eigenes Gerät entwickelt, den «CoatMaster».[5]
An dieser Stelle möchte ich allen Mitarbeitern unseres Instituts für ihr grosses Engagement, ihre Begeisterungsfähigkeit und die tolle gegenseitige Unterstützung ganz herzlich danken.

Thomas Hocker
Institutsleiter

[1] www.swissnuclear.ch/upload/cms/user/MM_Eckwertstudie.pdf
[2] en.wikipedia.org/wiki/Fukushima_Daiichi_nuclear_disaster
[3] www.drs.ch/www/de/drs/tagesthema/272551/275400.nationalrat-beschliesst-atomausstieg.html
[4] www.sbf.admin.ch/htm/dokumentation/publikationen/forschung/11.06.06.NFO.StandPerspektivenEnergieforschung_d.pdf
[5] www.winterthurinstruments.com/

Preface

In what type of energy technology do you believe?

«The confidence in nuclear power is increasing» was the title of a press release by the expert group «swissnuclear» in 2008.[1] In spring 2011 the outcome of this telephone survey most probably would have been the opposite. The Fukushima disaster had just happened and was a shock to the whole world. It definitely undermined our trust in the safety and manageability of nuclear power.[2]
In the past Switzerland relied on hydro-electric and nuclear power as primary electricity sources. However, later in 2011, both the Swiss Federal Council and the Swiss Parliament decided to abandon nuclear power in the long run.[3] To develop alternatives new concepts and ideas are now in urgent demand. It is already clear that there is no simple solution. There won't be a single new technology to substitute today's nuclear power capacities. Instead a mix of new technologies in the fields of energy efficiency, energy storage, and electricity transmission seems to be our best bet.[4] Large, central power stations most probably will be complemented by decentralized and custom-made combined heat and power applications.
Researchers at our Institute of Computational Physics (ICP) have already worked for many years on solutions for decentralized energy supplies. Projects are performed on mobile and stationary applications of fuel cells (chapter 2) as well as on new types of solar cells (chapter 3). The efficient usage of electricity is a key feature of displays and illuminants based on organic semiconductors (OLEDs) discussed in chapter 3.
Since our research has a highly practical component there is no danger in loosing grip. This is not only true for our work on energy topics, but also for example for our thermography applications. In collaboration with our spin-off company Winterthur Instruments, we developed the «CoatMaster», a device for the non-destructive measurement of coating thicknesses.[5]
At this point I would like to thank my colleagues for their strong commitment, their enthusiasm and mutual support.

Thomas Hocker
Head of the institute

[1] www.swissnuclear.ch/upload/cms/user/MM_Eckwertstudie.pdf
[2] en.wikipedia.org/wiki/Fukushima_Daiichi_nuclear_disaster
[3] www.drs.ch/www/de/drs/tagesthema/272551/275400.nationalrat-beschliesst-atomausstieg.html
[4] www.sbf.admin.ch/htm/dokumentation/publikationen/forschung/11.06.06.NFO.StandPerspektivenEnergieforschung_d.pdf
[5] www.winterthurinstruments.com/

Sensors, Actuators and More

1.1 Characterisation of thermally induced damages in CRFP

Contributors: M. Bonmarin, N.A. Reinke

Partners: IDP-ZHAW, IMPE-ZHAW
Funding: ZHAW School of Engineering (SoE), internal funding
Duration: 2011 – 2012

The high stiffness, strength, the good fatigue properties and low weight make carbon reinforced fibre plates (CRFP) a material of choice for the aeronautical industry. Nonetheless, the exposition of CRFP to high temperatures can durably affect their performance. The detection and the characterisation of those temperature-induced damages are crucial.
Involving three Institutes of the School of Engineering of the ZHAW (IDP, ICP and IMPE), this project intends to detect thermally induced damages and characterise their consequences on the performance of carbon reinforced fibres.
Small variations of the thermal properties of CRFP resulting from the exposition to high temperature are investigated using highly sensitive active thermography methods such as lock-in and pulsed thermography (see Fig. 1).

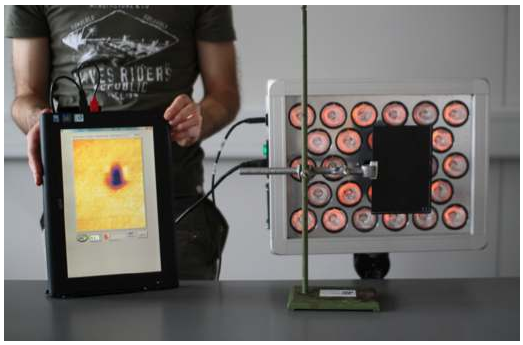


Fig. 1: Compact measurement system for lock-in thermography

The modification of the performance consecutive to heat exposition are characterised with the help of analytical methods and mechanical tests. A powerful, compact measurement system has been developed, which allows field application of lock-in thermography.

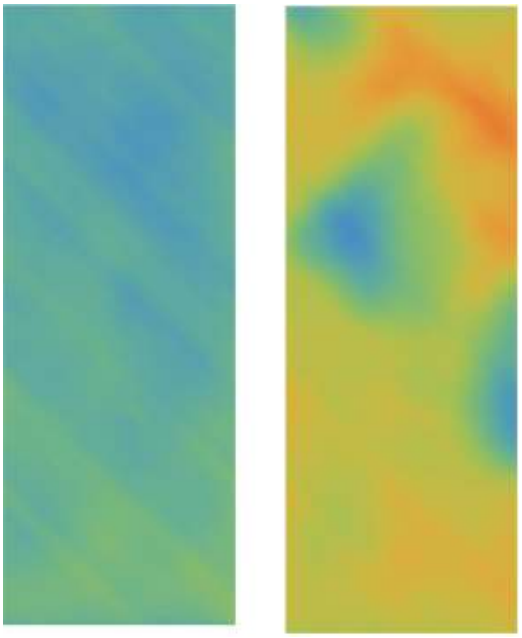


Fig. 2: Lock-in thermographic images of CRFP before (left) and after (right) exposition to high temperature (60 seconds at 300 °C)

1.2 Beschichtungskontrolle mit thermischer Schichtprüfung

Contributors: N.A. Reinke

Partners: IDP-ZHAW, Winterthur Instruments GmbH
Funding: Winterthur Instruments GmbH
Duration: 2011 – 2012

Heutzutage trägt nahezu jedes Objekt eine funktionelle oder dekorative Beschichtung. Dabei sind die Aufgaben dieser Beschichtung so vielfältig wie der Verwendungszweck des Gegenstandes selbst. Die Beschichtung, bestimmt nicht nur das Aussehen, sondern beeinflusst seine mechanischen Eigenschaften und seine Korrosionsbeständigkeit.
Eine kontinuierliche Kontrolle des Beschichtungsprozesses ermöglicht eine gezielte Einsparung von Beschichtungsmaterial und ist damit sowohl von ökonomischer als auch von ökologischer Bedeutung. Der CoatMaster der Firma Winterthur Instruments GmbH ermöglicht die berührungslose und zerstörungsfreie Prüfung von Beschichtungseigenschaften wie Schichtdicke und thermische Eigenschaften.

Fig. 1: CoatMasterOne

Der CoatMaster basiert auf der thermischen Schichtprüfung, die an der Zürcher Hochschule für Angewandte Wissenschaften entwickelt wurde. Hierbei handelt es sich um eine innovative Untersuchungsmethode, bei der die Oberfläche einer Beschichtung mit einer Lichtquelle erwärmt wird, um Rückschlüsse auf die Eigenschaften der Beschichtung zu ziehen. Nach einer kurzzeitigen Erwärmung um wenige Grad Celsius erfolgt die Abkühlung der Oberfläche durch Wärmeleitung in tiefere Bereiche. Der Verlauf der Abkühlung hängt von den physikalischen Eigenschaften der Beschichtung und der Unterlage ab.
Die Oberflächentemperatur klingt umso schneller ab, je dünner die Beschichtung ist, sofern sie eine geringere thermische Leitfähigkeit als der Untergrund hat. Ebenso bewirkt ein schlechtes Haftungsverhalten eine Verzögerung der Abkühlung, weil an der Grenzfläche ein starkes Temperaturgefälle entsteht. Es kommt zu einem Temperaturstau in der Beschichtung. Aus dem zeitlichen Verlauf der Oberflächentemperatur kann also auf die Dicke und Materialeigenschaften der Beschichtung geschlossen werden.

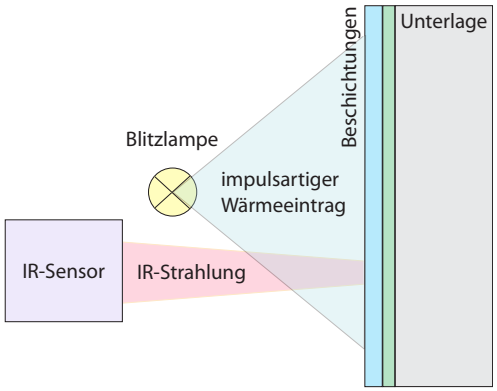


Fig. 2: Messprinzip

Der CoatMaster ermöglicht die Bestimmung von relativen Schichtdicken ohne Kenntnis der thermischen Eigenschaften der Beschichtung. Absolute Schichtdicken, können mittels einer Referenz bestimmt werden.
Zudem können Beschichtungsparameter wie Dicke oder Materialeigenschaften von mehrlagigen Schichtsystemen in Abstimmung mit der Firma Winterthur Instruments GmbH untersucht werden. Die Genauigkeit der Messung hängt vom thermischen Kontrast der Materialeigenschaften der Beschichtung und des Substrats ab. Für einen dunklen Pulverlack auf einem metallischen Substrat liegt die Reproduzierbarkeit bei 2% vom Messwert.
Unsere Kunden setzen den CoatMaster für die tägliche Prüfung von Beschichtungen auf Kunststoff, Keramik, Metall, Holz sowie Beschichtungen auf Papier ein.

1.3 Automatic algebraic mesh generation

Contributors: G. Sartoris, M. Robbiani

Partners: ZHAW, ZAMP-ZHAW, NM-Numerical Modeling GmbH
Funding: Gebert Ruef Stiftung
Duration: 2008 – 2011

The solution of a partial differential equation by the finite-element (FE) method depends in a crucial way on a grid which corresponds to a discretization of the underlying physical domain. Therefore, the most time-consuming part of the solution process of a partial differential equation may be devoted to the generation of an adequate grid. The task becomes even more challenging when the underlying physical domain is to be dynamically varied by the user. For the FE-simulation there are two main approaches to 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 approach allows the treatment of complex geometries with relatively little user interaction but it is counterbalanced by the fact that unnecessarily large grids are generally created. The second approach is time consuming, requires quite a bit of skill to discover appropriate maps but has an inherent mathematical description enabling easy variations of the geometry and a better control of the numerical error.
This project aims to develop new methods for algebraic automatic grid generation which are relevant to practical applications, in particular to dynamical grid generation. 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. The calculus of variations provides an excellent framework for the generation of structured grids by the algebraic method. The idea is to model the essential properties of a grid through an appropriate functional such that optimal grid qualities lead to extremal values of that functional. Thus the determination of the ideal grid reduces to an optimization process to which a broad range of numerical methods apply. In particular, we may again use FE methods to find approximate solutions to these saddle-point problems. For the selection of a functional, there exist many reasonable choices. In particular, the functional can depend on first or higher order derivatives of the deformation gradient. However, in order to minimize computational time, we focus on functionals depending exclusively on first order derivatives, i.e. on the metric tensor. Functionals determining the quality of the grid as smoothness, orthogonality or conformality are well known in the literature, but in practice several qualities need to be satisfied so that one actually works with a combination of these functionals - the relative weight of the functionals being prescribed by the user.
During the course of the project, it was soon apparent that the major problem is the lack of univocity of the diffeomorphism, a property that must be guaranteed in order to successfully apply the algebraic method for mesh generation. Mathematically just for 2D domains and some simple shapes one can guarantee this one-to-one property, so that for the general case, we have to work with approximations thereof. In particular, a viable practical solution consists in working with functionals showing a strong singular behavior when the determinant of the metric tensor goes to zero. Such functionals are strongly non-linear and a dynamic homotopic approach is required to find numerical solutions.

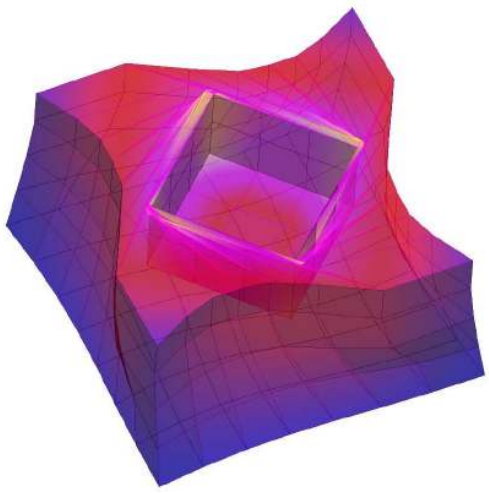


Fig. 1: Dynamically deformed grid due to the rotation of the inner block and continuously adapted outer mesh.

1.4 Computergestützte Karamellproduktion

Contributors: R. Axthelm

Partners: Max Felchlin AG
Funding: Swiss Food Research
Duration: 2012

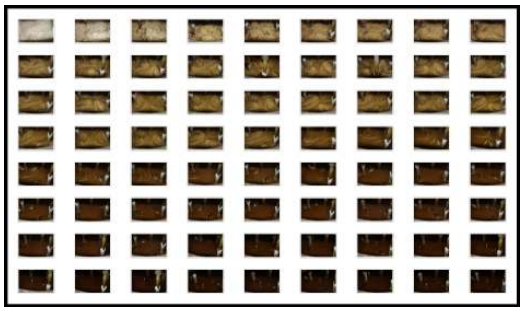


Fig. 1: Farbentwicklung bei Karamellschmelze

Karamell ist eine beigefarbene, feste oder cremige Masse, die im Wesentlichen aus geschmolzenem Zucker besteht. Bei etwa 135 °C beginnt Kristallzucker zu schmelzen, wobei erst bei Temperaturen um 150 °C das eigentliche Karamellisieren einsetzt, bei dem sich Farbe und Geschmack verändern. Für den starken Bruch, sind Temperaturen von 180 bis 200 °C notwendig. Je nach Temperatur verfärbt sich der Karamell dabei goldgelb bis tiefbraun (siehe Fig. 1) und entwickelt ein typisches, mehr oder weniger herbes Röstaroma. Allerdings ist nicht nur die Temperatur sondern auch die Schmelzdauer von Bedeutung. Beginnt der Zucker zu schmelzen, dauert es nur wenige Sekunden, bis der Karamell eine dunkle Farbe annimmt - die Herstellung verlangt entsprechend ständige Aufmerksamkeit. Damit die Masse anschliessend nicht erstarrt, wird sie, wenn der gewünschte Bräunungsgrad erreicht ist, mit Rahm abgelöscht.
Während des Karamellisierens findet eine Reihe chemischer Prozesse statt. Kohlenhydrate verbinden sich zu verschiedenen Polymeren, von denen einige für die braune Färbung und den bitteren Geschmack verantwortlich sind. Karamell schmeckt umso herber, je dunkler er gebrannt ist. Dabei spielen bereits kleine Nuancen (siehe Fig. 2) eine grosse Rolle.
Der Moment bei dem der Karamell abgelöscht wird ist entscheidend. Verpasst man diesen so ist das Produkt nicht mehr verwertbar und die verwendete Menge an Zucker ist verloren. Bei der Firma Felchlin ist zur Abpassung des richtigen Moments ein Mitarbeiter verantwortlich, der mit geschultem Auge den ungefähr zehn Minuten andauernden Prozess überwacht.

Fig. 2: Nuancen in der Farbgebung

Die Vermutung ist, dass nicht etwa der absolute Farbwert des Karamells massgeblich ist für die Bestimmung des optimalen Ablöschzeitpunktes, sondern ein Moment innerhalb der zeitlichen Farbentwicklung. Wahrscheinlich, und das gilt es in diesem Projekt herauszufinden, sind dies Geschwindigkeit und Beschleunigung des Schmelzprozesses, was über die Farbentwicklung gemessen werden kann.
Der Schmelzprozess wird gefilmt und der mittlere Farbwert in Abhängigkeit der Zeit aus dem Videomaterial ermittelt. Im YUV-Farbraum nehmen die Farbwerte eine charakteristische Form (siehe Fig. 3) an. Nachdem die so ermittelte Kurve geeignet entrauscht wurde können weitere Eigenschaften des Karamellisierens ermittelt und untersucht werden.

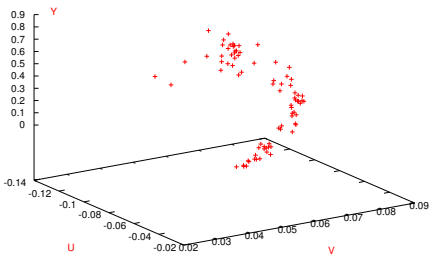


Fig. 3: Farbentwicklung von Karamell im YUV–Farbraum

Ziel des Projektes ist die Konstruktion eines Heizkessels mit eingebauter Kamera, an die ein Computer angeschlossen ist. Eine eigens für diesen Zweck implementierte Software soll zum richtigen Zeitpunkt einen Signalton abgeben, womit der entsprechende Mitarbeiter, zusätzlich zu seinem geschulten Auge, Unterstützung erhält.

1.5 Fussgängersimulation bei hohen Personendichten

Contributors: R. Axthelm

Partners: ASE GmbH
Funding: ICP-ZHAW
Duration: 2013

Fig. 1: Duisburger Loveparade *(SZeit online", 04.08.2010)*

Seit dem Unglück bei der Loveparade in Duisburg 2010 wird der Begriff Crowd-Management im deutschen Sprachraum öffentlich verwendet. Er beinhaltet die systematische Planung und Überwachung einer geordneten Bewegung oder Versammlung von Menschen. Zur Verbesserung dieser Planungen könnten Simulationen von Fussgängerströmen dienen. Zum einen liessen sie sich bei der räumlichen Planung von Zu– und Abgängen einsetzen und zum anderen zur Kontrolle wärend des Veranstaltungsablaufs, wobei die Simulationsergebnisse sich dann zusätzlich auf Realdaten stützten.
Der Anwendungsbereich solcher Simulationsrechnungen lässt sich nicht nur auf andere Grossveranstungen wie z.B. Fussballspiele erweitern, sondern auch auf Planungen und Konzeptionierungen von Gebäuden wie Bahnsteige, Bahnhofs- oder Flughafenhallen.
Die Firma ASE ist spezialisiert auf videobasierte Erfassung von Personenströmen, agentenbasierte Simulation realistischer Szenarien und die ereignisorientierte Simulation der Auslastung von Serviceplätzen. Solche sogenannten mikroskopischen Simulationen, die jeden Fussgänger einzeln darstellen, stossen bei hohen Personendichten schnell an Grenzen, so dass keine zuverlässige Analyse mehr möglich ist. Makroskopische Modellansätze versprechen in solchen Situationen bessere Rechenergebnisse. Bis heute ist aber keine kommerzielle Lösung verfügbar.
Der makroskopische Modellansatz von Personendichten basiert zum einen darauf die Menschenmasse als Kontinuum anzusehen und zum anderen auf drei Hypothesen die für Personenbewegungen in grossen Dichten aufgestellt werden:

1. Die Geschwindigkeit eines einzelnen Individuums wird durch die benachbarten Personen und das Verhalten der Menge bestimmt.

2. Die Fussgänger haben ein gemeinsames Ziel, das sie verfolgen.

3. Die Fussgänger nähern sich auf dem direktesten Weg zu ihrem Ziel, wobei sie grössere Personendichten zu vermeiden versuchen.

Anhand dieser drei Hypothesen lassen sich die Bewegung und die Dichteentwicklung der Menschenmasse als Kontinuum mit der folgenden Gleichung beschreiben:

$$\varrho_t + \nabla \cdot (\varrho\, u) = 0\,,$$

wobei ϱ für die Dichte und u für die vektorielle Geschwindigkeit der Personenmasse steht. Die Geschwindigkeit hängt sowohl von der Dichte, denn jeder versucht hohe Menschenansammlungen zu vermeiden, als auch von der Position des Ziels, in der Regel der Ausgang oder die Konzertbühne, ab. In den verschiedenen Literaturen werden an dieser Stelle verschiedene Ansätze gemacht. Herauszufinden, welche dieser Ansätze für die zu betrachteten Situationen die besten Ergebnisse erzielen, ist neben der numerischen Berechnung einer entsprechenden Lösung Teil dieses Projektes. Fig. 2 zeigt ein erstes Simulationsergebnis, welches zunächst nur eine einfache Variante des eigentlichen Modellansatzes darstellt.

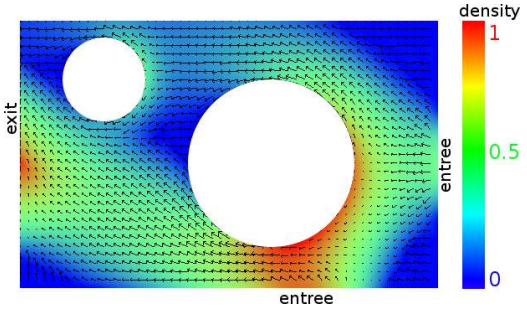


Fig. 2: Bewegungsrichtung und Dichteverteilung in einem Raum mit Hindernissen.

Electrochemical Cells and Energy Systems

2.1 Belenos Fuel Cell Stack: Simulation and Freezing

Contributors: B. Perucco, A. Gentsch, F. Büchi, J. Roth, J.O. Schumacher

Partners: Paul Scherrer Institut, Belenos Clean Power
Funding: Swiss Federal Office for Energy (SFOE), Belenos Clean Power
Duration: 2010 – 2014

The project aims at providing fundamental knowledge for future fuel cell and system developments. One aspect is the operation of a proton exchange membrane fuel cell on H_2 and O_2 below ambient pressure. This topic is approached by model validation and calibration with a numerical one-phase 2+1D model, developed by the ICP, while the PSI is providing the experimental background for validation and calibration.

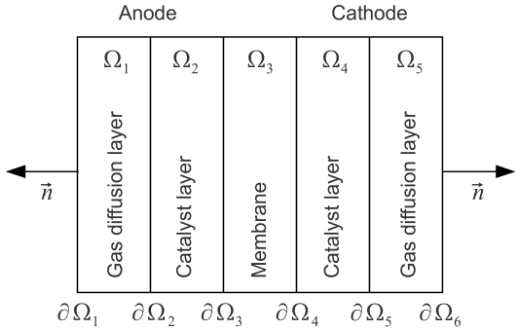


Fig. 1: Geometry of the 1D MEA model. The electrochemical reactions are simulated in the catalyst layers. The model accounts for the transport of oxygen, hydrogen, water vapour, dissolved water, electrical charge, and heat.

At the ICP, the model developement is divided into three subtasks. One subtask addresses the development of a flow-field model that describes the gas flow distribution within the bipolar plates. A model reduction is performed that allows to solve a two-dimensional flow problem of the gas distribution channels instead of a full three-dimensional problem. This reduces the computational time to solve the Navier-Stokes equations. The generation of a discretization mesh of the flow-field was achieved with the multiphysics software SESES. A customized 2D mesh generator was built which uses NURBs (non uniform rational B-splines) to represent curved gas distribution channels.
The second subtask includes the development of a 1D model of the transport processes through the membrane electrode assembly (MEA). The transport of electrons, protons, oxygen, hydrogen, water vapour, dissolved water, and heat through the MEA are described by the model. The MEA model consists of the five layers along the through-plane direction depicted in Fig. 1. Different model versions are tested and a simulated current-voltage curve where pure oxygen and air is used to operate the fuel cell is shown in Fig. 2.
We implemented a numerical solution algorithm to solve the partial differential equations of the 1D MEA model. This solution algorithm can be combined with the 2D flow-field model in SESES. The development of this combined 2+1D model is adressed in the third subtask. A Galerkin Finite Element method is used to discretize the partial differential equations of the model. The nonlinear system of equations is solved by the Newton-Raphson method that is implemented in a runtime efficient C code library. For example, a single point on the current-voltage curve is calculated within about 40 ms depending on the discretization. In a next step, the C code library will be loaded in SESES in order to solve a numerical one-phase 2+1D model.
Furthermore, a two-phase flow model was developed describing the water transport in the gas diffusion layer (GDL) and catalyst layer (CL) of a proton exchange membrane fuel cell (PEMFC). The influence of the treatment of the GDL with a hydrophobic polymer (PTFE) on the saturation was investigated. Thereby, we studied different types of boundary conditions to correctly model the flux of water from the gas diffusion layer into the gas channel (GC).

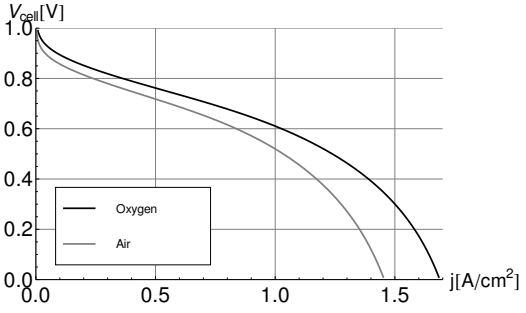


Fig. 2: Simulated current-voltage curves of proton exchange membrane fuel cells. Operation with pure oxygen and air to operate the fuel cell was compared. The assumptions are: pressure: P = 2.6 bar for H_2, P = 2.5 bar for O_2, P = 0.53 bar for air, temperature: T = 74 °C, dewpoint: DP = 60 °C

2.2 Development of membrane mechanics in micro SOFC

Contributors: Y. Safa, T. Hocker

Partners: ETH-NIM, ETH-LTNT, EPFL-SAMLAB, CSEM, NTB
Funding: Swiss National Science Foundation (SNSF) Sinergia
Duration: 2010 – 2012

The aim of ONEBAT project is the development of a miniaturized Solid Oxide Fuel Cell (micro-SOFC) power source for portable electronic devices used in industrial and medical fields.
This new type of energy converting device based on liquid gas has the advantage of high flexibility (geographical independence, immediate charging) and an expected large increase in energy density.
The design of micro sofc built upon multi-layer ceramic films may exhibit some functional problems. It has a low resistance against peeling stress at the interface between different layers where cracks (delamination) may occur. In addition, the membrane is subjected to in-plane compressive stresses, and then, it may undergo an instability transition by buckling. Both buckling and cracks reduce the load carrying capacity of the structure. Furthermore, crack propagation can lead to a failure mode limiting the service life of the fuel cell. The compression in the film can arise during the deposition process from uniform temperature changes, in case of thermal expansion mismatch between the layers.
In the framework of thermo-mechanical research activities during 2011 we mention: experimental tests to investigate conditions of the buckling patterns are handled by Nonmetallic Inorganic Materials Group at ETH Zurich, optical measurement of the curvature of membrane and advanced measurement of the buckling amplitudes are achieved at SAMLAB Laboratory at EPFL Lausanne. The main contribution to this work at ICP ZHAW was focused on the numerical analysis and the physical modelling of buckling and delamination phenomena in the thin film. On the light of Rayleigh-Ritz method which is implemented in the in-house Mathematica code the deformation of the thin film is analyzed as superposition of buckling modes. The energy minimization concept has allowed the justification of the buckling shape based on the energy storage modes.
A post-processing routine is developed for the calculation of the principal stresses in order to derive yielding conditions for the post-buckling stage according to the Mohr-Coulomb criterion. The holding of the buckling shape under heating conditions is analyzed numerically and analytically based on the spectrum of the Hessian of post-buckling energy. The input values for the simulation are determined by measurements achieved by NIM-ETHZ and at SAMLAB EPFL (cf. Figs. 1 and 2).
On the other hand, a new semi-analytical method for the prediction of the buckling driven delamination phenomena is formulated and implemented in Mathematica. This new formulation leads to an innovative contribution for the primary design of similar applications (e.g. thermal barrier coatings).

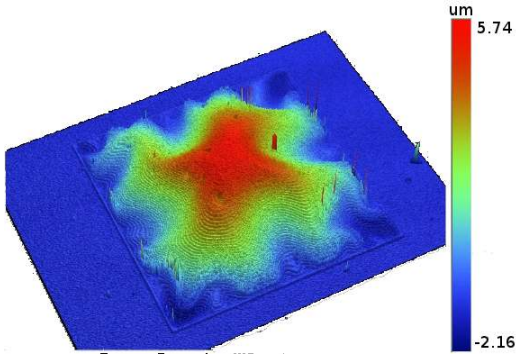


Fig. 1: 3D view of an 8YSZ membrane at room temperature taken with white light interferometry at SAMLAB EPFL

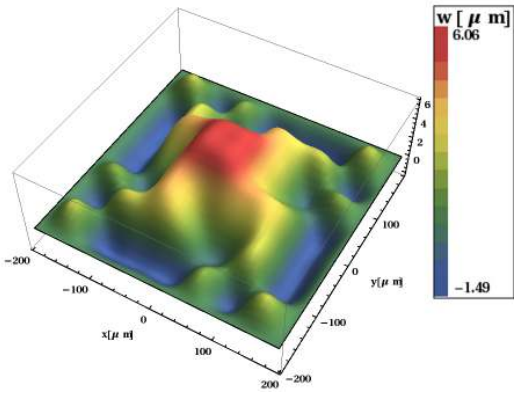


Fig. 2: Numerical simulation corresponding to 800 MPa residual compressive stress. An octopus-like pattern with branched buckling folds is obtained

2.3 Weiterentwicklung SOFC Brennstoffzellenmodul

Contributors: P. Diggelmann (IEFE), T. Hocker, Ch. Meier

Partners: Hexis AG Winterthur
Funding: Swiss Federal Office of Energy (SFOE), Swiss Electric Research
Duration: 2011 – 2013

Zur Reduktion von Material- und Montagekosten entschied sich die Firma Hexis AG zur Neukonstruktion ihres Brennstoffzellenmoduls (BZM). In das BZM integriert sind nebst Zellstack und Reformer auch wärmetauschende Elemente, welche die Betriebstemperatur sowie die Temperaturgradienten an der Zelle beeinflussen. Die thermisch-fluidische Auslegung des neuen Designs wird vom ICP, zusammen mit dem Institut für Energiesysteme und Fluid-Engineering (IEFE), durch Modellbildung unterstützt.
In der Konzeptphase konnte durch Analyse der Massen- und Energieströme, der Charakterisierung der wesentlichen Systemkomponenten sowie der Abbildung des BZM-internen Wärmetauschernetzwerkes ein optimierter Betriebspunkt identifiziert werden (Fig. 1). Dieser sollte mit reduzierten Wärmetauscherflächen die geforderten Betriebstemperaturen garantieren, wodurch die BZM-Konstruktion wesentlich vereinfacht werden kann. Erste experimentelle Untersuchungen bestätigten die getroffenen Annahmen.

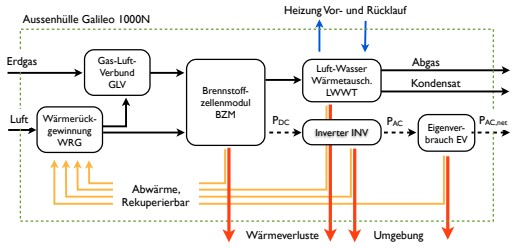


Fig. 1: Fliessdiagramm der Massen- und Energieströme

Die laufende Konstruktionsphase soll nun durch dreidimensionale, numerische Strömungssimulation (CFD) in *Ansys CFX* unterstützt werden. Berechnet werden das Strömungs- und das Temperaturfeld unter Berücksichtigung von Strahlungswärmetransport (Fig. 2).
Eine primäre Anforderung an unsere Strömungssimulation ist eine verkürzte Berechnungsdauer im Vergleich zu früheren CFD Modellen. Eine einzelne Berechnung nahm mehrere Tage in Anspruch, da die Strömungskanäle im Stack geometrisch voll aufgelöst wurden. Das neue Modell bedient sich stattdessen eines von CFX angebotenen Ansatzes für Strömungen in porösen Medien, wodurch der Stack zu einem mehrphasigen, dafür kontinuierlichen, Berechnungsgebiet wird.
Die Strömung und der Wärmetransport im Stack wurden zunächst in CFD-Simulationen einer einzelnen, geometrisch voll aufgelösten Stack Repeat Unit untersucht. Effektive Wärmeleitfähigkeiten sowie Strömungswiderstände wurden aus dem Detailmodell extrahiert und in das Gesamtmodell eingefügt.
Durch die besagten geometrischen Vereinfachungen, der Reduktion der Anzahl Fluid-Solid-Interfaces sowie einer 1:1-Gittergenerierung konnte die Berechnungsdauer bei verbessertem Konvergenzverhalten auf rund 2 Stunden reduziert werden. Somit können umfangreichere Material- und Designparameterstudien innert nützlicher Frist durchgeführt werden.

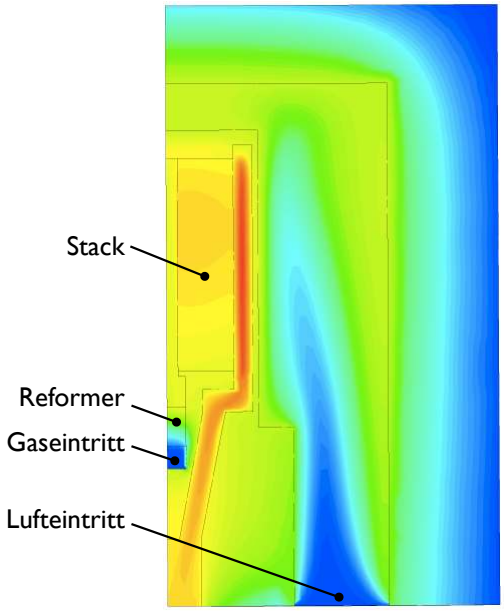


Fig. 2: Temperaturfeld des BZM (numerische Strömungssimulation in *Ansys CFX*)

2.4 An interdisciplinary study of electrode degradation in solid oxide fuel cells (SOFC)

Contributors: L. Holzer, T. Hocker, B. Iwanschitz, B. Muench, P. Gasser

Partners: Hexis AG Winterthur, EMPA Dübendorf, ETH-EMEZ
Funding: Swiss Electric Research, Swiss Federal Office of Energy (SFOE), EU-FP7
Duration: 2011 – 2014

Increasing the life time represents a key issue for a successful market entry of solid oxide fuel cell (SOFC) systems. In recent years considerable progress was achieved due to detailed investigations of the involved material components, of their chemical and structural stabilities and of the compatibility among those components. Of particular importance thereby is the microstructure stability of the porous electrodes, which is the focus of this project. The study combines microstructure analysis (i.e. electron microscopy, nanotomography, image analysis) with multi-physics simulations (finite element modeling) and with experimental investigations (variation of electrode compositions, fabrication parameters and operating conditions).
Quantitative analyses of the microstructure lay the foundations of these degradation studies. New analytical methodologies were developed over the last years using FIB/SEM-nanotomography (see Fig. 1) and image modeling. Based on these developments it is now possible to measure the microstructure parameters, which are critical for charge and mass transport

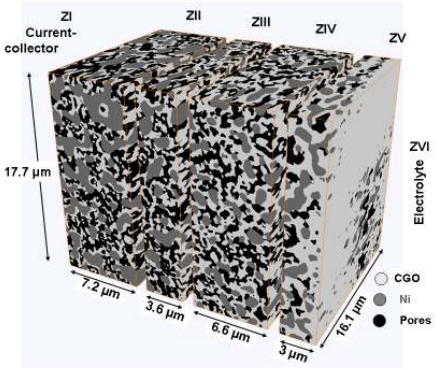


Fig. 1: Visualization of 3D microstructure in a Ni-CGO anode based on FIB/SEM-tomography.

(i.e. tortuosity and constrictivity) and for the electrochemical activity (i.e. surface area, interfaces, TPB, connectivity). By means of time lapse tomography even the time dependent changes of these parameters can be described (see Fig. 2).
Microstructure modeling was then introduced at ICP in order to study the effects of morphological changes on the electrode performance. The data from microscopy is used as structural input for finite element modeling. In these simulations, electrochemical reactions are coupled with charge and mass transport. These multi-physics simulations allow the calculation

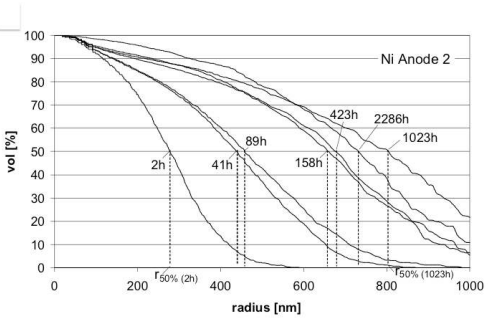


Fig. 2: Change of Nickel particle size (r50) during degradation at 850 °C in humidified hydrogen fuel.

of area specific resistances distinguishing between ohmic and polarization components, as a function of the specific microstructures as observed by microscopy. Including the information from time lapse tomography, the FE-simulations allow for a time dependent description of the electrode performance as a function of the corresponding operating conditions (i.e. temperature, fuel composition, water vapour content, current density).
These investigations are then complemented with systematic degradation experiments that are performed by our industrial partners (Hexis AG) and by an international consortium in the framework of an ongoing european project (SOFC life).
The interdisciplinary approach opens new possibilities to study degradation on a quantitative level and to understand the complex interplay between materials and fabrication parameters, operating conditions and their influence on the degradation kinetics. The quantitative description of the degradation kinetics also represents the basis for systematic improvements of a new generation of SOFC electrodes with longer life time and higher efficiency.

2.5 Structural Segmentation and Stochastic 3D Modeling of $La_{0.6}Sr_{0.4}CoO_{3-\delta}$-cathodes

Contributors: M. Neumann, L. Holzer, T. Hocker, G. Gaiselmann, V. Schmidt, M. Prestat

Partners: Ulm University, ETH-NIM, EMPA Dübendorf
Funding: Swiss National Science Foundation (SNSF)
Duration: 2011 – 2014

In this joint project between Ulm University, EMPA Dübendorf and ZHAW Winterthur the microstructure of $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ cathodes (LSC) in solid oxide fuel cells (SOFC) is investigated. A parametric stochastic 3D simulation model is developed by Ulm University, which is able to describe the geometry of a two-phase microstructure. Hereby, one phase is completely connected and consists of spherical particles. Microstructures with these properties appear e.g. in SOFC-electrodes, that are produced from LSC nanopowder manufactured with flame spray synthesis (see Prestat et al. (2010), *Electrochemistry Communications 12*, 292-295).
The stochastic model is developed to detect correlations between the production process (e.g. variation of sinter temperatures and/or change of pore former contents) and the resulting microstructures as well as the corresponding electrode performance. It is based on image data of LSC-cathodes with different sinter temperatures, that is to say 750°C, 850°C and 950°C, gained by high resolution FIB-SEM tomography (see Fig. 1).

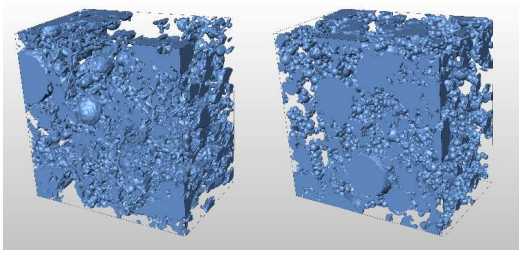


Fig. 1: Left: Real data from LSC-cathode with sinter temperature 850°C. Right: Realization of the model with sinter temperature 850°C.

On the 3D-images one can see, that the LSC-phase is dominated by a dense packing of spherical particles. This phase is represented by a union of moderately overlapping spheres in a first step, whereas the proceeding is similar to the one for segmentation of porous electrode material in Li-ion batteries (see Thiedmann et al. (2011), *Computational Materials Science*, 50, 3365-3376).
Based on the sphere representation, the LSC-phase is modelled with ideas from stochastic geometry and graph theory. The model consists of a random sphere system, where the midpoints are realizations of a complex 3D point process. In order to assure the perfect connectivity of the sphere system, a modified version of the relative neighborhood graph is introduced, which controls the radii of the random spheres.
Finally the stochastic model of the LSC-phase is described by certain parameters, which are fitted to three different microstructures of LSC-cathodes, produced of sintering temperatures 750°C, 850°C and 950°C. For each constellation of parameters corresponding 3D-microstructures can be realized. The model is then validated by comparing structural characteristics (e.g spherical contact distribution function, continuous pore size distribution) from the 3D-realizations and the FIB-tomographs. For all three sinter temperatures a good fit is achieved (see Fig. 2).

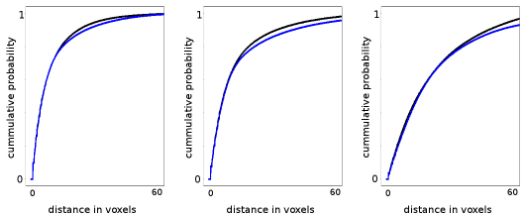


Fig. 2: Comparison of the spherical contact distribution functions from the binarized FIB-SEM data (black) and realizations of the model for different sinter temperatures (blue). From left to right: 750°C, 850°C, 950°C.

2.6 Calibration of Hexis fuel gas-to-air flow controller

Contributors: M. Linder

Partners: Hexis AG Winterthur
Funding: Hexis AG Winterthur
Duration: 2010 – 2011

The Hexis fuel cell system Galileo 1000 N provides the electrical energy and heat demand of single family homes from natural gas. For fuel cell operation, an upstream gas reformation is necessary to convert the natural gas, i.e. mostly methane, into hydrogen and carbonmonoxide. This conversion is realized by a catalytic partial oxidation (CPOx) process. The challenge for the CPOx-process is to accurately control the fuel-to-air ratio to avoid soot generation and CPO-catalyst overheating. Both cause efficiency losses and damages to the fuel cell and the reformer. The Hexis gas-to-air ratio controller (GARC) uses two hot film anemometers. Since this measurement principle relies on the thermo-physical properties of the respective gas mixture such as its heat capacity and its heat conductivity, unavoidable variations in the natural gas composition can lead to significant flow deviations.
The aim of this work was to develop a new strategy for the GARC calibration and the initial operating settings to avoid both soot generation and excessive performance losses for different natural gas compositions. For this purpose, several tests with different gas compositions and flow rates were conducted. The results are shown in Fig. 1. One sees that for certain gas compositions the deviation of the flow rate from its set point is quite large. Based on these results, it first seemed rather unrealistic to find a practicable way to run the Hexis Galileo system with different gas qualities.
Nevertheless we started tackling the problem by looking for a systematical relationship between the observed flow deviations and the physical properties of the tested fuel gas compositions. Therefore different regression models and data transformations were compared and tested. As shown by the red marks in Fig. 2, we finally found appropriate correlations for the flow deviations based on the specific heat capacity and the heat conductivity of the fuel gas. The purple marks show the correlated fuel-to-air ratio, which includes flux deviation and changes in ideal fuel-to-air ratio caused by varying fuel gas compositions. To avoid soot generation we have to ensure a positive fuel-to-air ratio. To achieve this, we applied an additional safety factor that leads in any case to a positive deviation as shown by blue marks.
The introduced approach for the GARC calibration and determination of initial set point is currently in use at Hexis. From the field engineers there are not any reports about nameable incidents known so far.

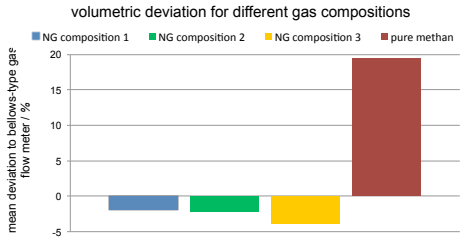


Fig. 1: Measured GARC flow deviation for different natural gas compostions

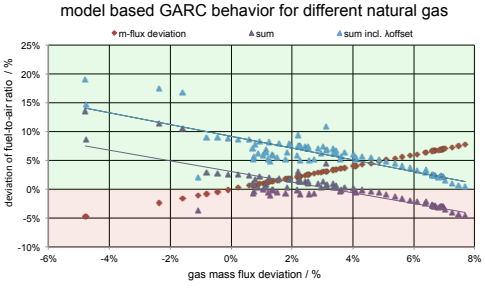


Fig. 2: Cumulated fuel gas-to-air ratio deviation for different natural gas compositions

2.7 Thermogradientenprüfstand für Brennstoffzellen

Students: P. Lehnherr, D. Wild

Category: Projektarbeit, Studiengang Maschinentechnik MT
Mentoring: T. Hocker, L. Kaufmann
Handed In: Dezember 2011

Diese Projektarbeit beschäftigte sich mit dem Thermogradientenprüfstand der Firma Hexis. Mit dem TGP können die Brennstoffzellen des Brennstoffzellen-Heizgerätes Galileo 1000 N auf ihr thermo-mechanisches Bruchverhalten untersucht werden. Ziel dieser Arbeit war es, ein überarbeitetes Design des TGP aufzubauen und in Betrieb zu nehmen. Nach Inbetriebnahme sollten Prüfstand- und Zellentests durchgeführt werden. Zudem sollte eine statistische Auswertung der Daten durchgeführt werden. Es wurde definiert, mit einem Probenumfang von 30 Zellen zu arbeiten, um ein realistisches Bild der Lebensdauer der Zellen zu erhalten. Der neue Prüfstand konnte nach einigen Anpassungen erfolgreich in Betrieb genommen werden. Es zeigte sich, dass die aktive Kühlung mittels Druckluft gut funktioniert. Durch diese Kühlung sowie durch die Reduktion der thermischen Masse konnte der Prüfzyklus gegenüber dem Vorgängermodell von ca. 50 min auf ca. 30 min reduziert werden. Nach ersten erfolgreichen Prüfstandtests, zeigte sich jedoch, dass mit der bestehenden Prüfstandkonstruktion nicht alle Probleme der Vorgänger-Konstruktion behoben werden konnten und noch keine rationelle Prüfung der Zellen durchgeführt werden kann. Während den Belastungstests der Zellen treten nach wie vor Störsignale auf, weshalb viele Zellentests vor Ende des Prüfvorgangs abgebrochen wurden. Dies führte dazu, dass im Rahmen dieser Projektarbeit nur wenige auswertbare Messresultate aufgenommen werden konnten. Deshalb kann aufgrund der Auswertung der Daten mittels Weibull-Analyse keine verlässliche Aussage über die Stabilität der Zellen gemacht werden. Damit das Ziel einer rationellen Zellenprüfung mit dem TGP erreicht wird, sind noch weitere Verbesserungen am Prüfstand nötig. Für das weitere Vorgehen wird empfohlen, das Design oder die Materialwahl des Deckels zu überarbeiten um die Entstehung der Störgeräusche zu verhindern. Zudem sollte die Heizung im Bezug auf Isolation zum Gehäuse und der Langlebigkeit überarbeitet werden.

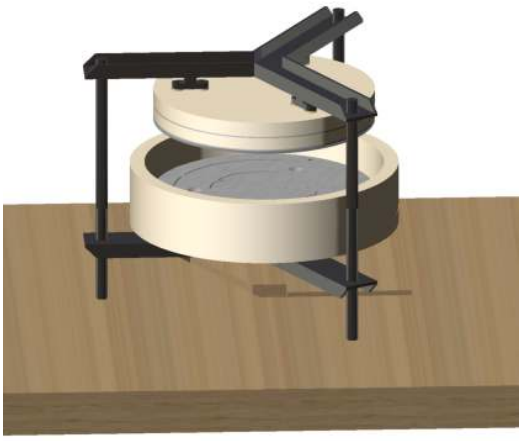


Fig. 1: CAD Modell des überarbeiteten Thermogradientenprüfstand

Organic Electronics and Photovoltaics

3.1 Exploring and Improving Durability of Thin Film Solar Cells (DURSOL)

Contributors: B. Ruhstaller, T. Lanz, S. Züfle, M. Neukom, M. Schmid

Partners: EMPA, EPFL, CSEM, SUPSI, ZHAW, Alcan
Funding: Competence Center Energy and Mobility (CCEM-CH), Swiss Electric Research
Duration: 2011 – 2013

The CCEM-CH project DURSOL aims at joining the competences of several partners in micromorph silicon, compound semiconductors, dye sensitized and organic thin film solar cells. The project objectives are focussed towards the understanding of fundamental degradation phenomena in thin film solar cells. Degradation is due to complex mechanisms related to inherent material stability, interdiffusion across junctions, and due to external influences such as ambient atmosphere and solar light, and it certainly depends on the type of semiconductors being used in the devices and how the solar cells are encapsulated. The task for the ICP within this project is to advance its numerical models of the various solar cell techniques being investigated: the dye-sensitized solar cells (DSCs), organic photovoltaics (OPVs) and thin film silicon solar cells. This is done within collaborations with experimental groups (EPFL-LPI, CSEM and EPFL-PVLab). The progress made during the first project year is summarized below:

Model-based analysis of dye-sensitized solar cell degradation

We extended our coupled optical and electrical model for the dye-sensitized solar cell (DSC) in such a way that several transient experiments can be simulated (transient photovoltage/photocurrent decay, impedance spectroscopy, intensity modulated photovoltage and photocurrent spectroscopy (IMVS/IMPS)). This allows to compare a combined set of steady state and transient measurements to the corresponding simulations and to extract accurate values for the model parameters. This procedure will be applied to DSCs of different electrolyte composition and on aged cells at different stages of the aging process.
The electrical part of the DSC model is based on the continuity equations for electrons in the conduction band of the TiO_2 and for triiodide and iodide species in the electrolyte. It describes the diffusive transport of these charge carriers in the TiO_2 conduction band (electrons) and within the pores of the nanoporous TiO_2 and bulk electrolyte layers (triiodide and iodide). Trapping at an exponential distribution of band gap states is taken into account within the framework of the quasi-static approximation. Recombination is modelled by a sublinear power law dependence. In addition, charge transfer at the counter electrode is taken into account. The whole model results in a set of three coupled non-linear partial differential equations (PDEs), which are solved numerically. For the simulation of small perturbation transient experiments the system of PDEs is expanded around the steady state solutions and the perturbation equations are solved. The DSC test cells are produced and measured by EPFL-LPI. In the first step, the ICP obtained a set of measurements on three different cells with three different dyes (C101, Z907 and N719). On these cells, IV-curves and impedance spectra were measured from 0.01Hz to 1MHz in the dark and under illumination. This combined set of measurements is used to extract the model parameters by comparing the measurements to simulated data. This is shown for a single measurement in the figure below.

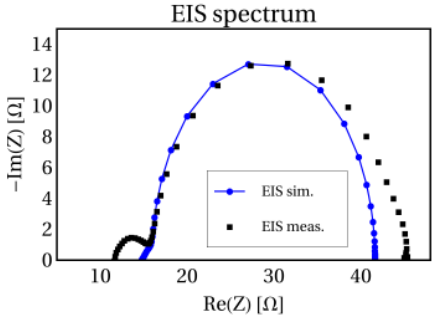


Fig. 1: Measured (black) and simulated (blue) impedance spectrum of a DSC test cell.

Spectral reflectometry and electroabsorption in organic solar cells

The ICP has launched the development of an advanced characterization setup for electroabsorption and examined organic solar cells fab-

ricated at CSEM. The electroabsorption (EA) technique investigates the change in the absorption spectrum of a semiconductor under the influence of an applied electric field. This change can be explained by the macroscopic Stark effect. Since the effect is small it can only be measured by a sophisticated setup, using a small signal response and lock-in technique. A voltage consisting of a dc and a modulated (ac) part is applied to the electrodes of the solar cell. Then the reflected or transmitted light is measured by a photodiode. We use the so-called reflection geometry as the back electrode is intransparent. When an external dc+ac voltage is applied, an electric field inside the organic semiconductor is formed in addition to the built-in field. The measured signal of the photodiode is then deconvoluted into the dc-part and the ac-part on the first or second harmonic of the modulation frequency, using a phase-sensitive lock-in amplifier. Our light source combined with a monochromator allows us to measure the spectral electroreflectance signal in the spectral range of 400 to 1000 nm with sufficient resolution (see Fig. 2).

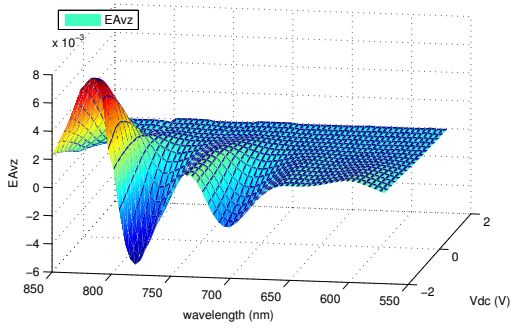


Fig. 2: Measured EA spectrum versus DC voltage.

The ICP has a strong expertise in the modeling of organic electronic devices both for advanced characterization and device optimization. The simulation-based description of electro-absorption measurements will allow us to better extract material parameters and confirm results of electrical device simulations. The direct extraction of the built-in voltage from EA measurements has been shown many times by just looking for the dc voltage at which the EA signal vanishes. Also the electric-field profile in a multilayer organic device can be estimated. But charge injection and space-charge effects can render this analysis quite difficult, necessitating a simulation approach.

Extended light scattering model for thin film silicon solar cells

Thin film solar cells based on amorphous and microcrystalline silicon suffer from significant aging of the active layer. Therefore one must resort to even thinner films. This requires the use of suitable light trapping schemes. We have extended an existing scalar light scattering model for coherent layers and experimentally validated it in a collaboration with the EPFL-PVLab. The cell under consideration and the comparison of the spectral quantum efficiency is shown in the two figures below. The planar cell is compared to the one with a structured ZnO interface. Improved absorption is observed for the cell with a rough ZnO interface. The simulations agree nicely with the experiment.

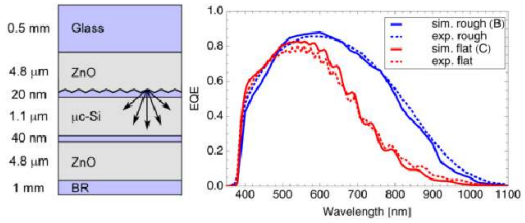


Fig. 3: Comparison of measured and simulated spectral quantum efficiency of a single-junction microcrystalline silicon solar cell.

3.2 APOLLO - Efficient areal organic solar cells via printing

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

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

The APOLLO project with several international academic and industrial partners was carried out from 2008 to 2011. It aimed of combining plastic electronic expertise to empower printed electronics applications. The focus therein is on single and tandem organic solar cells comprising newly developed donor materials. During the project period a comprehensive device model for the study and interpretation of measured data has been developed at the ICP. Thus the whole process chain from light absorption, exciton dissociation, charge carrier transport and collection by the electrodes is covered. The institute's expertise could so be extended from OLED to OPV modelling. Simultaneously our experimental capabilities have been strongly extended, allowing for comprehensive measurements joined with simulations and thus enabling a better understanding of the underlying physics.
During the last year of the project, the CELIV (charge extraction by linearly increasing voltage) method has been extensively used in addition to the steady-state current-voltage (JV) curves. By applying various transient and steady-state measurement techniques and comparing them to simulations it is possible to fit important material parameters like the charge carrier mobility or injection barriers with higher accuracy. For example, in a measurement series we could ascribe different extracted mobility values to different morphologies. A tool to fit multiple curves of different measurement techniques has been developed for this task. Fig. 1 shows the fitting of multiple curves with the same set of parameters.
Temperature-dependent measurements also constitute a promising approach for validating the physical models included in the simulation. The temperature strongly influences injection as well as transport. Therefore a systematic investigation important. Fig. 2 depicts the dependence of the open-circuit voltage on the variable temperatures and illumination intensities and shows a linear behaviour.
Through this project the international collaboration has been strengthened and the expertise of the ICP in modelling organic electronic devices could be increased and extended by experimental experience.

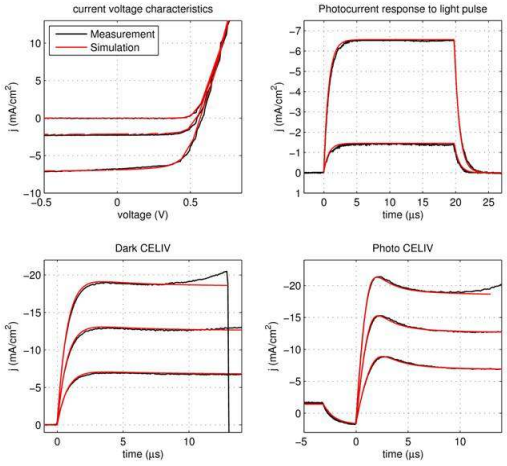


Fig. 1: Fit of transient and steady-state measurements at varying illumination intensities and bias voltages.

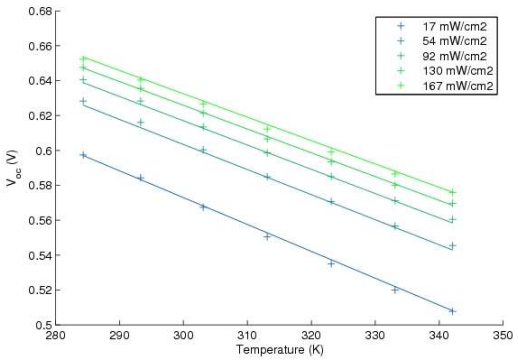


Fig. 2: Temperature-dependence of the open-circuit voltage for different illumination intensities.

3.3 Improving amorphous silicon solar cells by model-based characterization

Contributors: T. Lanz, B. Ruhstaller

Partners: Korea Advanced Institute of Technology
Funding: Swiss State Secretariat for Education and Research
Duration: 2011

In recent years, thin-film solar technology has increased its market share thanks to improvements in module conversion efficiencies as well as improved reliability. Further improvements in conversion efficiency on the solar cell level are still possible, thus offering the potential for even lower $/Watt prices for modules. This project aims to improve the performance of pin type amorphous silicon (a-Si) thin-film solar cells by model-based characterization and development of advanced processing methods for high stabilized efficiency. The single-junction a-Si solar cell is sophisticated enough to be industry relevant, yet simple enough to be scientifically examined by physics-based models.

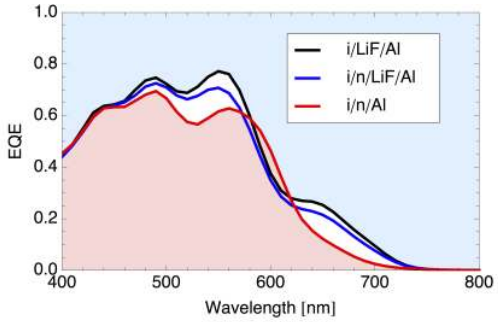


Fig. 1: Measurements of the external quantum efficiency (EQE) for three different types of amorphous silicon solar cells.

Within this project we were able to improve the understanding of the role of thin layers of lithium fluoride (LiF) that are used together with aluminum as back reflectors in thin-film a-Si solar cells. Measurements of the external quantum efficiency (EQE) for three types of a-Si solar cells with and without LiF are shown in Fig. 1. LiF/Al back reflectors are commonly used in organic solar cells. Recently, they were proven suitable for highly efficient a-Si pin type solar cells [Fang *et al.*, IEEE T-ED, 58(9), 2011]. The role of the LiF is twofold: due to its low refractive index it increases the reflectivity of the back reflector and it creates a surface passivation of the Si/Al interface. Using our recently validated optical model [Lanz *et al.*, JAP, 110(3), 2011] we studied the influence of thin layers of LiF on the optical intensity distribution within these solar cells. A visualization of the computed energy flux, denoted by the Poynting vector, within the intrinsic layer of the a-Si solar cell containing a LiF-based back reflector is shown in Fig. 2.

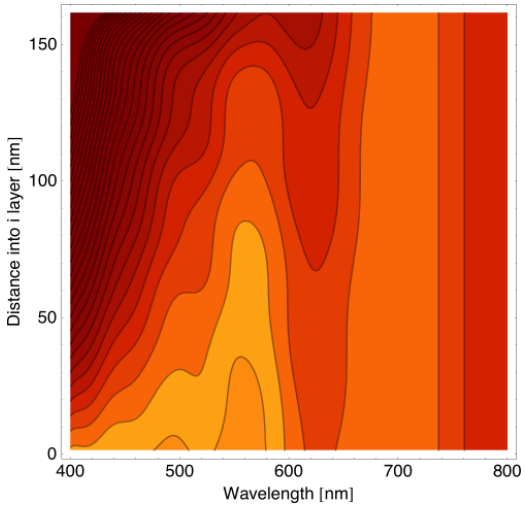


Fig. 2: Visualization of the computed energy flux (Poynting vector) within the intrinsic layer of the amorphous silicon solar cell.

The use of dedicated samples, deposited on flat substrates, leads to pronounced interferences in the spectral response (see Fig. 1). These interferences are highly sensitive to the thicknesses of the layers as well as the reflectivities of the interfaces. By comparing the measurement results with the optical simulations we may assess the impact of the LiF on the optical intensity distribution and distinguish between gains associated with the increased reflectivity of the back reflector and the influence of the LiF on the electrical cell characteristics. We find that, for cells on flat substrates, the increased reflectivity of the LiF/Al back contact accounts for a 7% increase in short circuit current, a gain that may be attributed solely to the optical impact of the LiF. Our findings thus help to assess the commercial viability of LiF/Al back reflectors.

3.4 Characterizing Large Area Tandem Thin-Film PV-Modules

Contributors: T. Lanz, B. Ruhstaller, D. Schär, F. Baumgartner

Partners: IEFE-ZHAW
Funding: ZHAW School of Engineering (SoE), internal funding
Duration: 2011 – 2012

Thin-film solar module technology has by now reached a 20% share of the worldwide installed solar modules. This technology still offers the potential for substantial reductions in production costs, thus lowering the specific $/Watt prices. Compared to standard crystalline silicon solar cells, thin-film solar cells reach lower conversion efficiencies. Combining two different types of solar cells in a serial interconnection to a tandem solar cell allows increasing the efficiency by about 25%, as a larger proportion of the solar spectrum can be absorbed. However, the deposition of such multiple layer successions with laterally homogeneous thicknesses over large areas is challenging. Furthermore, characterizing tandem modules and determining their nominal power requires more advanced equipment than standard single-junction modules and, as of today, there is no reliable and fast method for large numbers of samples. Thus, the scope of this project is the development of a novel spectral characterization of tandem solar modules.

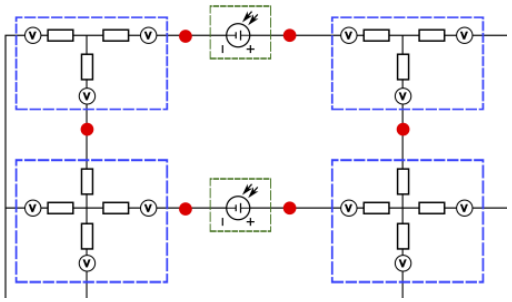


Fig. 1: Excerpt of the circuit diagram describing the interconnection of thin-film solar cells in a solar module used in SPICE modeling.

The responsibility of ICP within the project is the development of an electro-optical model of the tandem thin-film solar module. For the optical model we employ our recently validated optical light-scattering model [Lanz *et al.*, JAP, 110(3), 2011], that was developed in collaboration with the PVLAB of EMPL IMT-NE. For the electrical model we consider equivalent circuit modeling using SPICE, see Fig. 1, as well as finite element modeling using seses. Our model takes into account the different spectral responses of the top and bottom solar cells, as well as light scattering at rough interfaces, as found in all commercially viable modules. Further, the model considers charge transport in the transparent electrodes over the entire module area. The model thus allows studying the overall influence of lateral inhomogeneities of the deposited layer thicknesses as well as defects such as vertical short circuits, see Fig. 2. We intend to validate the coupled model with measurements of tandem solar modules and support the development of the measurement setup to be integrated into the Solarbus.

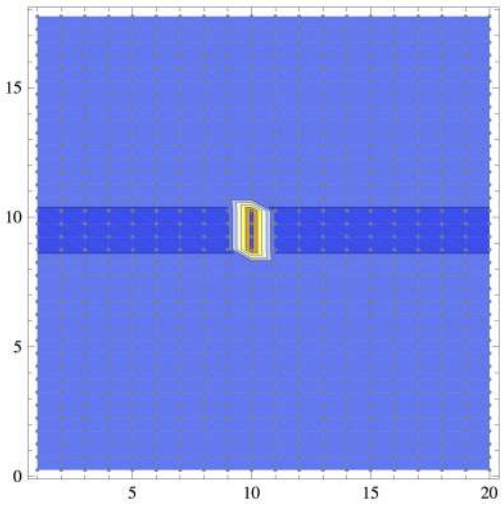


Fig. 2: Visualization of the calculated current densities in a thin-film solar module that contains a vertical short circuit (a pinhole).

The validated model combined with the spectral measurement setup shall be used to detect lateral inhomogeneities on the module level, as well as identify and quantify quality and aging issues. Further, the model can be used to optimize the layout of modules, such that module performance indicators become insensitive to manufacturing tolerances.

3.5 AEVIOM - Advanced Experimentally Validated Integrated OLED Model

Contributors: B. Ruhstaller, B. Perruco, E. Knapp

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

In March 2011 the EU-funded project AEVIOM (2008-2011, www.aeviom.eu) ended. It focused on the modeling of organic light-emitting devices. Fig. 1 shows the difference in form factor between OLEDs and conventional light sources.

Fig. 1:OLEDs in comparison with conventional light sources

During the last three years a “second generation” OLED model which takes the consequences of the disordered nature of realistic organic semiconductor OLED materials into account was realized. An advanced three-dimensional (3D) supercomputer Monte Carlo charge transport and recombination model was developed by our project partners. The 3D-results were “translated” to accurate one-dimensional expressions, and using these expressions fast PC-software tools were developed by ZHAW and Fluxim. Intensive experimental studies have been used to validate the models developed. Experimental characterization methods such as current-voltage curves, dark injection transient current measurements and impedance spectroscopy for OLEDs can be reproduced with the software as shown in Fig. 2.

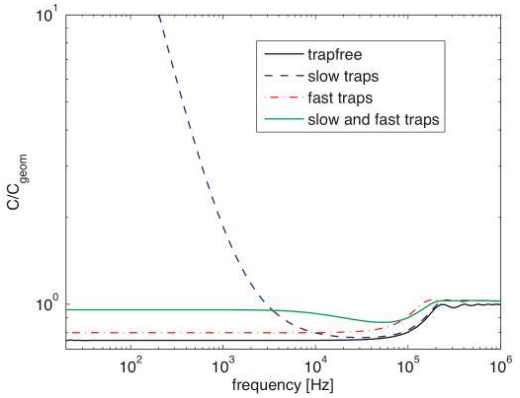


Fig. 2: Frequency-dependent capacitance of different OLEDs

It shows the frequency-dependent capacitance for trapfree OLEDs and trap-affected ones. Further, applications of this second-generation OLED modeling tool have been demonstrated for a complete “hybrid-white” OLED, based on experimentally determined hole and electron mobility functions, using the world’s first full 3D Monte Carlo OLED modeling as a benchmark. The model has also been used to support OLED lifetime and color stability studies. Predictive modeling has been demonstrated for single-layer OLEDs, and the realization of such a demonstration is in good progress for multi-layer OLEDs.

3.6 Integrated Multidisciplinary & Multiscale Modeling for Organic Light-Emitting Diodes (IM3OLED)

Contributors: M. Loeser, E. Knapp, K. Lapagna, B. Ruhstaller

Partners: Holst Centre (Eindhoven, NL), Philips Research Laboratory (Aachen, D), Fluxim (CH), Moscow Engineering Physics Institute (MEPhI), Kintech Lab, Photochemistry Center of the Russian Academy of Sciences (PCC RAS)
Funding: FP7 of the European Commission
Duration: 2011 – 2014

The EU-funded IM3OLED project, being an international collaboration between European and Russian partners, aims at developing a software toolset for multiscale OLED modeling. Such a tool would help the OLED industry escape today's "trial-and-error" development and accelerate towards the goal of 150 lumens per Watt devices.

Overall OLED efficiency depends on many factors: the properties of the light emitting molecules, deposition onto the substrate, integration into a device, extracting the light from the active layer and the device, heat management and more. Complicating things further, many of these factors are interlinked. For example, how the device heats up in operation may affect the molecule's ability to generate light and the way light travels through the device. This makes it extremely difficult to predict how innovations in one area will affect performance in others, leading to a trial-and-error approach in R&D.

IM3OLED aims to help the OLED industry speed up development by creating new modeling software that allows a more systematic R&D process. This software toolset will predictively model OLEDs in 3D and at all length scales – from molecular to large-area devices. It will include molecular calculations, electrical and optical simulation, 1D-3D light extraction and scaling / integration effects. Importantly, the tool will incorporate a dynamic feedback loop, enabling developers to accurately predict how changes in one area of OLED development affect other areas. This will allow multiple OLED properties to be optimized simultaneously.

Together with its spin-off company Fluxim AG, the Institute of Computational Physics (ICP) constitutes two Swiss partners among the four European partners funded by the European Commission's seventh framework program (FP7). While Fluxim commercializes simulation software as an easy-to-use tool, the ICP develops numerical algorithms. The tasks of the Swiss partners are the electrical modeling of charge transport in the continuum approach, the light-outcoupling of planar and structured OLEDs as well as the electrothermal aspects of large-area OLED panels.

3.7 Numerical simulation and design of extremely thin absorber solar cells

Contributors: M. Loeser, K. Lapagna, B. Ruhstaller

Partners: EMPA Thun
Funding: Swiss Federal Office of Energy (SFOE)
Duration: 2011 – 2012

This project is a joint research effort among the Laboratory for Mechanics of Materials and Nanostructures of the EMPA Thun and the Institute of Computational Physics of the Zurich University of Applied Sciences, to investigate and improve - both numerically and experimentally - the optical characteristics of nano-structured, extremely-thin absorber solar cells.
In recent years extremely thin absorber (ETA) solar cells have received considerable attention, and despite their yet low efficiencies, ranging about 2.5%, they are considered as promising novel devices for converting sunlight into electric energy. The use of extremely thin absorber layers has numerous advantages. The probability that two optically generated carriers recombine before they reach the contact electrodes and are thus lost for energy conversion strongly decreases with the width of the absorber layer. In traditional photovoltaic (PV) applications this issue was dealt with by employing very expensive absorber materials with excellent electronic characteristics. ETA solar cells do not only require a strongly decreased amount of absorber materials but also allow for the use of absorbers with significantly poorer electronic properties that come at a strongly reduced price.
However, the efficiency of ETA solar cells is not only determined by their electrical, but also by their optical characteristics. The ability to efficiently trap and convert incident sunlight is a key feature that decides about economic success. In many cases the percentage of the incident light that is converted into free charges depends exponentially on the absorber thickness. In order to combine the advantages inherent to thin absorbers with the necessity of high optical absorption efforts must be made to enlarge the optical path in such way that the solar cell can absorb a significant fraction of the incident sunlight. To gain deeper understanding of the underlying complex optical processes and to obtain optimal device designs numerical simulations of the complete three-dimensional (3-D) problem are indispensible, as ill-chosen microstructures can even decrease the device performance.

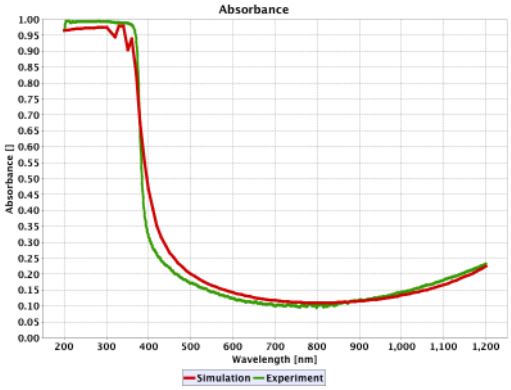


Fig. 1: Fitting refractive index model parameters to the measured absorption spectra for the layer structure glass/FTO/ZnO.

Yet, due to the combination of large devices and small micro-structures the accurate multi-dimensional simulation of such structures is challenging. At the ICP we developed a 3-D simulation software that solves Maxwell's equations at greatly reduced computational cost thanks to a novel numerical method. This software allows to obtain full-wave solutions for geometries that so far could not be numerically analyzed due to their large size.
Prior to comparing the reflection and absorption spectra obtained from spectral measurements and three-dimensional optical simulations we ensured that we employ the correct material parameters (above all, the refractive indices). We extracted the refractive indices of the relevant materials (in particular from FTO and ZnO) from the measured data. The procedure of parameter extraction is based on fitting absorption and transmission spectra that are obtained from one-dimensional transfer-matrix calculations (using the software SETFOS) to the measured spectra. The numerical values that were obtained for n and k agree reasonably well with what is reported in literature.
As the foundation for a comparison between numerical and experimental data has now been laid, we can start the benchmarking procedure with the full-wave simulations.

Appendix

A.1 Student Projects

- P. Lenherr, D. Wild: *Thermogradientenprüfstand für Brennstoffzellen*, Betreuer: L. Kaufmann, T. Hocker, Firmenpartner: Hexis AG, Winterthur (2011)

- M. König, P. Zuber: *Thermische Analyse eines Schokoladen-Kühlkanals*, Betreuer: T. Hocker, M. Suter, Firmenpartner: Max Felchlin AG, Schwyz (2011)

- H. Schmitt: *Monte-Carlo Simulation von organischen photovoltaischen Zellen*, Betreuer: N.A. Reinke, M.T. Neukom

- P. Baur, S. Ernst: *Entwicklung eines LED-Screens für Werbung unter Eisflächen in Hockeyarenas*, Betreuer: N.A. Reinke, R. Ritzmann

A.2 Scientific Publications

1. S. Wenger, M. Schmid, G. Rothenberger, A. Gentsch, M. Grätzel, J.O. Schumacher: *Coupled optical and electronic modeling of dye-sensitized solar cells for steady state parameter extraction*, J. Phys. Chem. C, 115 (20), pp 10218-10229 (2011).

2. M. Neukom, N.A. Reinke, B. Ruhstaller: *Charge extraction with linearly increasing voltage: A numerical model for parameter extraction*, Solar Energy 85, 6, 1250-1256 (2011).

3. T. Lanz, B. Ruhstaller, C. Battaglia, C. Ballif: *Extended light scattering model incorporating coherence for thin-film silicon solar cells*, J. Appl. Phys. 110, 033111 (2011).

4. L. Holzer, B. Iwanschitz, T. Hocker, B. Münch, M. Prestat, D. Wiedenmann, U. Vogt, P. Holtappels, J. Sfeir, A. Mai, Th. Graule: *Microstructure degradation of cermet anodes for solid oxide fuel cells: Quantification of nickel grain growth in dry and in humid atmospheres*, J Power Sources, 196, 12791294 (2011).

5. L. Holzer, B. Münch, B. Iwanschitz, M. Cantoni, T. Hocker, Th. Graule: *Quantitative relationships between composition, particle size, triple phase boundary length and surface area in nickel-cermet anodes for Solid Oxide Fuel Cells*, J Power Sources, 196, 7076 7089 (2011).

6. L.M. Keller, L. Holzer, R. Wepf, Ph. Gasser: *3D geometry and topology of pore pathways in Opalinus clay: Implications for mass transport*, Applied Clay Science, 52, 85-95 (2011).

7. M. Linder, T. Hocker, R. Denzler, A. Mai, B. Iwanschitz: *Automated, Model-Based Analysis of Uj-Data for Electrolyte-Supported SOFC Short-Stacks*, Fuel Cells, vol. 11, pp. 573-580 (2011).

8. E. Knapp, B. Ruhstaller: *Numerical impedance analysis for organic semiconductors with exponential density of localized states*, Appl. Phys. Lett. 99, 9, 093304 (2011).

9. E. Knapp, B. Ruhstaller: *Numerical analysis of steady-state and transient charge transport in organic semiconductor devices*, Optical and Quantum Electronics (2011).

10. D. Rezzonico, B. Perucco, E. Knapp, R. Häusermann, N.A. Reinke, F. Müller, B. Ruhstaller: *Numerical analysis of exciton dynamics in organic light-emitting devices and solar cells*, Journal of Photonics for Energy, 1, 011005-1-11 (2011).

A.3 News Articles

1. N.A. Reinke: *Bericht über Winterthur Instruments*, Swiss Equity Magazin, 2011
2. N.A. Reinke: *Bericht über Winterthur Instruments*, Technopark Leaders, 2011
3. N.A. Reinke: *Moderne Methoden der Schichtprüfung*, Journal für Oberflächentechnik, 2011
4. N.A. Reinke: *Moderne Methoden der Schichtprüfung*, besser lackieren!, 2011
5. N.A. Reinke: *einLeuchtEnD*, Aktuelle Technik, März 2011
6. N.A. Reinke, A. Bariska: *Schichtdickenmessung*, Malerblatt, Mai 2011
7. N.A. Reinke, A. Bariska: *Schichtparameter zuverlässig bestimmen*, Journal für Oberflächentechnik, April 2011
8. A. Bariska, N.A. Reinke: *Berührungslose thermische Schichtprüfung*, Swiss Engineering, März 2011

A.4 Book Chapters

1. Y. Safa: *Helium Thermodynamics, Analytical Model.* Book Chapter, Helium: Characteristics, Compounds, and Applications / Becker Lucas A. (Hrsg.) - Hauppauge, New York, USA: Nova Science Publishers , ISBN/ISSN: 978-1-61761-213-8, 2011.
2. B. Ruhstaller, E. Knapp, B. Perucco, N.A. Reinke, D. Rezzonico, F. Müller: *Advanced Numerical Simulation od Organic Light Emitting Devices.* Book Chapter, Optoelectronic Devices and Properties, Oleg Sergiyenko (Ed.), ISBN 978-953-307-204-3, 2011.

A.5 Exhibitions

1. Thurgauer Technologietag 2011, Arbon, April 2011
2. Hannover Messe, Hannover, April 2011
3. Control Messe, Stuttgart, May 2011
4. Winterthurer Nacht der Technik, ZHAW, Winterthur, June 2011
5. Blue-Tech Fachkongress, Casinotheater, Winterthur, September 2011

A.6 Conferences and Workshops

1. Y. Safa, T. Hocker: *A new model for detailed simulation of multiple transport and conversion processes in SOFC stack repeat units*, 8th Symposium on Fuel Cell Modeling and Experimental Validation, Bonn (Germany), March 2011.
2. A. Evans, R. Tölke, M. Prestat, Y. Safa, T. Hocker, L.J. Gauckler: *Free standing yttria stabilised zirconia micro solid oxide fuel cell membranes*, EMRS, Nice (France), June 2011.
3. B. Ruhstaller: *Parameter extraction by simulation-based characterization of organic solar cells*, Large Area, Organic and Printed Electronics Conference (LOPE-C), Frankfurt (Germany), June 2011.

4. T. Lanz: *Light scattering simulation for thin film silicon solar cells. invited talk*, International Simulation Workshop on Organic Electronics and Photovoltaics, Winterthur (Switzerland), June 2011.

5. E. Knapp: *Impedance Analysis of Organic Light-Emitting Devices*, International Simulation Workshop on Organic Electronics and Photovoltaics, Winterthur (Switzerland), June (2011).

6. B. Ruhstaller, B. Perucco: *On the exciton profile in OLEDs - seamless optical and electrical modelling*, International Simulation Workshop on Organic Electronics and Photovoltaics, Winterthur (Switzerland), June 2011.

7. M. Neukom: *Charge extraction with linearly increasing voltage: A numerical model for parameter extraction*, International Simulation Workshop on Organic Electronics and Photovoltaics, Winterthur (Switzerland), June 2011.

8. M. Schmid: *Modeling and simulation of small amplitude transients and impedance spectra in DSCs*, International Simulation Workshop on Organic Electronics and Photovoltaics, Winterthur (Switzerland), June 2011.

9. A. Evans, R. Tölke, J. Martynczuk, M. Prestat, L.J. Gauckler, Y. Safa, T. Hocker: *Thin films for micro solid oxide fuel cells*, SSI, Warsaw (Poland), July 2011.

10. L. Holzer: *Microstructure effects on the activity of SOFC electrodes: basic principles and preliminary results*, Swiss-Korean Workshop, Thin Films for Solid Oxide Fuel Cells, ETHZ, Zurich (Switzerland), July 2011.

11. Y. Safa: *Buckling-Driven Crack Growth in Elastic Plate Devices*, 21. Symposium Simulationstechnik der Arbeitsgemeinschaft Simulation (ASIM), Winterthur (Switzerland), September 2011.

12. L. Holzer, L. Keller, B. Münch: *Quantitative microstructure analysis in materials science*, Lectures at Summer Academy of Ulm University: Stochastic Analysis, Modelling and Simulation of Complex Structures, Soellerhaus, Kleinwalsertal (Germany), September 2011.

13. L. Holzer, T. Hocker, B. Iwanschitz: *Microstructure analysis and modelling related to degradation of SOFC-electrodes*, 2nd int. Workshop on fuel cell degradation, Thessaloniki (Greece), September 2011.

14. B. Perucco, J.O. Schumacher, J. Roth, F.N. Büchi: *Two-phase modelling of the membrane electrode assemblyof PEMFCs*, European Fuel Cell–Piero Lunghi Conference, Rome (Italy), December 2011.

15. S. Schönenberger, M. Neukom, B. Ruhstaller: *Numerical model and parameter fitting for more insight into BHJ organic solar cell operation*, European Materials Research Society (E-MRS) Symposium, Nice (France), 2011.

16. Y. Safa: *Mathematica Implementation of New Simulation Codes for Challenging Industrial Applications*, Der XIII. Mathematica-Tag, Berlin (Germany), 2011.

17. T. Hocker: *Assessing the performance and degradation behavior of high-temperature solid oxide fuel cells*, Symposium about Trends in Thermodynamics and Materials Theory, Berlin (Germany), 2011.

18. M. Neukom, S. Züfle, N.A. Reinke, B. Ruhstaller: *Charge extraction with linearly increasing voltage: A numerical model for parameter extraction*, DPG Frühjahrstagung 2011, Dresden (Germany), 2011.

19. A. Evans, R. Tölke, J. Martynczuk, M. Prestat, Z. Yáng, M.V.F. Schlupp, L.J. Gauckler, Y. Safa, T. Hocker: *Development of miniaturized solid oxide fuel cells on silicon chips*, ECERS, Stokholm (Sweden), 2011.

A.7 Prizes and Awards

1. N.A. Reinke and A. Bariska, *Heuberger Winterthur Jungunternehmerpreis 2011*
2. N.A. Reinke and A. Bariska, *VentureKick-Award* $I\&II\&III$
3. N.A. Reinke and A. Bariska, *Invited Exhibitor @ Innovation Japan 2011*
4. N.A. Reinke and A. Bariska, *Volkswirtschaft-Stiftung Förderung*
5. N.A. Reinke and A. Bariska, *Invited Exhibitor @ Sonderschau Berührungslose Messtechnik Control 2010 & 2011*
6. N.A. Reinke and A. Bariska, *Top 20 Innovation Hannover Messe 2011*
7. N.A. Reinke and A. Bariska, *VentureLeaders Award*
8. B. Ruhstaller, *Invited Exhibitor @ PV Expo 2011*, Tokyo, Japan

A.8 Teaching

Bachelor of Science

- Analysis $I\&II$ – *R. Axthelm*
- Lineare Algebra I – *R. Axthelm*
- Lineare Algebra I – *M. Schmid*
- Mensch Technik Umwelt – *T. Hocker*
- Organische Elektronik und Photovoltaik – *B. Ruhstaller*
- Thermo-Fluiddynamik III – *T. Hocker*
- Physik Felder & Wellen – *M. Bonmarin*
- Physik I – *M. Bonmarin*
- Physik $I\&II$ – *N.A. Reinke*
- Physik $I\&II$ – *M. Schmid*
- Physik $I\&II$ – *J.O. Schumacher*
- Sensorik – *N.A. Reinke*

Master of Science

- Applied Photonics – *B. Ruhstaller*
- Multiphysics Modelling and Simulation – *J.O. Schumacher*
- Advanced Thermodynamics – *J.O. Schumacher*
- Mathematical Methods (www.pv-master.com) – *J.O. Schumacher*

Summer Schools

- SOFC Modeling and Design, Joint European Summer School for Fuel Cell and Hydrogen Technology (Italy) – *T. Hocker*

A.9 Spin-off Companies

www.nmtec.ch

Numerical Modelling GmbH works in the field of Computer Aided Engineering (CAE) and offers services and simulation tools for small and medium enterprises. Our core competence is knowledge transfer: we bridge the gap between scientific know-how and its application in the industry. With our knowledge from physics, chemistry and the engineering sciences we are able to profoundly support your product development cycle. Numerical Modelling speaks your language and is able to conform to given constraints with respect to time and budget.
We often create so-called customer specific CAE tools in which the scientific knowledge required for your product is embedded. In this form, it is easily deployed within your R&D department and supports actual projects as well as improving the skills of your staff. Ask for our individual consulting service which covers all areas of scientific knowledge transfer without obligation.

www.fluxim.com

FLUXiM is a provider of device simulation software to the display, lighting, photovoltaics and electronics industries worldwide. Our principal activity is the development and the marketing of the simulation software SETFOS which was designed to simulate light emission from thin film devices such as organic light-emitting diodes (OLEDs), thin film solar cells (organic and inorganic) and organic semiconducting multilayer systems.
Our company name FLUXiM is derived from flux simulation. Our software products are used worldwide in industrial and academic research labs for the study of device physics and product development. Check out our references and testimonials for more info. We develop swiss-made software in Switzerland and in addition also provide services such as consulting, training and software development, see services page for more details.

www.winterthurinstruments.ch

Winterthur Instruments GmbH develops measurement systems for fast non contact and non destructive testing of industrial coatings. These measurement systems can be used to determine coating thicknesses, material parameters (e.g. porosity) and contact quality (e.g. to detect delamination). The system is based on optical-thermal measurements and works with all types of coating and substrate materials. Our measurement systems provide the unique opportunity of non-contact and non-destructive testing of arbitrary coatings on substrates.

A.10 ICP-Team

Name	Function	e-Mail
Dr. Rebekka Axthelm	Research Associate	rebekka.axthelm@zhaw.ch
Dr. Mathias Bonmarin	Research Associate	mathias.bonmarin@zhaw.ch
Kai Brossi	Research Assistant	kai.brossi@zhaw.ch
Dr. Peter Cendula	Research Associate	peter.cendula@zhaw.ch
Samuel Hauri	Research Assistant	samuel.hauri@zhaw.ch
Prof. Dr. Thomas Hocker	Lecturer, Head ICP	thomas.hocker@zhaw.ch
Dr. Lorenz Holzer	Research Associate	lorenz.holzer@zhaw.ch
Lukas Kaufmann	Research Assistant	lukas.kaufmann@zhaw.ch
Dr. Lukas Keller	Research Associate	lukas.keller@zhaw.ch
Evelyne Knapp	Research Associate	evelyne.knapp@zhaw.ch
Thomas Lanz	Research Assistant	thomas.lanz@zhaw.ch
Kevin Lapagna	Research Assistant	kevin.lapagna@zhaw.ch
Markus Linder	Research Assistant	markus.linder@zhaw.ch
Christoph Meier	Research Assistant	christoph.meier@zhaw.ch
Omar Pecho	Research Associate	omar.pecho@zhaw.ch
Benjamin Perucco	Research Associate	benjamin.perucco@zhaw.ch
Prof. Nils Reinke	Lecturer	nils.reinke@zhaw.ch
Remo Ritzmann	Research Assistant	remo.ritzmann@zhaw.ch
Prof. Dr. Beat Ruhstaller	Lecturer, Dep. Head ICP	beat.ruhstaller@zhaw.ch
Dr. Yasser Safa	Research Associate	yasser.safa@zhaw.ch
Dr. Guido Sartoris	Research Associate	guido.sartoris@zhaw.ch
Dr. Matthias Schmid	Research Associate	matthias.schmid@zhaw.ch
Prof. Dr. Jürgen Schumacher	Lecturer	juergen.schumacher@zhaw.ch
Esther Spiess	Administrative Assistant	esther.spiess@zhaw.ch
Lilian Toniolo	Administrative Assistant	lilian.toniolo@zhaw.ch
Simon Züfle	Research Assistant	simon.zuefle@zhaw.ch

The following visiting scientists were staying at the ICP during the last year:

- Prof. Dr. Seung Jae Baik, research partner, Korea Advanced Institute of Technology (KAIST), South Korea
- Matthias Neumann, Ulm University, Ulm, Germany
- Felipe Augusto Brasileiro, IAESTE Exchange Student, Universidade Estadual de Campinas, Saõ Paulo, Brasil

A.11 Location

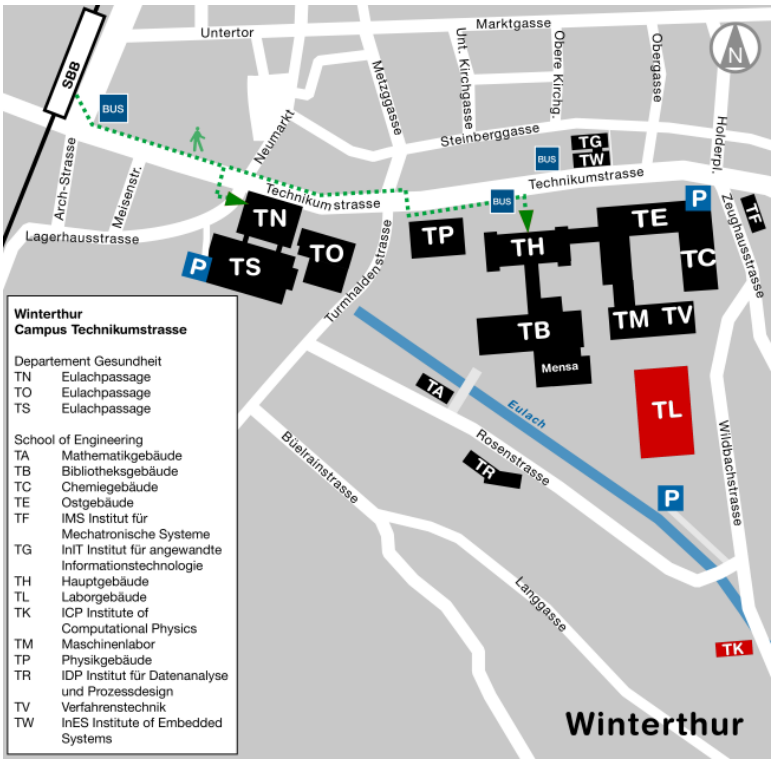
ICP Institute of Computational Physics

Technikumstrasse 9
P.O. Box
CH-8401 Winterthur

www.icp.zhaw.ch

Contact
Thomas Hocker
Phone +41 58 934 78 37
thomas.hocker@zhaw.ch

Administration
Lilian Toniolo
Phone +41 58 934 73 06
lilian.toniolo@zhaw.ch



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Zurich University
of Applied Sciences

School of Engineering

ICP Institute of
Computational Physics

Technikumstrasse 9
P.O. Box
CH-8401 Winterthur

Phone +41 58 934 71 71
info.engineering@zhaw.ch
www.icp.zhaw.ch