

## Proceedings of the

# ARGE Sensorik PhD-Summit 2011

June 29-30, 2011

Johannes Kepler University Linz,  
Science Park, Room MT 226/1

Edited by Bernhard Jakoby (Johannes Kepler University Linz)

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# Content

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## Preface

The Austrian Working Group on Sensors (ARGE Sensorik) was founded in 2006 aiming at the optimization of the joint utilization of sensor know-how and associated technology distributed over Austria. One major goal of the ARGE Sensorik is the initiation of joint research networks also involving industrial partners. The ARGE now serves as platform representing various facets of interdisciplinary sensor research in Austria. Its members are research institutes and centers of competence working on sensors or dealing with problems where sensors play a major role. The activities of the ARGE have been stimulated and financially supported by the Austrian Research Association (Österreichische Forschungsgemeinschaft, ÖFG) from the very beginning.

One of the main activities of the ARGE is the organization of workshops featuring the presentation of current research topics by major Austrian players in sensor research and leading to scientific exchange among them. This is done in plenary workshops but also in topically focuses small groups. For more information on the ARGE and current activities, please visit [www.arge-sensorik.at](http://www.arge-sensorik.at).

In 2009 the ARGE steering committee decided to have a plenary meeting where young researchers, in particularly those who are about to or have recently finished their PhD theses present their work. Due to the success of that event (held in Vienna) we decided to continue with another young researcher meeting in 2011, this time in Linz. The ARGE Sensorik Award was also presented at this occasion where the jury selection was based on the presentations at the workshop and one journal publication per participant submitted before the workshop. The award was presented to Roman Bruck and two special awards have been given to Norbert Reitinger and Thomas Voglhuber-Brunnmaier.

A selection of the contributions is presented in this electronic Proceedings volume.

At this occasion I would like to thank all individuals who helped to organize this event (in particular staff at the Institute of Microelectronics and Microsensors), our financial sponsors (Johannes Kepler University Linz, Austrian Center of Competence in Mechatronics ACCM, Österreichische Forschungsgemeinschaft ÖFG), and of course the contributors for presenting and discussing their work!

Linz, September 2011

Bernhard Jakoby

# Workshop Program

Time	Name	Affiliation	Topic*
09:00	B. Jakoby	JKU	Welcome and Introduction
09:15	Roman Bruck	AIT	Integrated polymer-based Mach-Zehnder interferometer label-free streptavidin biosensor compatible with injection molding
09:35	Norbert Reitinger	UG	Radiationless energy transfer in CdSe/ZnS quantum dot aggregates embedded in PMMA
09:55	Thomas Voglhuber	JKU	Modeling of an LFE piezoelectric fluid sensor as layered structure in the spectral domain
10:15	Wolfgang Buchegger	TUW	A highly uniform lamination micromixer with wedge shaped inlet channels for time resolved infrared spectroscopy
10:35			Coffee Break
11:00	Dominik Samson	TUW	Wireless sensor node powered by aircraft specific thermoelectric energy harvesting
11:20	Lukas Richter	AIT	Monitoring Cellular Stress Responses to Nanoparticles using a Lab-on-a-Chip
11:40	Michael Moser	TUG	Strong and Weak Electric Fields Interfering: Capacitive Icing Detection and Capacitive Energy Harvesting on a 220 kV High-Voltage Overhead Power Line
12:00			Lunch Break
13:00	Michael Rosenauer (ARGE Sensorik Award Winner 2010)	Osram	Introduces his research associated with the ARGE Sensorik Award 2010 and his current work with OSRAM
13:20	Moritz Eggeling	AIT	Low spin current-driven dynamic excitations and metastability in spin-valve nanocontacts with unpinned artificial antiferromagnet
13:40	Thomas Lederer	JKU	Utilizing a high fundamental frequency quartz crystal resonator as a biosensor in a digital microfluidic platform
14:00	Sander van den Driesche	TUW	A label-free indicator for tumor cells based on the CH2-stretch ratio
14:20			Coffee Break
14:40	Johannes Sell	ACCM, JKU	Real-time monitoring of a high pressure reactor using a gas density sensor
15:00	Markus Neumayer	TUG	Accelerated Markov Chain Monte Carlo Sampling in Electrical Capacitance Tomography
15:20	Nicola Moscelli	TUW	An Imaging System for Real-Time Monitoring of Adherently Grown Cells
15:40	Alexander Niedermayer	ACCM, JKU	Yet another precision impedance analyzer (YAPIA)—Readout electronics for resonating sensors
16:00			Short Break (Jury Meeting)
16:15	B. Jakoby, M.J. Vellekoop, F. Kohl	JKU, TUW,ÖAW	Presentation of the ARGE Sensorik Awards 2010 (M. Rosenauer) and 2011 (to be announced at this moment)
16:30	B Jakoby	JKU	Closing Discussion

\*indicated topics are titles of papers submitted for the ARGE Sensorik Award 2011, topics of talks may vary.

## **Selected Contributions**

Polymer-based photonic label-free biosensor, R. Bruck et al

Quantum dots in plasmonic systems for optochemical sensors, N. Reitinger

Modeling of an LFE piezoelectric fluid sensor as layered structure in the spectral domain, T. Voglhuber-Brunnmaier

A Highly Uniform Lamination Micromixer with Wedge Shaped Inlet Channels for Time Resolved Infrared Spectroscopy, W. Buchegger et al

Thermoelectric energy harvesting in aircraft for wireless sensors, D. Samson et al

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Yet another precision impedance analyzer - Readout electronics for resonating sensors, A.O. Niedermayer

### **Notes:**

*In this electronic compilation, the page format has not been unified but has been kept as provided by the individual authors. Thus in the remainder of this document the page format (size) varies, which may have to be kept in mind when printing selected contributions.*

*In the following, page numbers are given at the bottom of the respective pages (in red color if you view or print in color) - these were electronically imprinted on the documents provided by the authors (some contributions use independent page numbering).*

# Polymer-based photonic label-free biosensor

R. Bruck<sup>a</sup>, E. Melnik<sup>a</sup>, P. Muellner<sup>a</sup>, R. Hainberger<sup>a</sup>,  
M. Lämmerhofer<sup>b</sup>



<sup>a</sup> AIT Austrian Institute of Technology GmbH, Health & Environment Department, Nano Systems

<sup>b</sup> University of Vienna, Department of Analytical Chemistry



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30.6.2010 – Roman Bruck

# Polymer-based photonic label-free biosensor

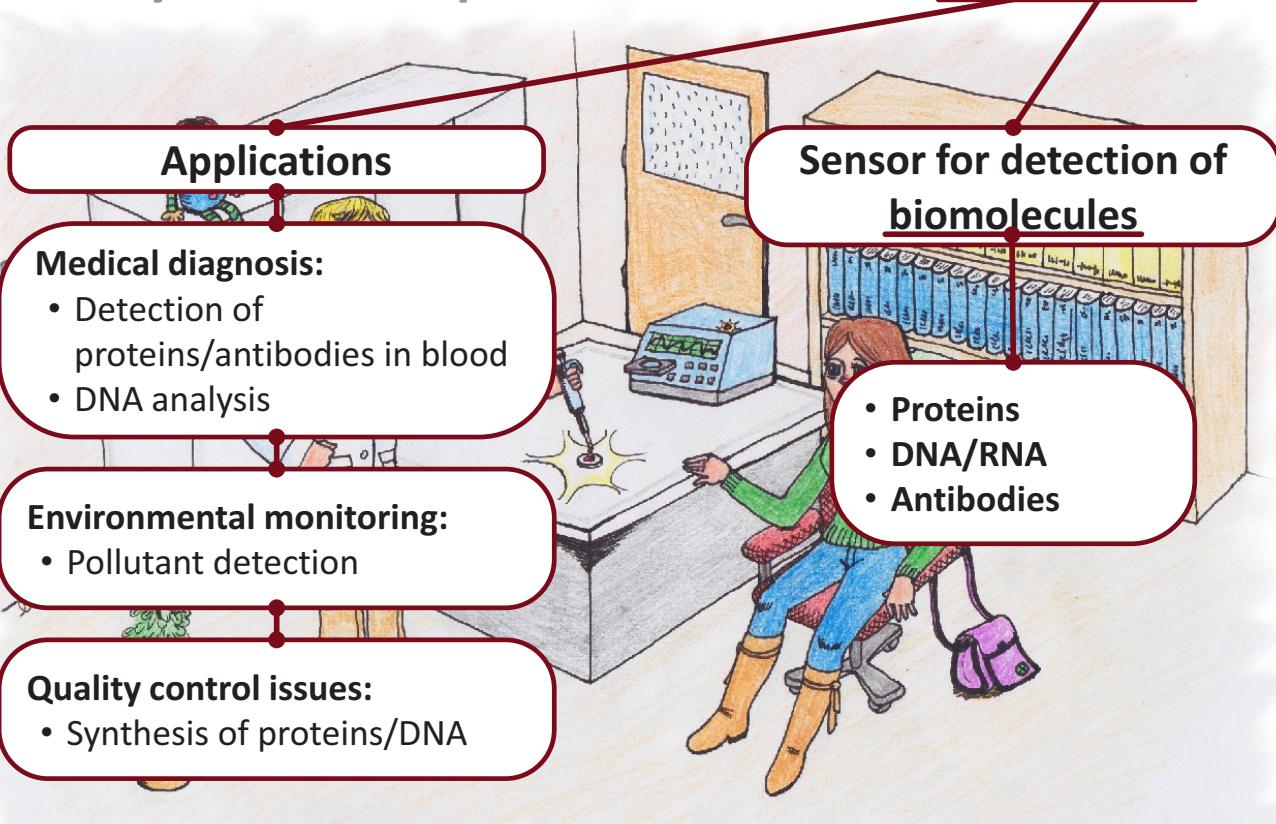
## Outline:

• What is a biosensor and what are its applications?

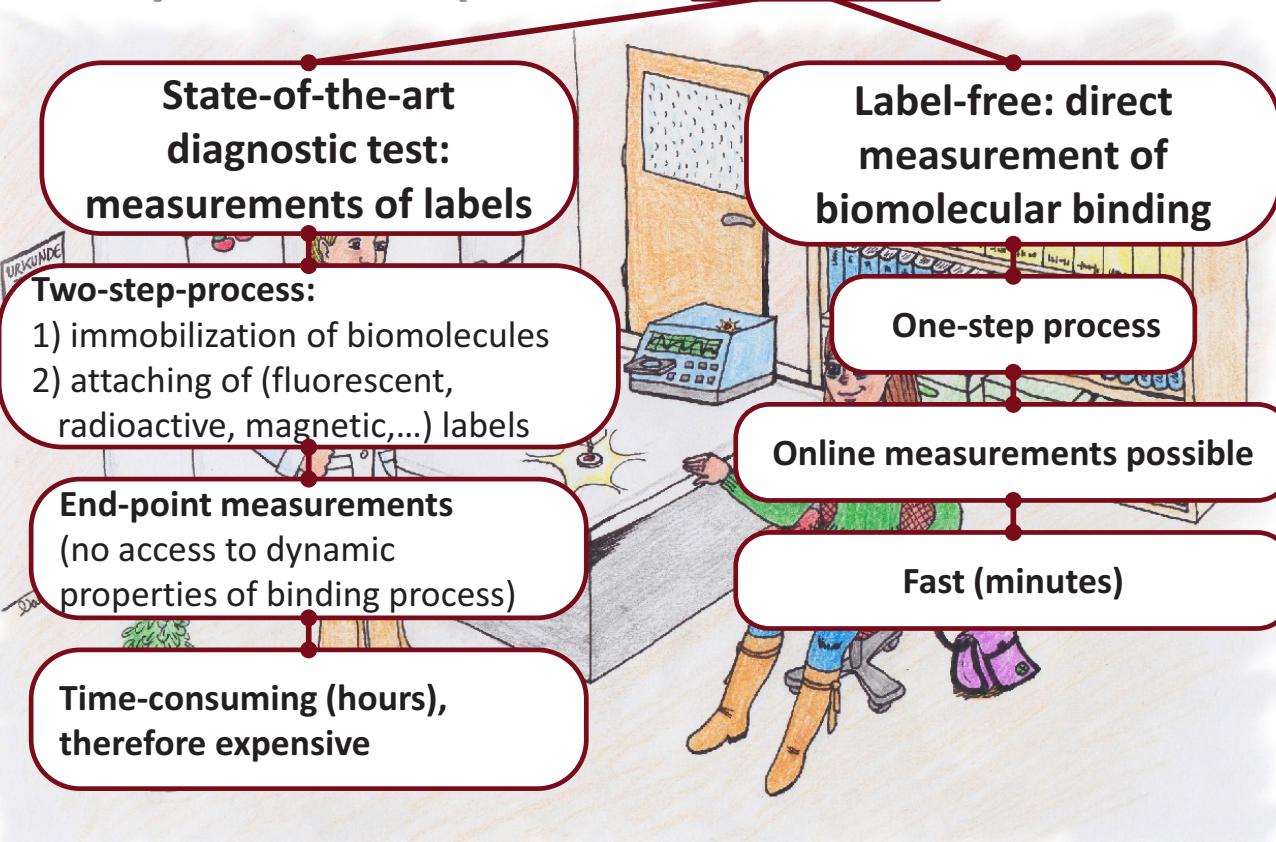
• Measurement principle & sensor concept

• Experimental results

# Polymer-based photonic label-free biosensor



# Polymer-based photonic label-free biosensor



## Polymer-based photonic label-free biosensor

**Using the properties of light to detect changes in the surrounding**

**No classical optics:**

Photonic sensors use new properties of light arising only when employing sub-wavelength structures

### Advantages:

- Highly sensitive
- Instantaneous sensor response
- Online measurement capability
- small device footprint
- parallel measurements

Evanescence waveguide sensor in a Mach-Zehnder interferometer configuration

## Polymer-based photonic label-free biosensor

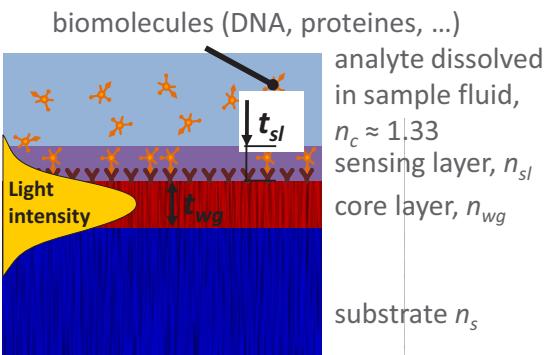
**cost efficient mass production (disposable devices in medicine!)**

**limited range of refractive indices (1.4-1.7), therefore limited sensitivity**

powerful technology platform for polymer processing , e.g. injection molding (e.g. CDs, DVDs, ...) and spin coating

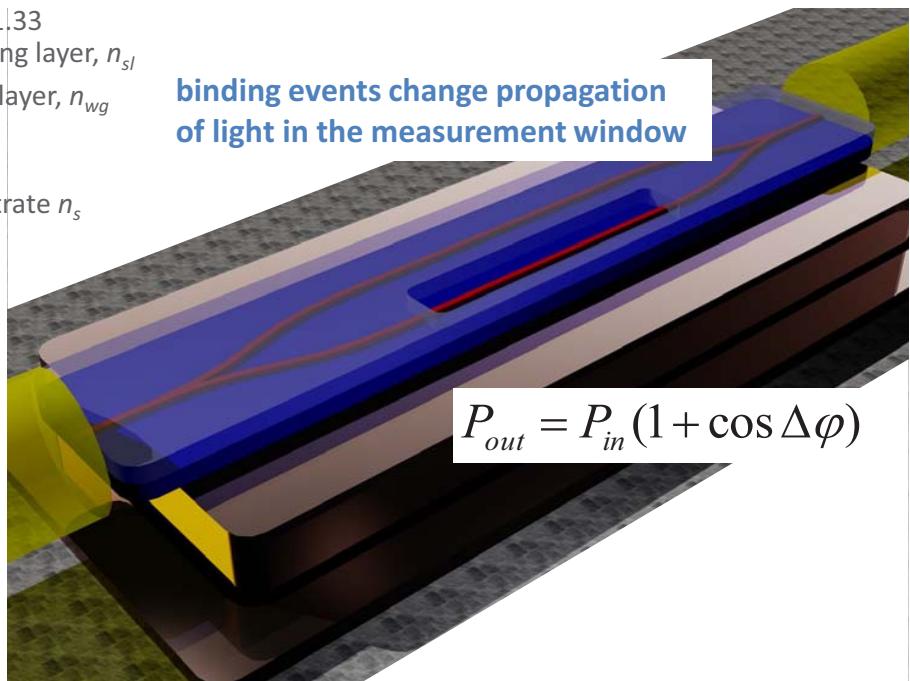
## Measurement principle:

### waveguide side view:



Biosensitive layer on top of waveguide provides selective binding and an enrichment of biomolecules on the sensor surface.

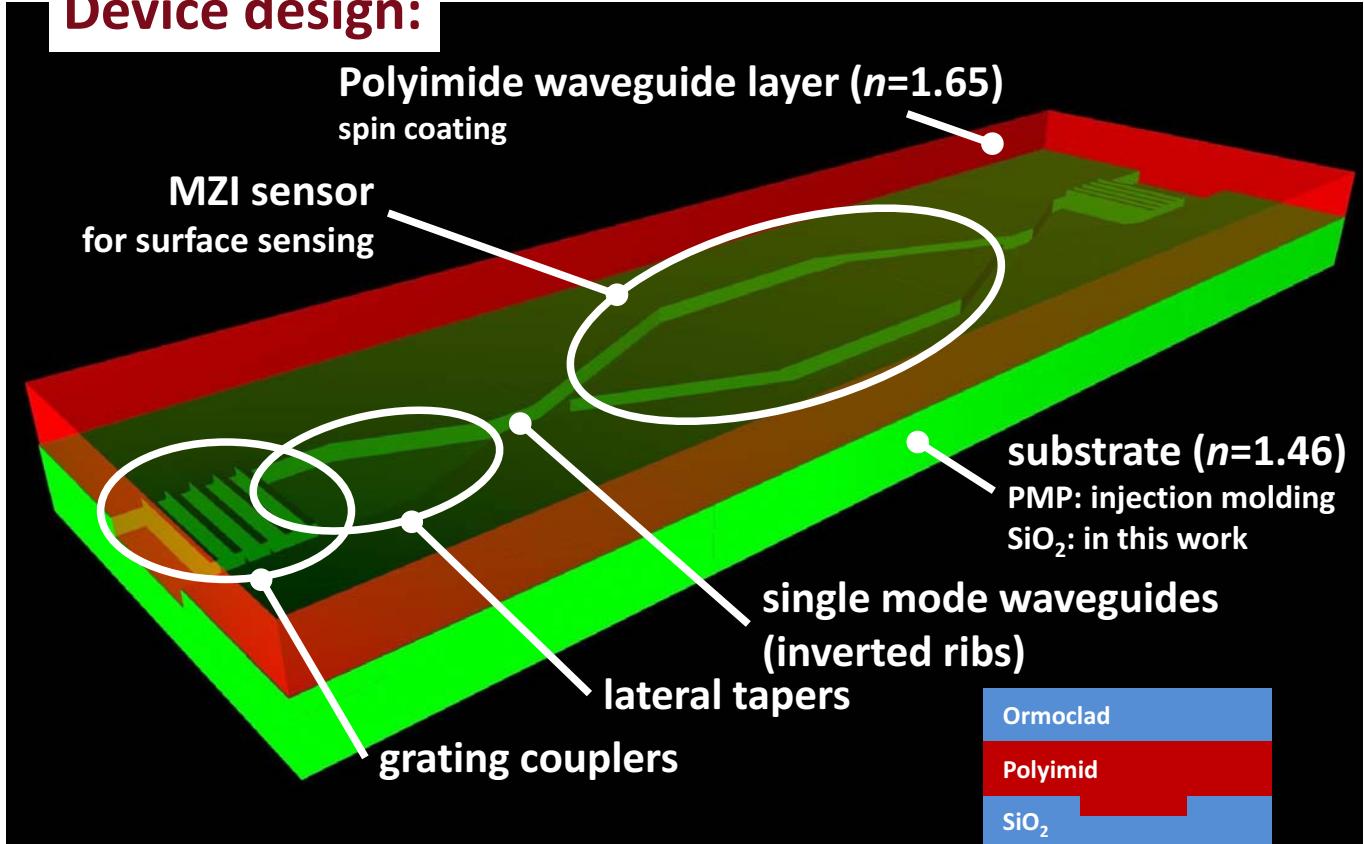
binding events change propagation of light in the measurement window



- Highly sensitive
- Simple & low-priced read-out system

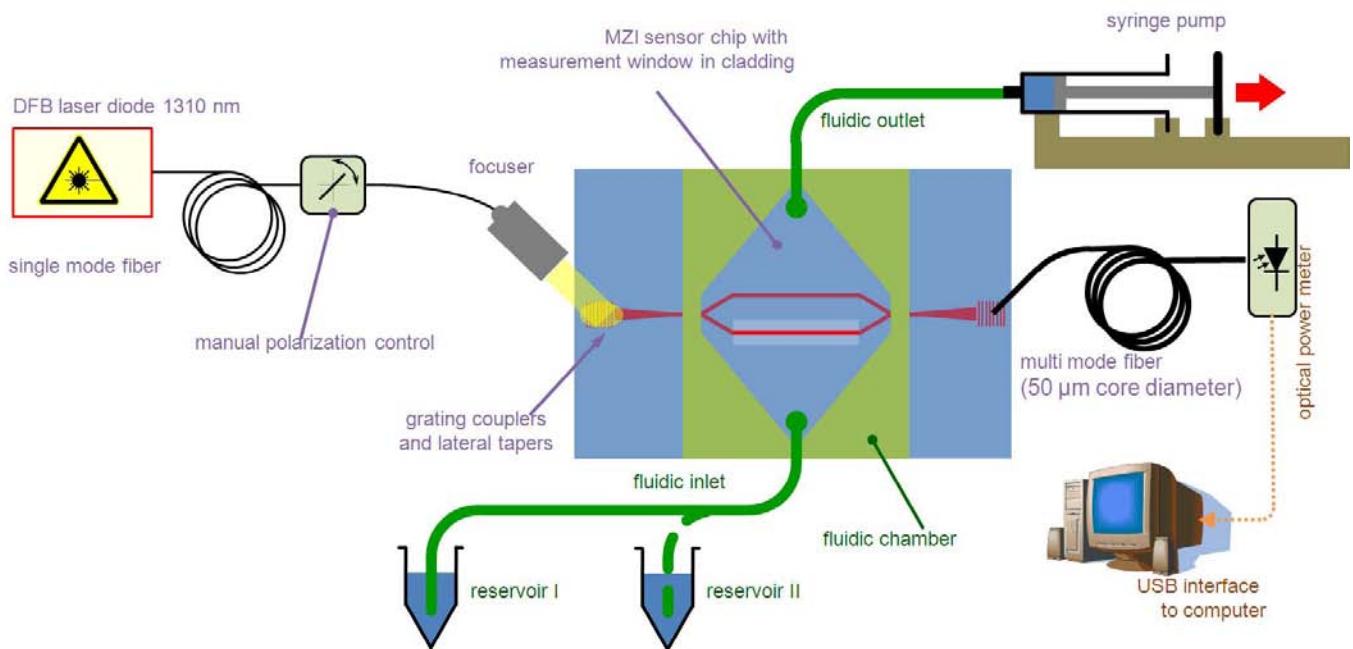
30.6.2010 – Roman Bruck

## Device design:



30.6.2010 – Roman Bruck

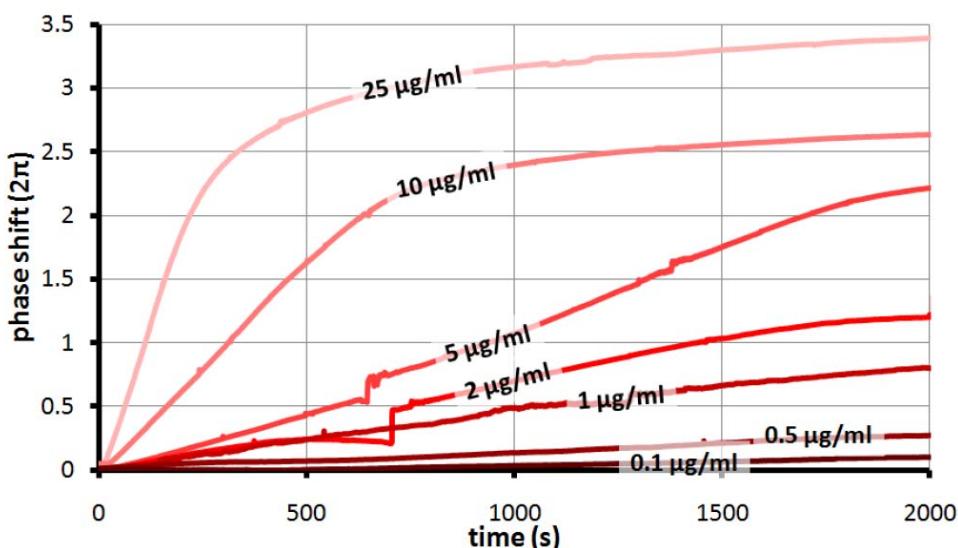
## MZI – measurement setup:



30.6.2010 – Roman Bruck

## Biotin-streptavidin measurements:

Biotin – streptavidin binding on non-blocked surfaces

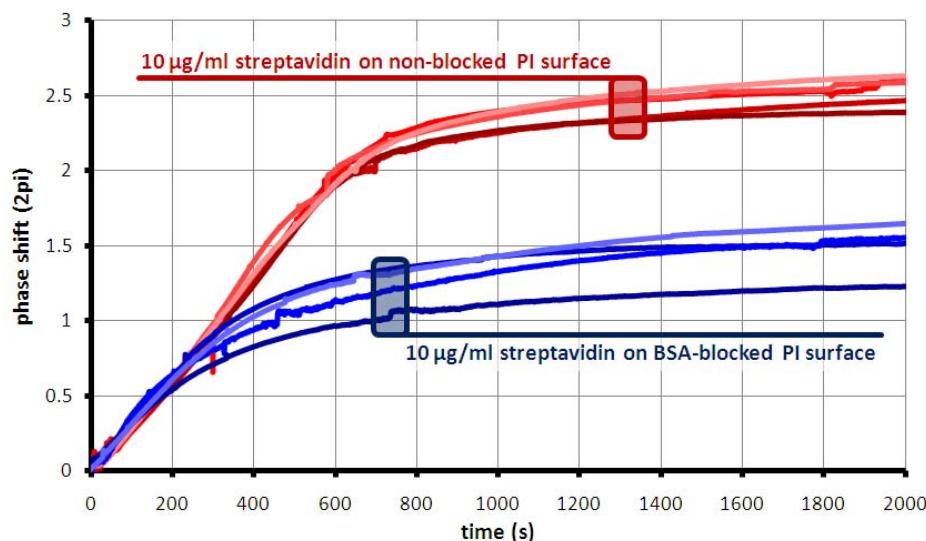


smallest concentration measured:  
0.1  $\mu\text{g}/\text{ml}$  = 1.6 nMol = 30 ppb

30.6.2010 – Roman Bruck

## Biotin-streptavidin measurements:

Reproducability – blocking – specificity



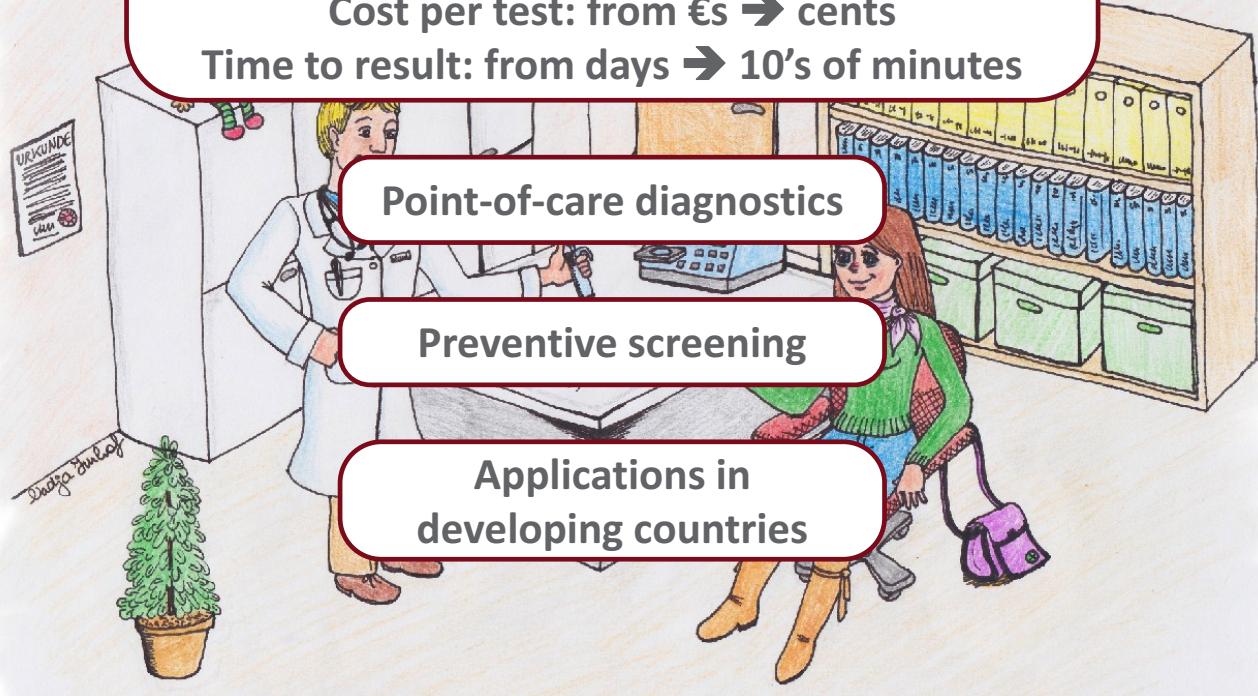
Standard deviation ~ 5%  
Sensor sensitivity varies max. 2%

Blocking:  
Signal reduced by about 40%  
BUT:  
No non-specific binding!

30.6.2010 – Roman Bruck

## A vision:

Price of read-out system: from 100k€ → k€  
Cost per test: from €s → cents  
Time to result: from days → 10's of minutes



# Quantum Dots in plasmonic systems for optochemical sensors

Norbert Reitinger

Nano-Optics Group

[nano optics.uni-graz.at](http://nano optics.uni-graz.at)

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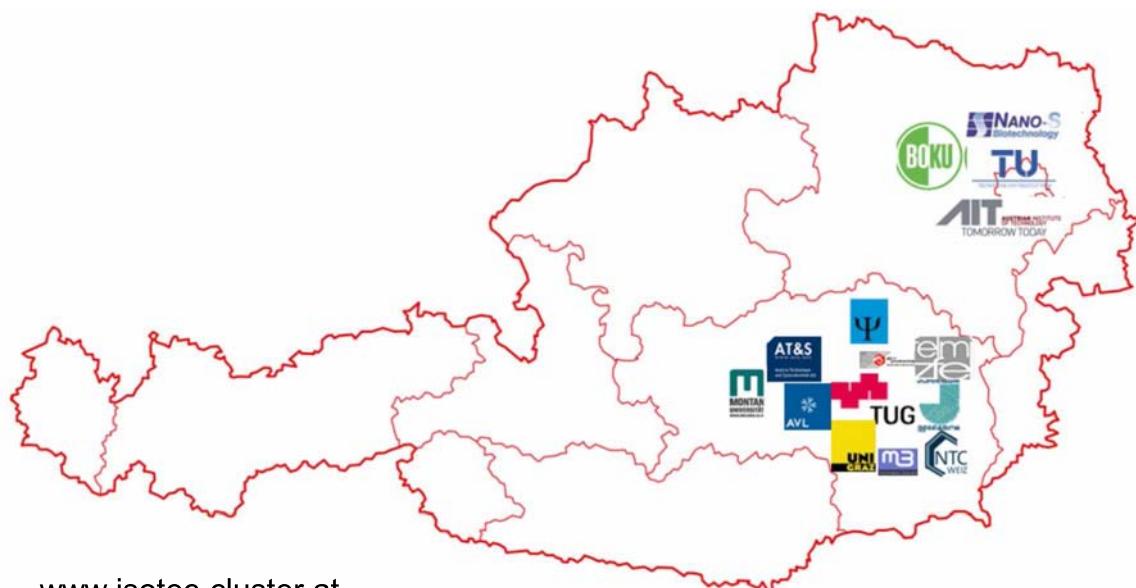
June 30, 2011

Institute of Physics, Karl-Franzens University Graz, Austria

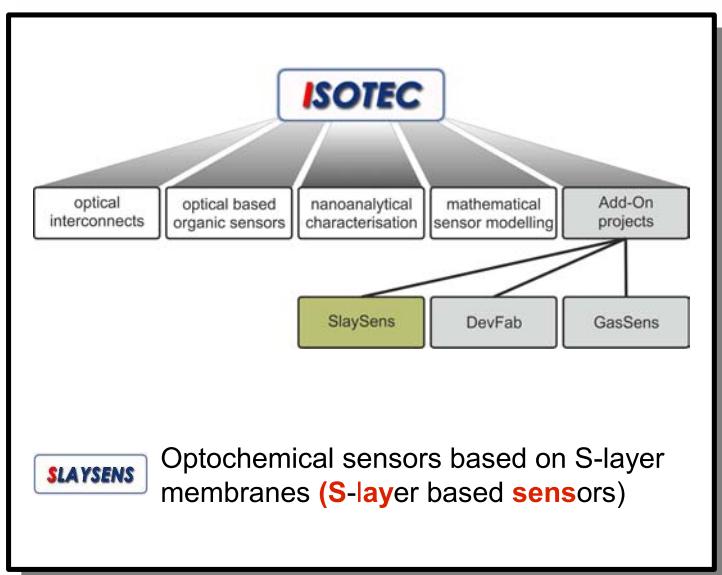
ISOTEC Research Cluster



**ISOTEC** Integrated Organic Sensor and Optoelectronic Technologies



[www.isotec-cluster.at](http://www.isotec-cluster.at)



## Contents

### Introduction

SlaySens -  
sensor principle  
  
quantum dots

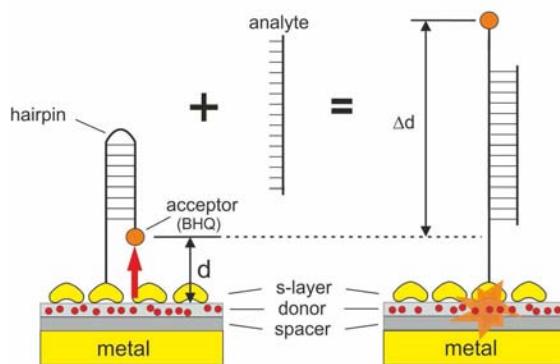
### Experiments

QD characterisation  
  
energy transfer  
  
emitter metal interaction

### Conclusion

summary  
  
outlook &  
applications

## Sensor Working Principle



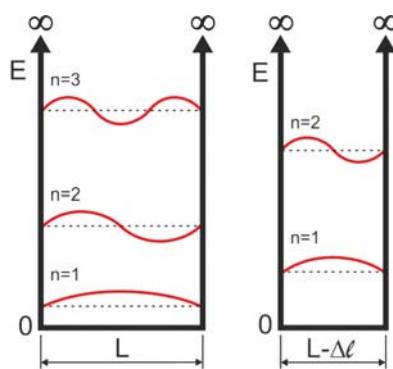
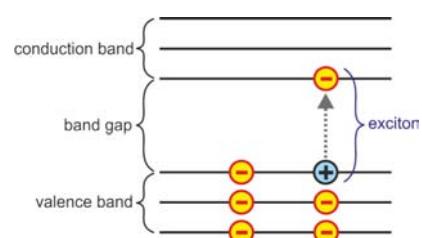
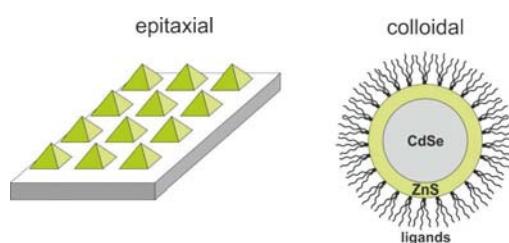
Scanning-force-microscope-surface-relief reconstruction of a crystalline protein S-layer from *Bacillus sphaericus*

© Center for Nanobiotechnology, University of Natural Resources and Applied Life Sciences, Vienna, Austria

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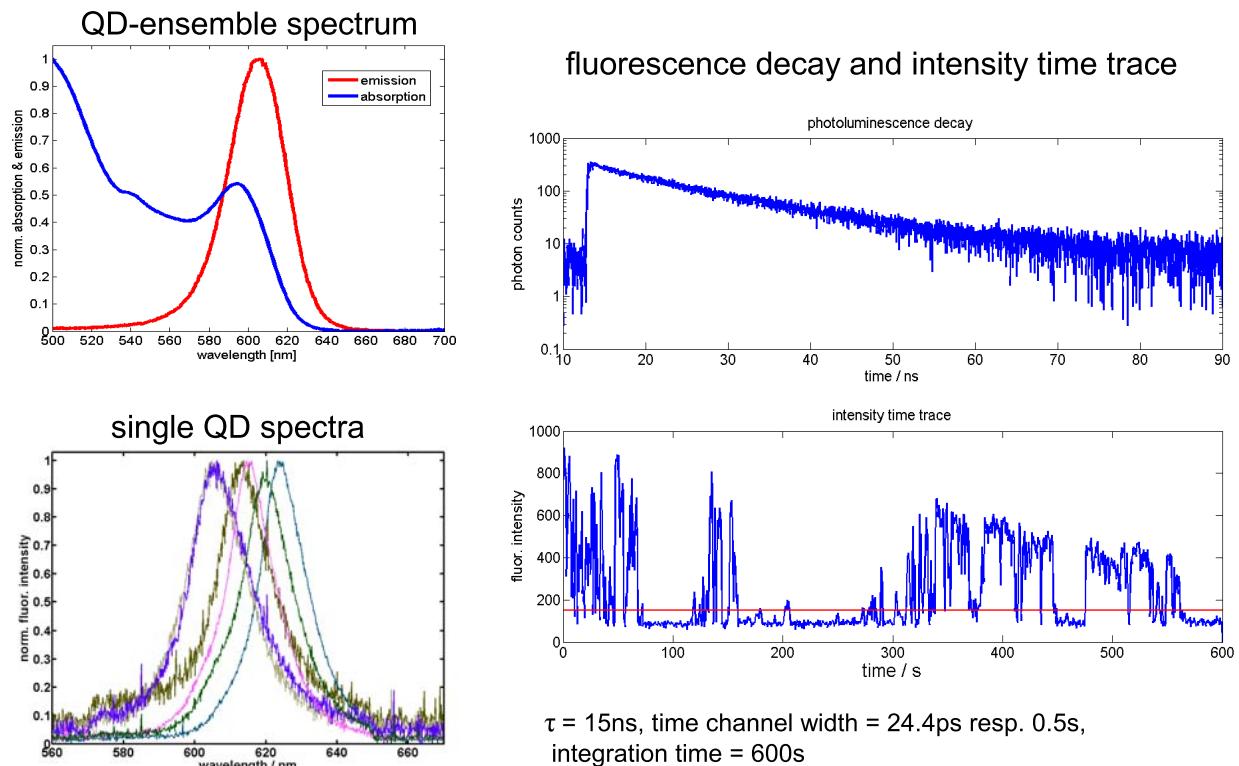
## Quantum Dots



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## QD characterization

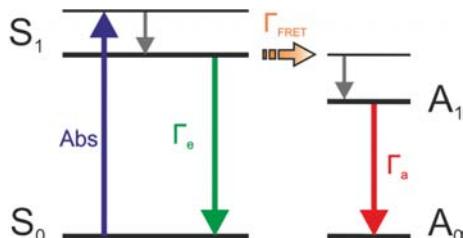


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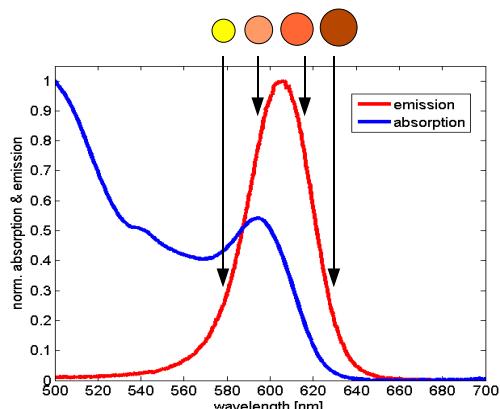
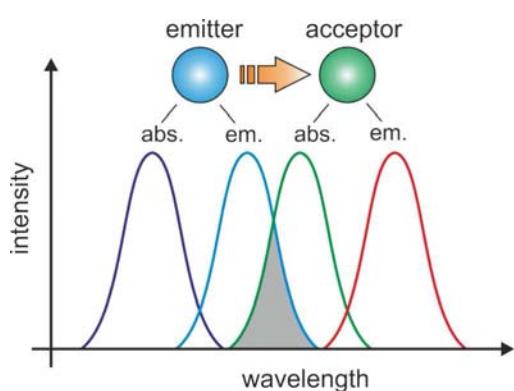


## FRET between Quantum Dots



$$\Gamma_{ET}(r) = \frac{1}{\tau_D} \left( \frac{R_0}{r} \right)^6 = \Gamma_D \left( \frac{R_0}{r} \right)^6$$

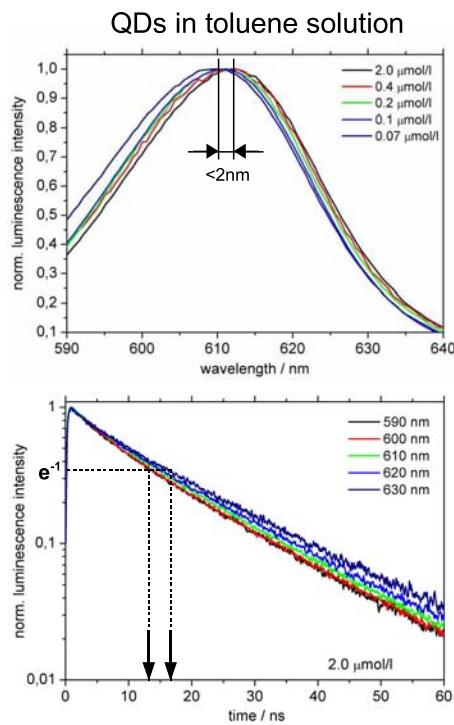
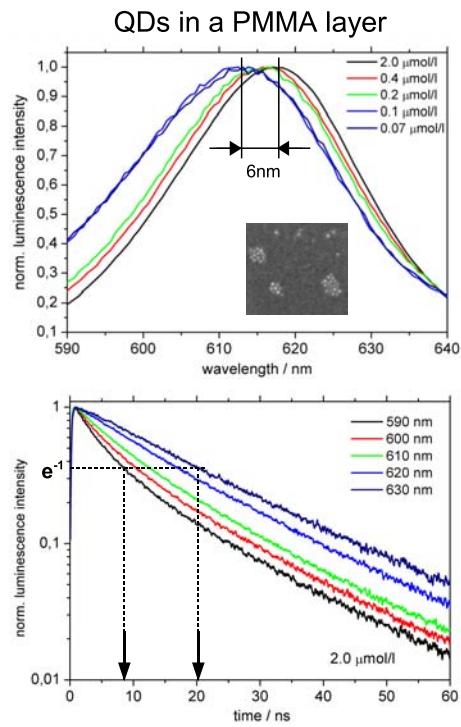
$$R_0^6 = 0.529 \frac{\kappa^2 Q_D}{n^4 N} J(\lambda)$$



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## FRET between Quantum Dots



N. Reitinger et al., Phys. Stat. Sol. A **208**, 710 (2011)

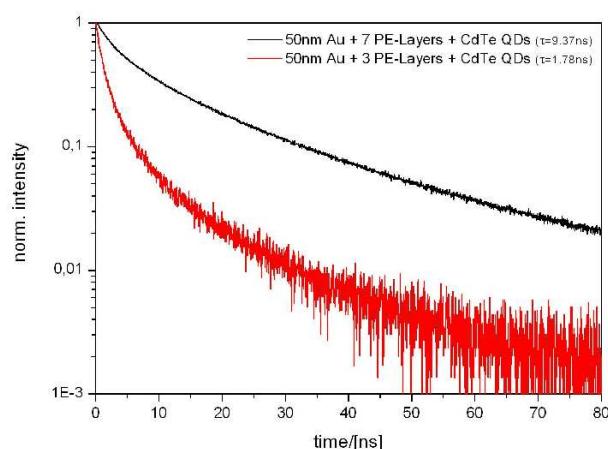
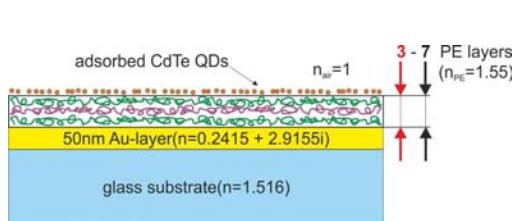
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## QD's and a flat metal film



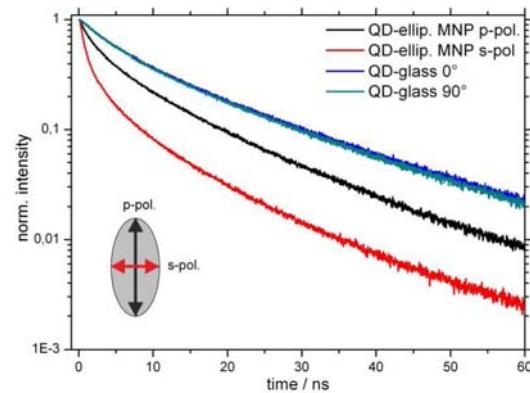
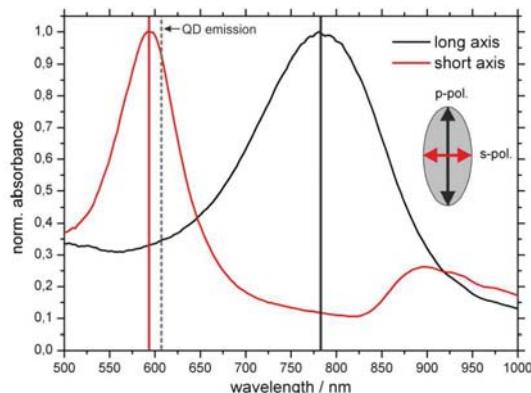
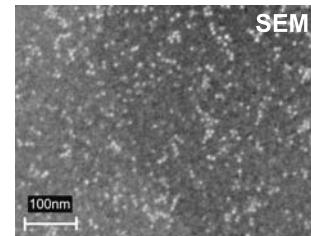
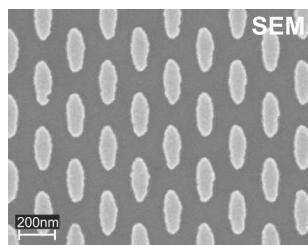
water-soluble CdTe QDs (EWL =630nm) (Prof. Dr. Xinhua Zhong, Department of Chemistry, East China University of Science and Technology, Shanghai)



$$I(t) = I_0 \cdot e^{-(t/\tau)^\beta}, \quad 0 < \beta \leq 1$$

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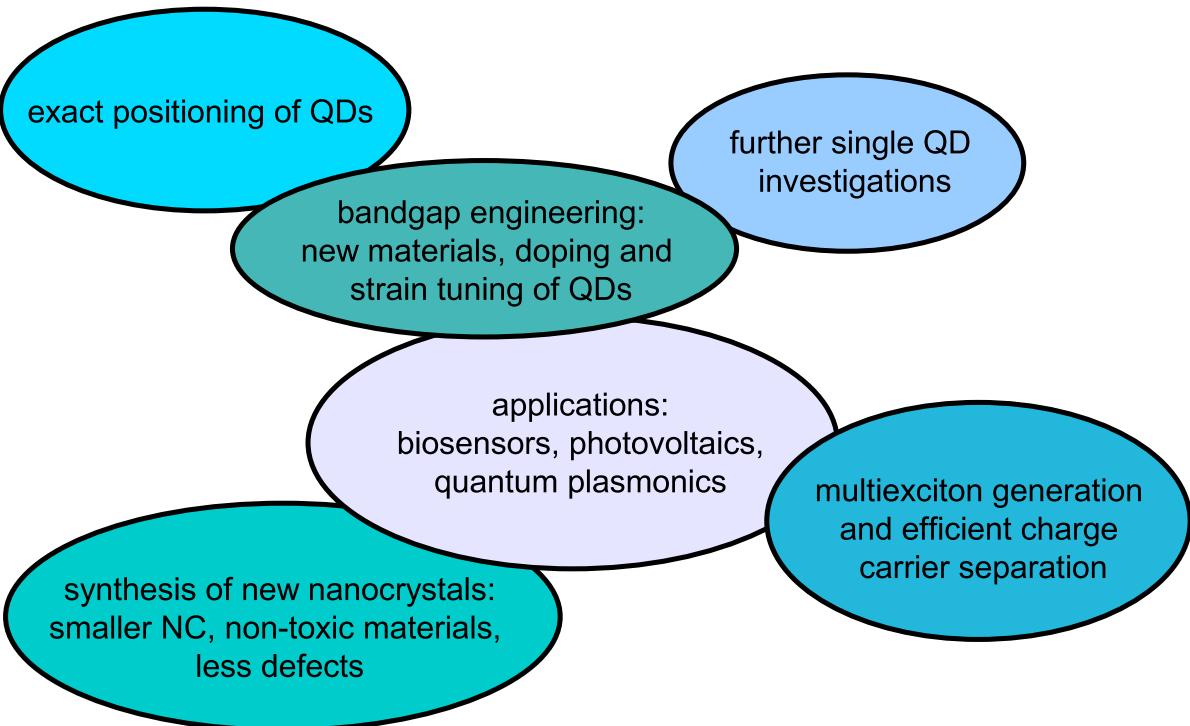


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## Summary

- fluorescence lifetime is suitable as sensor quantity
- but interpretation of decay curves can be difficult
- investigation of energy transfer between QD's
- interaction between QD's and metal



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Norbert Reitinger

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# Modeling of an LFE piezoelectric fluid sensor as layered structure in the spectral domain

Thomas Voglhuber-Brunnmaier

Institute for Microelectronics and Microsensors,  
Johannes Kepler University, Linz, Austria

## Liquid sensing

- Measure the parameters of a fluid  
E.g.: density, viscosity, permittivity, conductivity
- Thickness field excitation (TFE) vs. lateral field excitation (LFE)
- Modeled utilizing a semi-numeric spectral method

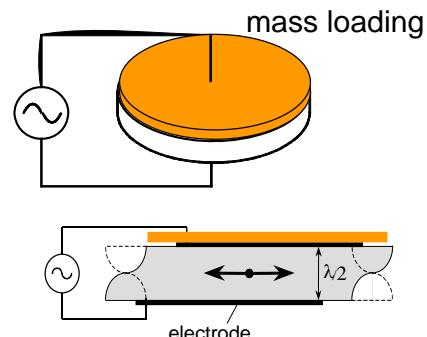
# Sensing utilizing piezoelectric structures

Sauerbrey (1959) (mass loading)

$$\Delta f = -\frac{2f_0^2}{A\sqrt{\rho c}} \Delta m$$

A...face area  
 $\rho$ ...density

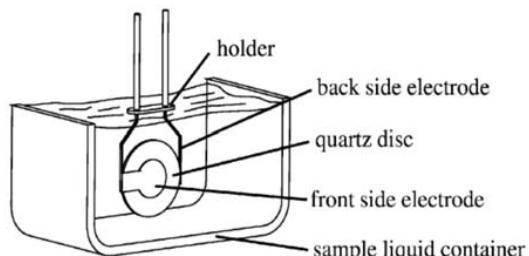
$\Delta m$ ...mass loading  
 $c$ ...shear modulus



Kanazawa, Gordon (1985) (viscous fluid loading)

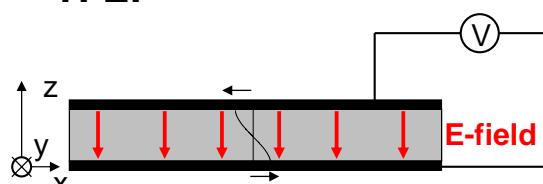
$$\Delta f = -f_0^{3/2} \sqrt{\frac{\rho' \mu}{\pi \rho c}}$$

$\rho'$ ...liquid density       $\mu$ ...shear viscosity



## Thickness Field vs. Lateral Field Excitation

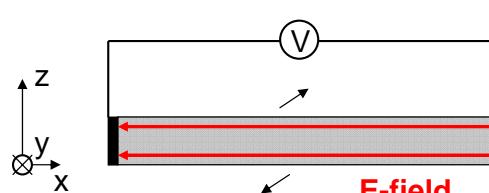
TFE:



stresses: piezoelectricity  
 (Quartz):

$$\begin{bmatrix} T_{xx} \\ T_{yy} \\ T_{zz} \\ T_{yz} \\ T_{xz} \\ T_{xy} \end{bmatrix} = \begin{bmatrix} e_{11} & 0 & 0 \\ e_{12} & 0 & 0 \\ e_{13} & 0 & 0 \\ e_{14} & 0 & 0 \\ 0 & e_{25} & e_{35} \\ 0 & e_{26} & e_{36} \end{bmatrix} \cdot \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

LFE:



$$\begin{bmatrix} T_{xx} \\ T_{yy} \\ T_{zz} \\ T_{yz} \\ T_{xz} \\ T_{xy} \end{bmatrix} = \begin{bmatrix} e_{11} & 0 & 0 \\ e_{12} & 0 & 0 \\ e_{13} & 0 & 0 \\ e_{14} & 0 & 0 \\ 0 & e_{25} & e_{35} \\ 0 & e_{26} & e_{36} \end{bmatrix} \cdot \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

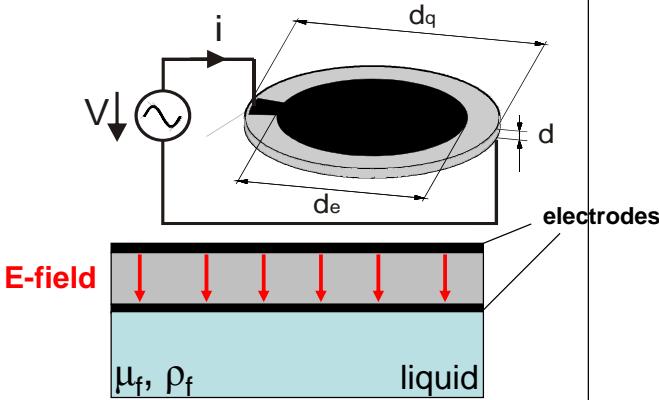
Coupling factors 330μm AT-Cut quartz :

	$k_{TE}$ in %	$k_{LE,0}$ in %	$k_{LE,90}$ in %	$v$ in m/s	$f_0$ in MHz
extensional	a	0	6.48	0	7009
fast shear	b	0	6.17	0	3801
slow shear	c	8.74	0	6.26	3326

(i.e., coupling strength between electrical and mechanical fields)

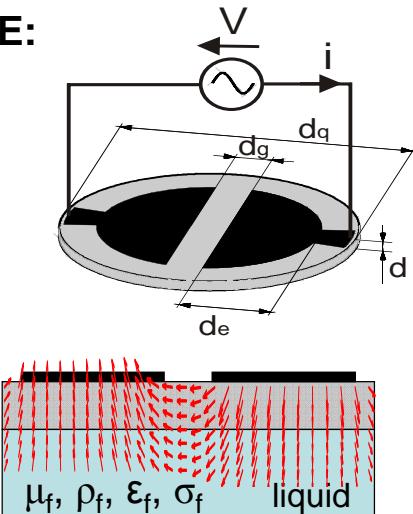
# Thickness Field vs. Lateral Field Excitation

**TFE:**



- only TFE - modes excited
- electric field confined in the piezo
- sensitivity to viscosity and density

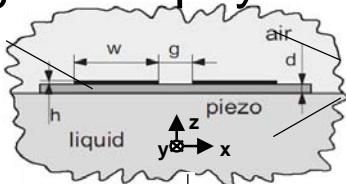
**LFE:**



- also LFE modes excited
- electric field propagates into liquid
- sensitivity also to permittivity and conductivity

## Modeling of the physical domains

piezoelectric equations +  
quasistatic approximation +  
equation of motion



linearized Navier Stokes +  
electrostatic Maxwell Eqn.

piezo equations:

$$\begin{aligned} \rho \ddot{\mathbf{u}} &= \nabla \cdot \mathbf{c}^E : \nabla_s \mathbf{u} + \nabla \cdot \mathbf{e} \nabla \varphi \\ \nabla \cdot \mathbf{e} : \nabla_s \mathbf{u} &= \nabla \cdot \mathbf{e}^S : \nabla \varphi \end{aligned}$$

$\mathbf{u}$  ... displacement vector,  $\varphi$  ... electric potential  
 $\rho$  ... mass density,  $\mathbf{c}^E$  ... elastic stiffness tensor  
 $\mathbf{e}$  ... piezoelectric stress tensor,  $\mathbf{e}^S$  ... permittivity tensor  
 $\nabla$  ... gradient operator,  $\nabla_s$  ... symmetric gradient operator

equations for liquid and air:

$$\begin{aligned} \rho \ddot{\mathbf{u}} &= \frac{1}{\zeta} \nabla (\nabla \cdot \mathbf{u}) + \mu \nabla \dot{\mathbf{u}} + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) \\ \nabla \cdot \left( \frac{\sigma}{\epsilon} \mathbf{D} + \dot{\mathbf{D}} \right) &= 0 \end{aligned}$$

$\mathbf{D}$  ... electric displacement vector,  $\zeta$  ... compressibility coefficient  
 $\mu$  ... shear viscosity coefficient,  $\lambda$  ... volume viscosity coefficient  
 $\sigma$  ... electrical conductivity,  $\epsilon$  ... isotropic permittivity

TABLE I

EQUATIONS DESCRIBING THE PIEZO MATERIAL AND DENOTATION OF THE INCLUDED QUANTITIES.

TABLE II

EQUATIONS DESCRIBING LIQUID AND AIR AND DENOTATION OF INCLUDED QUANTITIES.

time-harmonic, layered structure:

$$\frac{\partial}{\partial t} \circ \bullet \cdot i\omega, \frac{\partial}{\partial x} \circ \bullet \cdot (-ik_x), \frac{\partial}{\partial y} \circ \bullet \cdot (-ik_y)$$

spectral domain method

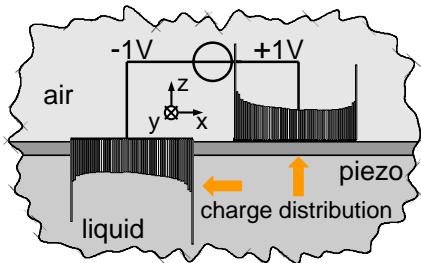
3 systems of ODEs of 1st order of dim 8:

$$\frac{\partial}{\partial z} \tilde{\psi}_{a,p,l}(k_x, k_y, z, \omega) = \tilde{A}_{a,p,l} \cdot \tilde{\psi}_{a,p,l}(k_x, k_y, z, \omega)$$

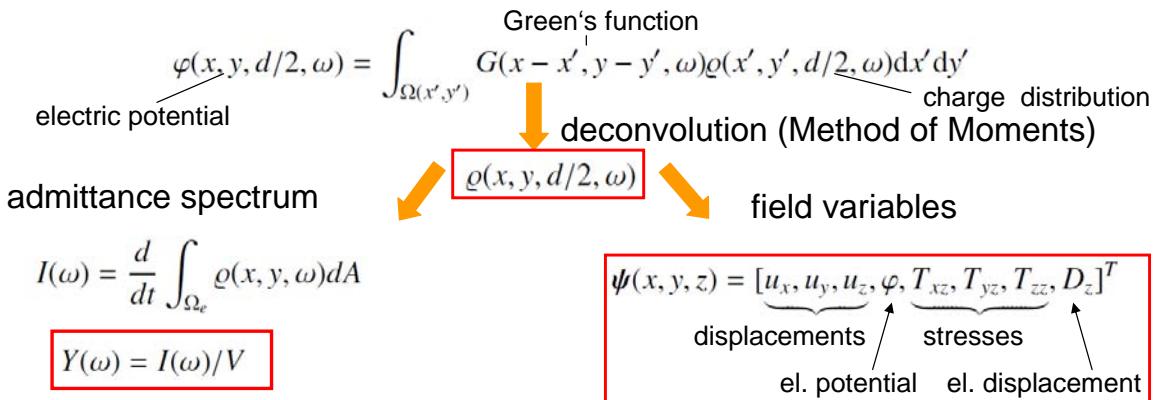
$$\tilde{\psi}_{a,p,l} = [\tilde{u}_x, \tilde{u}_y, \tilde{u}_z, \tilde{\varphi}, \tilde{T}_{xz}, \tilde{T}_{yz}, \tilde{T}_{zz}, \tilde{D}_z]_{a,p,l}^T$$

air piezo liquid

# Modeling of the electrodes: Green's function

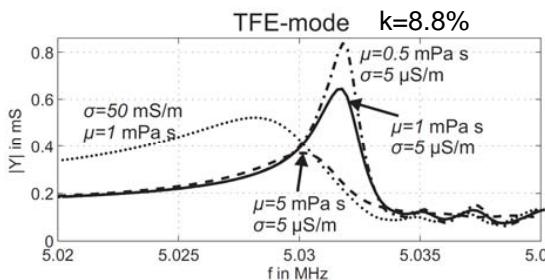


- electrodes modeled as purely electrical (mechanical loading of electrodes is neglected)
- determine the charge distribution necessary to produce the prescribed potential.
- Green's function ( $G$ ) is potential response due to point charge ( $G$  obtained from coupled ODEs in the spectral domain)

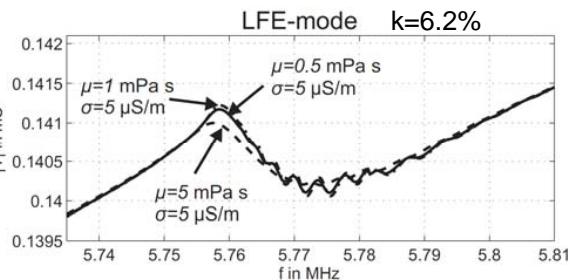


## Results for AT-cut quartz (ZXwlt 0°/54.75°/0°):

slow thickness-shear-mode (c-mode)



fast thickness-shear-mode (b-mode)



**piezoelectric disc:** 330 µm AT-cut quartz 5 MHz, shear displacement in x

**sample liquid:** pure ( $\sigma = 5 \mu\text{S}/\text{m}$ ) and tap water ( $\sigma = 50 \text{ mS}/\text{m}$ ). Shear viscosity of water ( $\mu = 1 \text{ mPa s}$ ) varied to  $\mu = 0.5 \text{ mPa s}$  and  $\mu = 5 \text{ mPa s}$ .

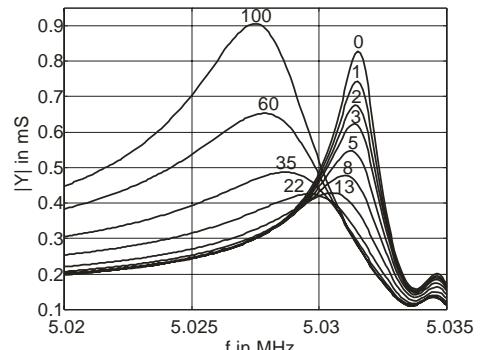
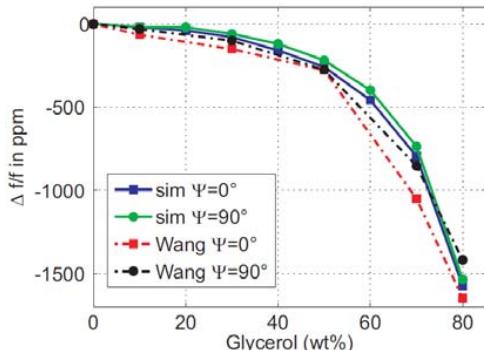
- slow shear mode shows good sensitivity to viscosity changes
- high cross-sensitivity to conductivity
- extensional and fast shear mode not useable
- **Coupling factors are not sufficient! Also geometry has to be considered!**

## Results for AT-cut quartz

	$k_{TE}$ in %	$k_{LE,0}$ in %	$k_{LE,90}$ in %	$v$ in m/s	$f_0$ in MHz	
a	0	6.48	0	7009	10.619	very weak
b	0	6.17	0	3801	5.759	weak
c	8.74	0	6.26	3326	5.034	strong

COUPLING FACTORS FOR  $a, b, c$ -MODES FOR TFE AND LFE, WAVE VELOCITIES, AND RESONANCE FREQUENCIES FOR A  $330\mu\text{m}$  DISC.

For AT-quartz only TFE mode is usable: **PSEUDO-LFE**



Admittance for varying conductivities of the liquid in mS/m.

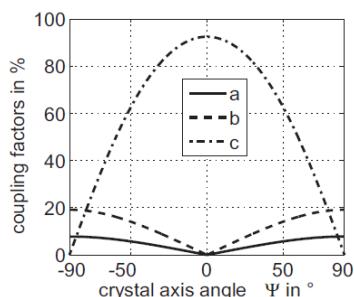
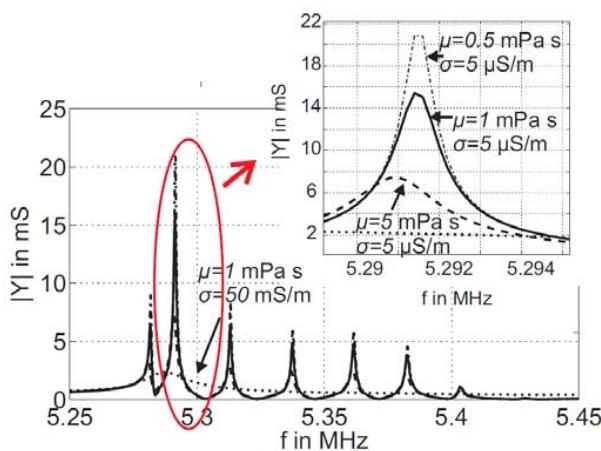
Experimental data from:

Wang, W.; Zhang, Z.; Zhang, C.; Liu, Y.; Feng, G. & Jing, G.  
Pseudo-LFE study in AT-cut quartz for sensing applications Proc.  
*IEEE Sensors*, **2008**, 1548-1551

## A pure LFE sensor: lithium niobate (YXwl 60°/58°)

	$k_{TE}$ in %	$k_{LE,0}$ in %	$k_{LE,90}$ in %	$v$ in m/s	$f_0$ in MHz
lithium niobate:					
a	31.9	0	7.8	7217	10.934
b	2.74	0	19.15	3993	6.050
c	0	92.51	0	3481	5.274

TABLE III  
COUPLING FACTORS FOR  $a, b, c$ -MODES FOR TFE AND LFE, WAVE VELOCITIES, AND RESONANCE FREQUENCIES FOR A  $330\mu\text{m}$  DISC.



# Summary

- + Method yields reasonable admittance spectra and fields
- + Fluid-structure interaction is fully modeled.
  - mechanical and electrical loading
- + Additional material layers can be applied easily
  - e.g. shielding electrode at bottom
- + Arbitrary piezoelectric materials and fluids can be simulated



# A Highly Uniform Lamination Micromixer with Wedge Shaped Inlet Channels for Time Resolved Infrared Spectroscopy

W. Buchegger<sup>1</sup>, C. Wagner<sup>2</sup>, B. Lendl<sup>2</sup>,  
M.Kraft<sup>3</sup>, M. Vellekoop<sup>1</sup>

<sup>1</sup>Institute of Sensor and Actuator Systems

<sup>2</sup>Institute of Chemical Technologies and Analytics

Vienna University of Technology

<sup>3</sup>CTR Carinthian Tech Research AG

## Outline

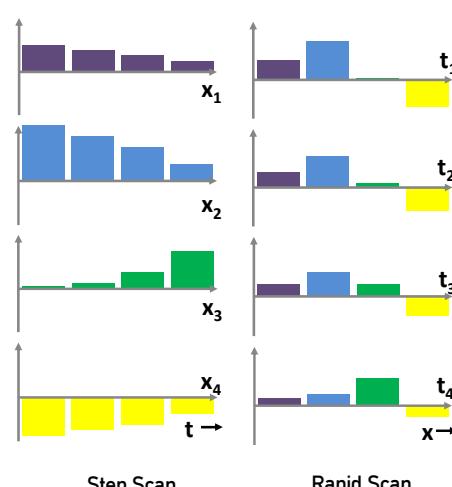
- Background
- Motivation
- Micromixer requirements
- Mixer designs and simulation
- Material and fabrication
- Measurement results
- Conclusion

## Background

- Many chemical and bio-chemical reactions have so far unknown transition states or kinetics (e.g. protein folding)
- Infrared Spectroscopy is a powerful method for time resolved analysis
- Current technologies
  - Step-Scan
  - Rapid-Scan

## Background

- Step Scan
  - Precise external trigger
  - Cyclic reactions
- Rapid Scan
  - Limited mirror velocity
  - Resolution 10ms



## Motivation

- Continuous flow micromixer to observe chemical reactions
- Mixing by diffusion (passive) in the low millisecond range
- Real-time information about reaction mechanisms and conformation changes of an analyte

## Micromixer requirements

- IR Spectroscopy requires shallow channels for aqueous solutions (about 10µm)
- Measurement spot of about 150x150µm<sup>2</sup>
- Strictly laminar flow  
Reynolds number :  $Re \leq 1$
- Mixing strongly depends on diffusion length
$$t_{mix} \propto \frac{l_{diff}^2}{D}$$
D... diffusion coefficient  
 $l_{diff}$ ... diffusion length
- Materials for mid-infrared wavelength

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## Micromixer design

- Two fluid channels
- Mixing channel on top
- Transparent cover
  - Two fluid layers are formed
  - Mixing times 5-10 ms

The diagram shows a cross-section of a micromixer. It consists of a transparent cover (red) and a blue substrate. Two inlet ports, Inlet A and Inlet B, are located at the bottom. An IR-Beam is directed downwards onto the mixing channel. The mixing channel is a rectangular groove in the substrate. The resulting mixed fluid exits from the right.

IR-Beam  
Inlet A  
Mixing Channel  
Inlet B

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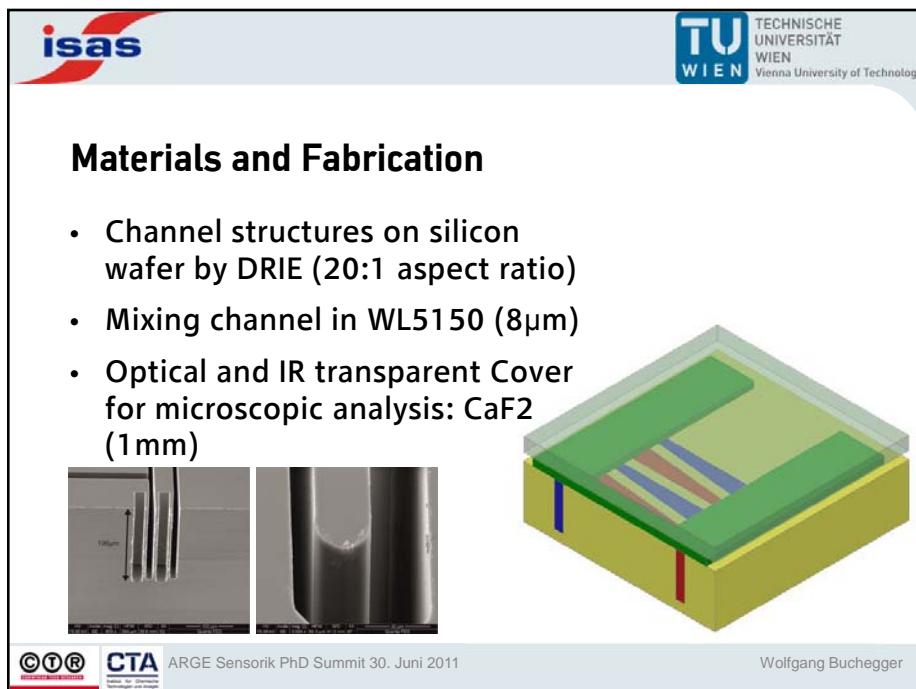
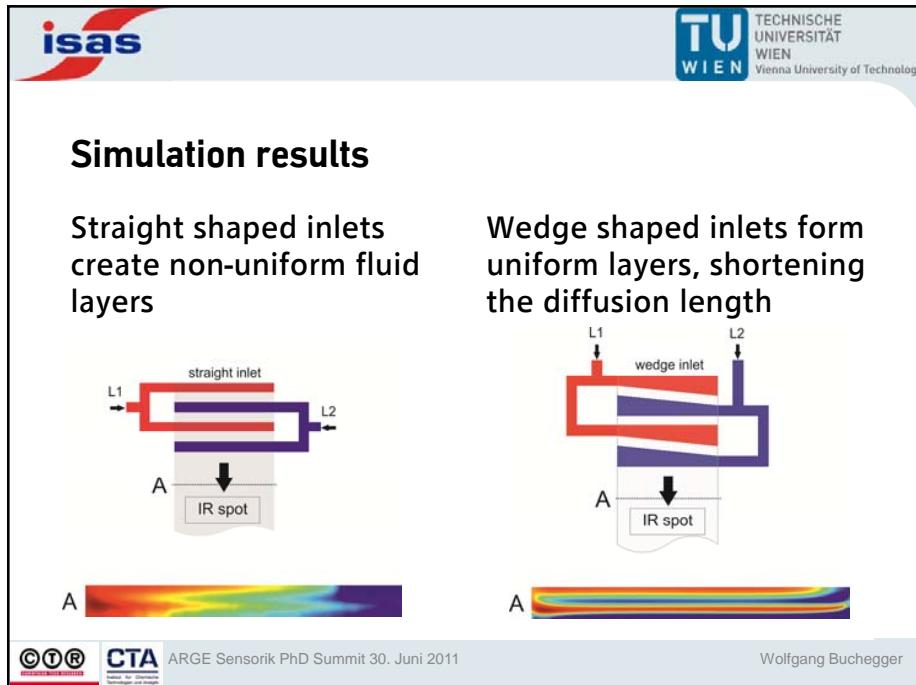
## Micromixer design

- Distribution network splits 2 liquid feeds into 4 streams
- Velocity optimized for each stream
  - Resulting in layers with different thickness
  - Accounts for diffusion layers

The diagram shows a more complex micromixer design. It features a distribution network that splits two liquid feeds, Inlet A and Inlet B, into four streams. These streams then enter a mixing channel. The mixing channel is a series of interconnected chambers. The resulting mixed fluid exits from the right. The diagram illustrates how the streams form distinct layers of different thicknesses within the mixing channel, accounting for diffusion layers.

Inlet A  
Mixing Channel  
Inlet B  
Liquid 2  
Liquid 1

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## Measurement principle

- Each measurement spot equals a time stamp
- Spot size about  $150 \times 150 \mu\text{m}^2$
- Flow rate determines the time between spots and the overall time range

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## Characterization

- Wedge shape
  - Mixing times of <1ms
- Testreaction:
  - Iron (III)  $[\text{Fe}^{3+}]$  and thiocyanate  $[\text{SCN}^-]$  form a dark complex
- Flow rates ranging from 1-30 $\mu\text{l}/\text{min}$

Equation	$y = A1 \cdot \exp(-x/t1) + y0$
x90	285 $\mu\text{m}$
t90	0,92 ms
adj. R-square	0,9912

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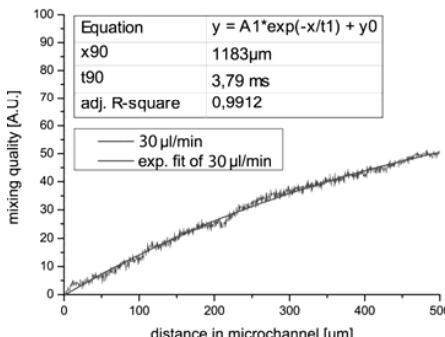
Wolfgang Buchegger

**Characterization**

- Straight shape
  - Mixing times of >3.5ms
- Testreaction:
  - Iron (III)  $[Fe^{3+}]$  and thiocyanate  $[SCN^-]$  form a dark complex
- Flow rates ranging from 1-30 $\mu$ l/min



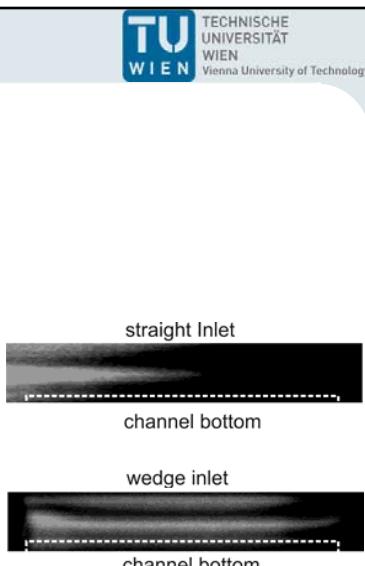
Equation	$y = A1 * \exp(-x/t1) + y0$
x90	1183 $\mu$ m
t90	3,79 ms
adj. R-square	0,9912



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**Characterization**

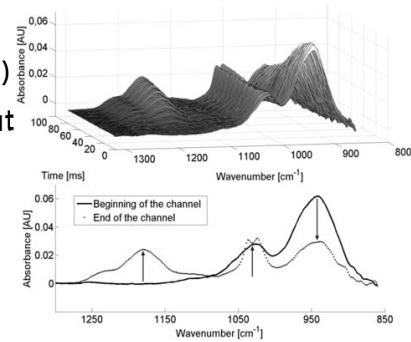
- Testreactions:
  - Fluorescent dyes to visualize the individual fluid layers
- Micromixer with a 25 $\mu$ m channel height
- Formation of fluid layers equals simulation results



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## Time resolved FTIR Measurement

- Sodium sulfite  $\text{Na}_2\text{SO}_3$  and formaldehyde solution HCHO
- Three changing bands
  - ( $942\text{cm}^{-1}$ ,  $1025\text{cm}^{-1}$ ,  $1180\text{cm}^{-1}$ )
- 86 recorded spectra in about 80 milliseconds

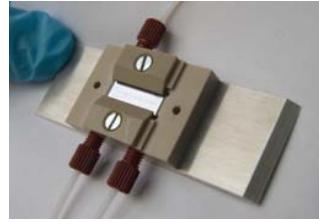


## Conclusion

- Passive mixing device applicable for IR-Spectroscopy enables continuous spectral analysis
- Short mixing times due to individual fluid layers formed by the distribution network and the wedge shaped inlets
- Mixing times in low millisecond range for aqueous solutions enable investigation of many chemical reactions

## Acknowledgements

Dr. Artur Jachimowicz  
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Peter Svasek  
Ewald Pirker  
Andreas Rigler



COMET Competence Center Program

## Thank you for your attention!

# Thermoelectric energy harvesting in aircraft for wireless sensors

Dominik Samson (EADS),

Thomas Becker (EADS),

Ulrich Schmid (TU Wien)

Linz, Austria 30/06/2011

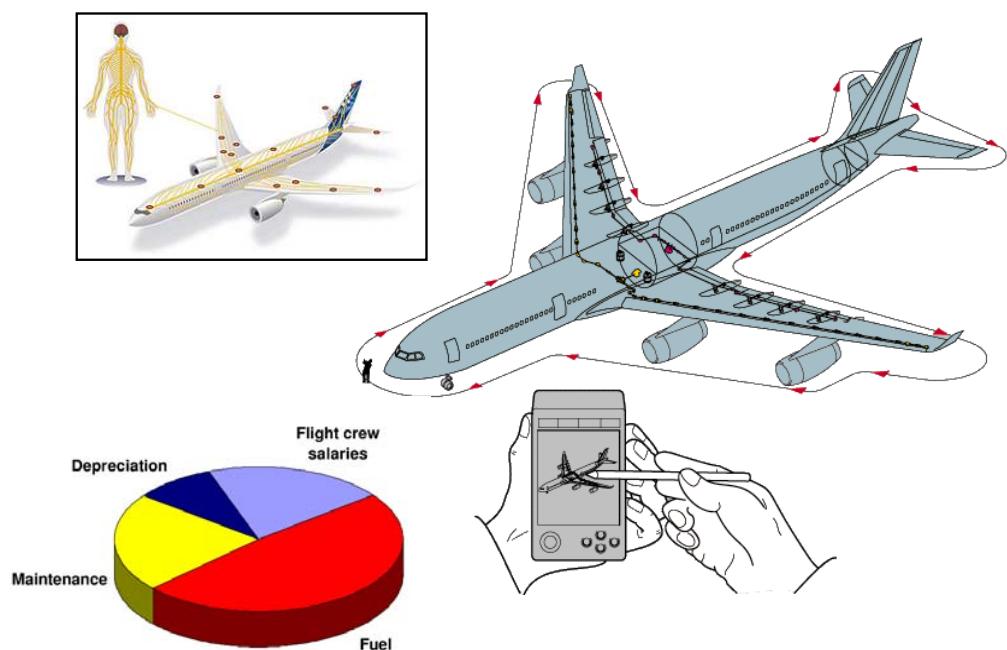


EADS Innovation Works - TCC4 "Sensors, Electronics & Systems Integration"

14 July 2011

## Scenario

Maintenance check by wireless sensor



## Scenario

How does Energy come to the sensor?

By cable:

- heavy
- difficult to install
- expensive to plan

By batterie:

- may not always work
- maintenance

Solution:

local power production at the sensor  
= **energy harvesting**



## Content

Introduction

Aircraft energy harvesting principles

Thermoelectric theory

Thermoelectric energy harvesting

Power management

Flight test

Conclusion

## EADS and IW



**IW Staff (2009)**  
Headcount : 524  
PhD/Thesis : 62



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Prof. Schmid



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**EADS**

## Energy harvesting

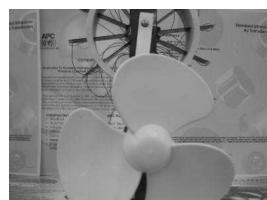
Possibilities for energy harvesting



Solar cell



Vibration  
Harvester



Windmill



Triboelectricity



Thermoelectric  
generator

- Sunlight
- External

- vibrations
- in aircraft
- not large

- Airflow
- External

- Airflow
- Fixed

- In/outside  $\Delta T$

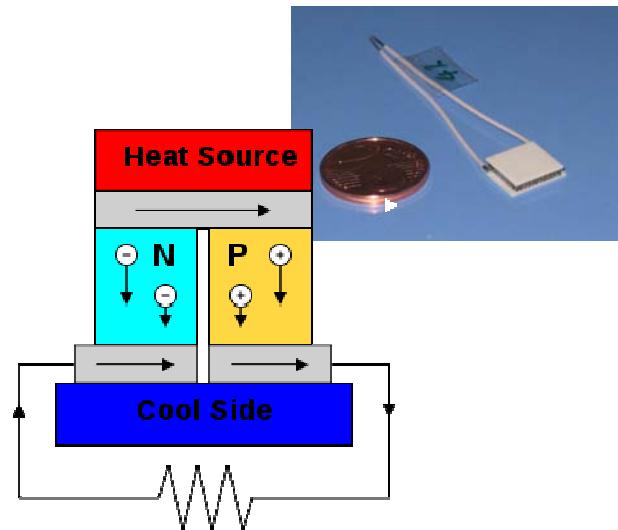
## Thermoelectric theory

Origin of the thermoelectricity

$$\text{Seebeck effect: } U = Q \cdot \Delta T$$

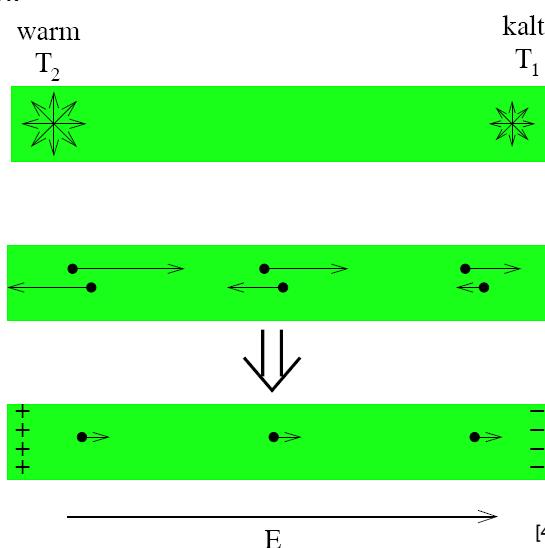
Thermoelectric Generator (TEG):

$$U = (Q_B - Q_A) \cdot \Delta T$$



## Thermoelectric theory

Model of Thermodiffusion:

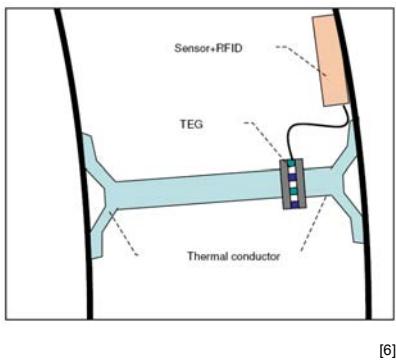


!!Source of thermoelectricity is the thermodiffusion!!

## Thermoelectric Energy Harvesting

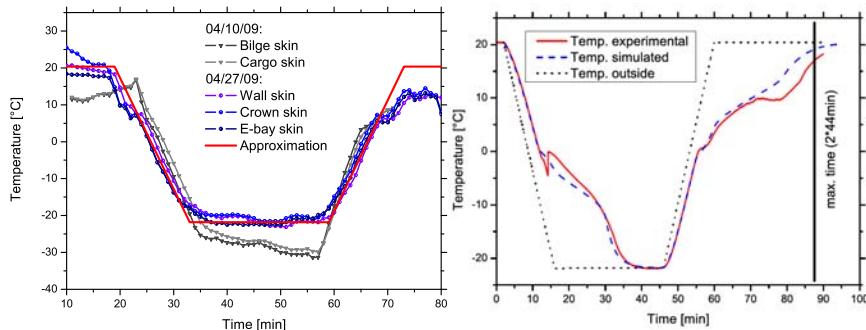
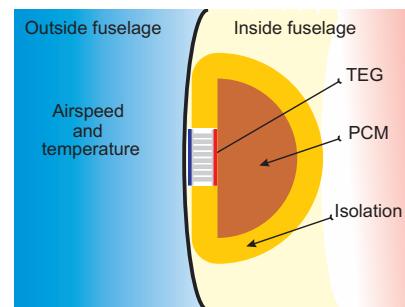
### Static harvesting

- inside: 24°C
- outside: -20°C
- + constant energy output
- difficult to install



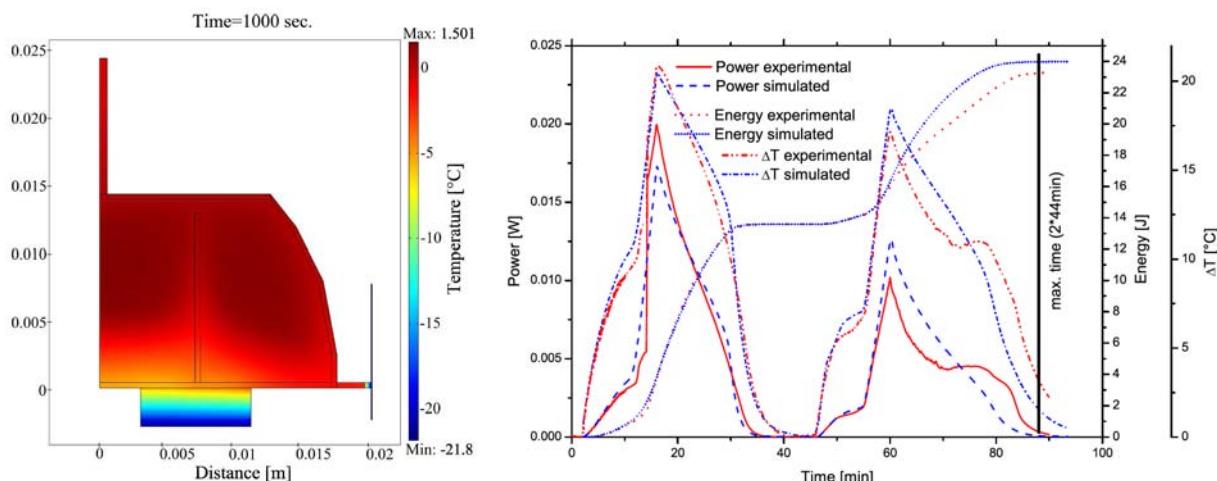
### Dynamic harvesting

- ground: 20°C
- cruise: -20°C
- peaked energy output
- + easy to install



## Thermoelectric phase changer

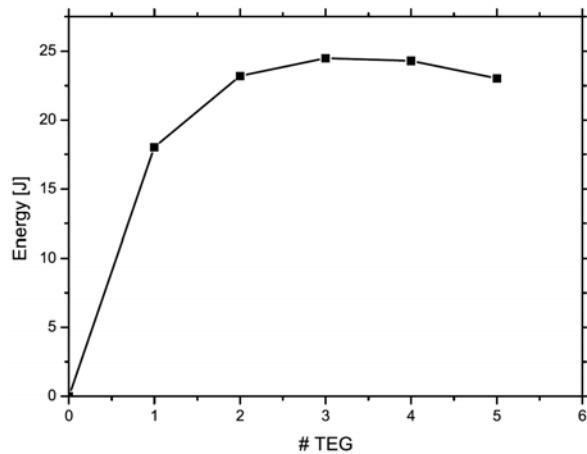
COMSOL FEM simulations for design parameters and energy output using general heat equation



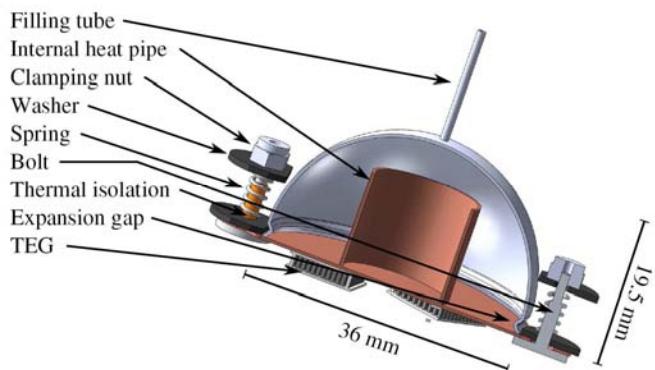
Energy output from 10g H<sub>2</sub>O ~ 6.5 mWh

## Thermoelectric phase changer

Optimization of the TEG heat conductivity



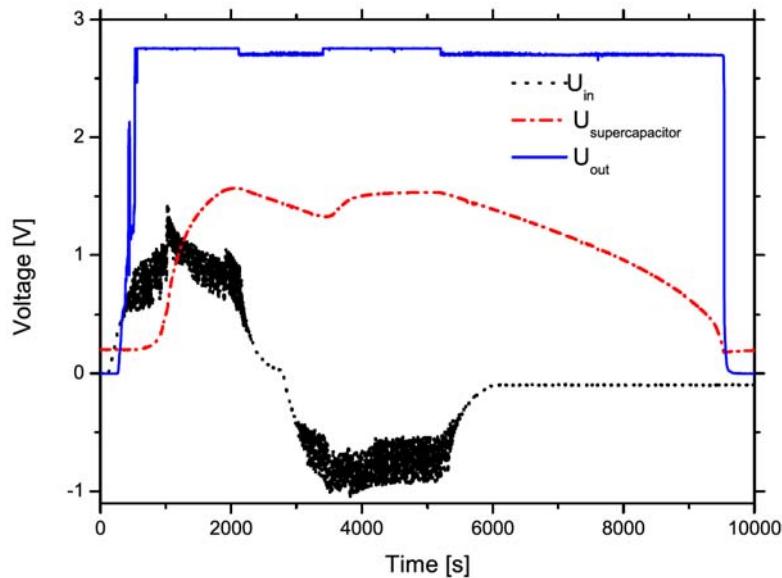
## Thermoelectric phase changer



N°	Short description	Energy output [J]   Weight (PCM + con- tainment, no TEG) [g]	PtW-ratio ( $t = 88\text{min}$ ) [W · kg $^{-1}$ ]
1	Double-walled, <u>no</u> internal heat pipe, 3 mounting bolts, simulation results	20.9   30.85	0.128
2	Double-walled, with internal heat pipe, 3 mounting bolts, experimental results	22.1   33.19	0.128
2b	Double-walled, with internal heat pipe, 3 mounting bolts, <u>with</u> vacuum isolation; experimental results	23.2   33.19	0.131
3	Double-walled, with internal heat pipe, 3 mounting bolts, 20 ml H <sub>2</sub> O, 8 TEGs, $R_t = 75\Omega$ , experimental results	60.5   57.5	0.199
4	Single-walled, with heat pipe, 2 mounting bolts, $\approx 10\text{mm}$ PU foam isolation; experimental results	30.9   27.9	0.210
4b	Single-walled, with heat pipe, 2 mounting bolts, $\approx 100\text{mm}$ PU foam isolation; experimental results	35   60	0.110
4c	N° 4 with Marlow TEG, simulated data	35.5   27.9	0.241

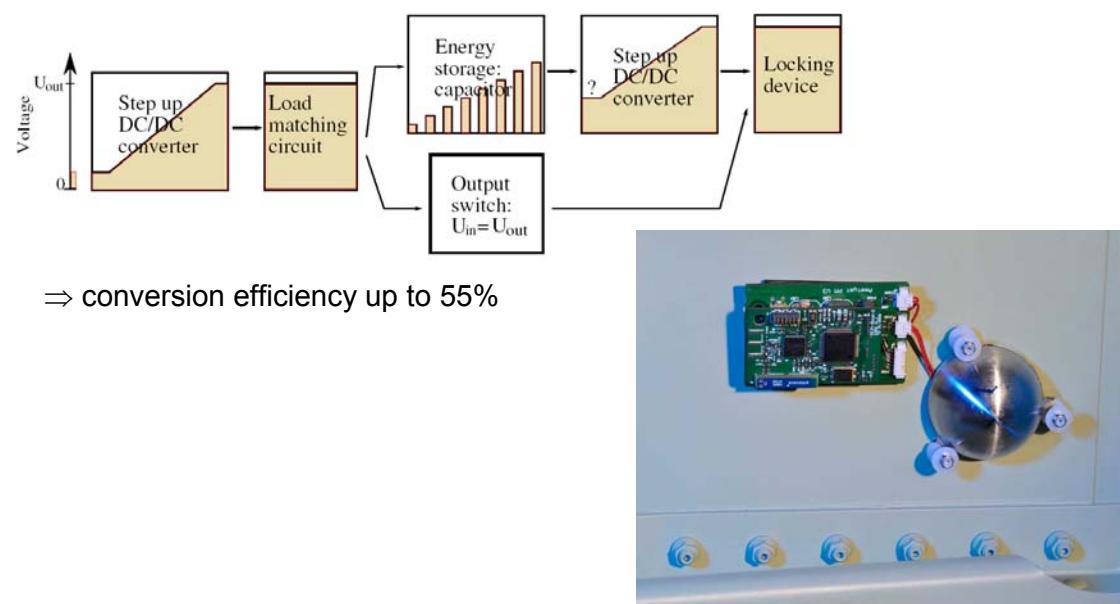
## Power management & Sensor node

Successful test in climate chamber, from one flight cycle sensor worked 2.5h @ 189  $\mu$ W



## Power management & Sensor node

Circuit to store and provide the power is necessary:



## Flight test

Flight test of the harvester:



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## Flight test

Flight test of the harvester:

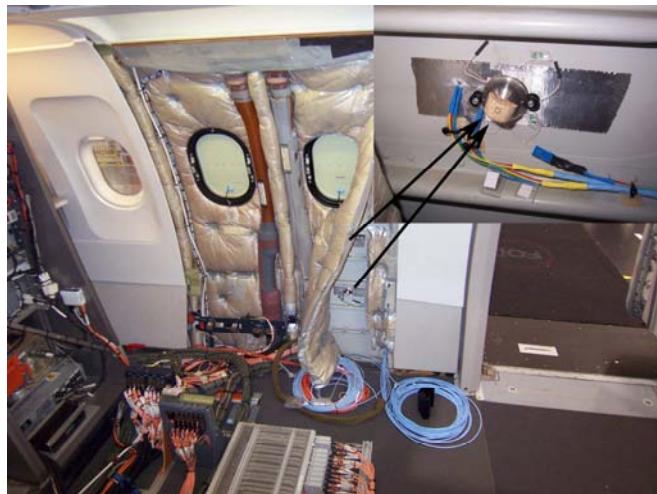


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## Flight test

Flight test of the harvester:



## Conclusion

- energy harvesting in aircraft is possible
- thermoelectricity is the most promising candidate
- efficient power management is needed
- flight test proved the concept

## References

- [1] Airline financial detail report.
- [2] Wiring tips up A380 schedule. International Herald Tribune, June, 14th 2006.
- [3] Darren FYE Shashank PRIYA, Chih-Ta CHEN and Jeff ZAHND. Piezoelectric windmill: A novel solution to remote sensing. Japanese Journal of Applied Physics, 44(3):104–107, 2005.
- [4] Ingo Hüttl Rolf Peister, Reinhard Pieper. Thermospannungen - Vielgenutzt und fast immer falsch erklärt! Physik und Didaktik in der Schule und Hochschule PhyDid, 1/4:10–22, 2005.
- [6] <http://www.amethyst-projekt.de/>

# Capacitive Icing Detection and Capacitive Energy Harvesting on a 220kV HV Overhead Power Line

Institute of Electrical Measurement  
and Measurement Signal Processing

Head of the Institute & Supervisor: Univ.-Prof. DI Dr. Georg Brasseur

in collaboration with   
AUSTRIAN POWER GRID  
STROM.GENOSI

Michael J. Moser

PhD Summit 2011, Linz, 30.6.2011

## Introduction

### What is „Icing of Overhead Power Lines“?

- atmospheric icing (aggregation of ice and/or snow)
- onto the surface of overhead conductors
- posing additional weight load (up to several kg/m) to the supporting towers



Source: NOAA, WRH, <http://www.wrh.noaa.gov>

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## Countermeasures



Source: Hydro Quebec  
<http://www.hydroquebec.com>



Source: Manitoba Hydro,  
[www.hydro.mb.ca](http://www.hydro.mb.ca)



Source: <http://www.lopour.cz>

Further measures:

- AC and DC currents
- dielectric coatings, hydrophobic coatings (CIGRÈ)

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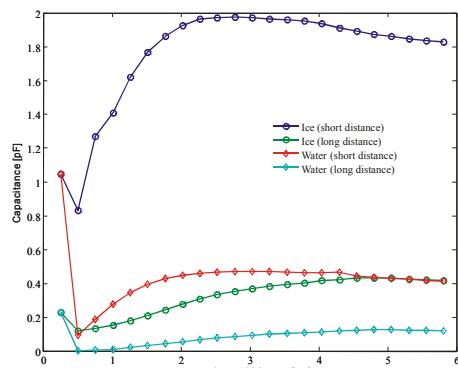
## How to detect icing?

- Weather monitoring on OHL towers
  - Optical, ultrasonic, microwave thickness or line sag measurement:
  - Conductor weight measurement
  - Optical inspection
- 
- **Aims for a new approach:**
    - Measurement on the surface of the conductor
    - Measurement of minimal quantities of ice
    - Autonomous, versatile device
    - Idea: Capacitive Measurement?

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## Field Simulation for a Capacitive Measurement Setup



Source: M.J. Moser, B. George, H. Zangl and G. Brasseur, „Icing Detector for Overhead Power Transmission Lines“, Proceedings of the 2009 IEEE Instrumentation and Measurement Technology Conference, pp. 1105-1109

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## Challenges with capacitive measurement

In general:

- Large offset + small signal changes
- Disturbers/EMC
- Ambiguities (Shielding and Coupling effects)
- Presence of metal (surfaces) adds additional offsets

Here:

- All of the above!
- Field Gradient: measurement of fF in an AC kV environment!

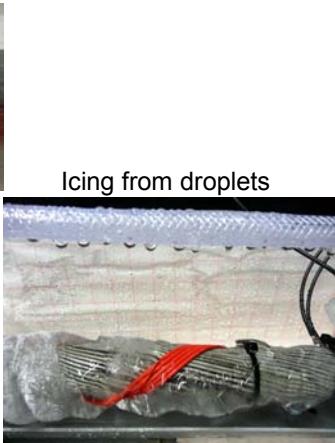
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## Laboratory Testbed



Melting of clear ice



Icing from droplets

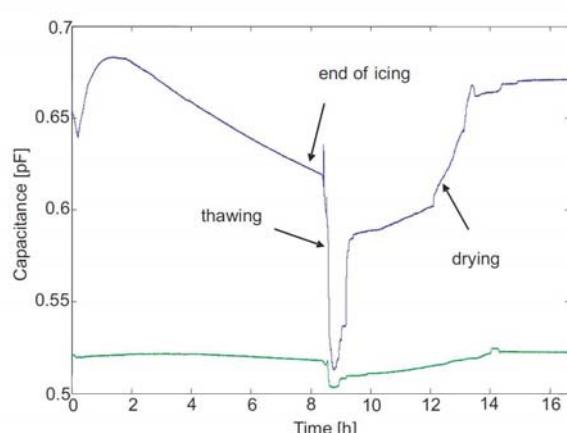


Clear ice layer

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## Laboratory Results



M.J. Moser, B. George, H. Zangl and G. Brasseur, „Icing Detector for Overhead Power Transmission Lines“, Proceedings of the 2009 IEEE Instrumentation and Measurement Technology Conference, pp. 1105-1109

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# Energy Harvesting

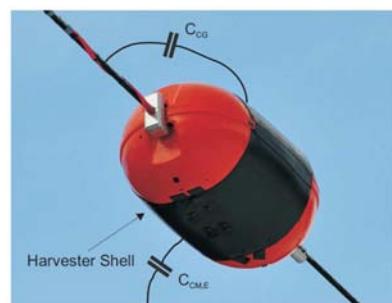
## How to get energy for autonomous operation?

- *Batteries*. Only for lowest power demands.
- *Current Transformer*. Depends on a minimum current in the line.
- *Solar panels*. Depend on sunlight, need much space, are comparatively inefficient. Suffer from pollution.
- *Capacitive Energy Harvesting?*

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# Capacitive Energy Harvester



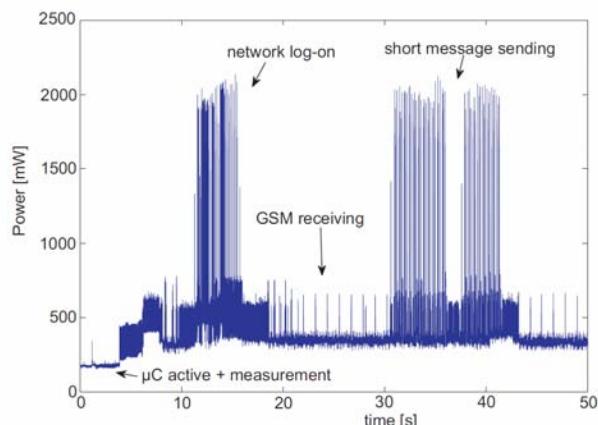
Source:

This device just needs a live power line but the line does not need to transport power (compared with current transformers).

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PhD Summit 2011, Linz, 30.6.2011

## Power Demand

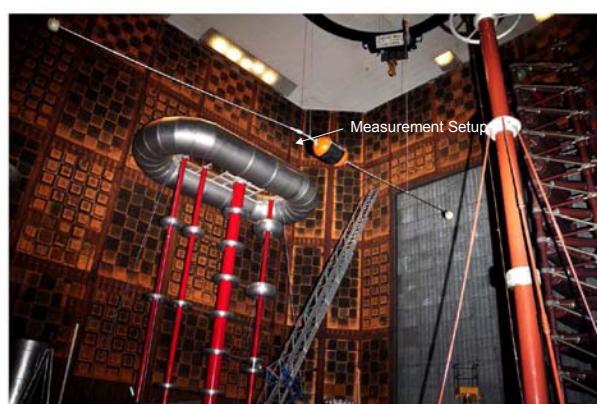


Source: M.J. Moser, T. Bretterklaiber, H. Zangl and G. Brasseur; „Strong and Weak Electrical Field Interfering: Capacitive Icing Detection and Capacitive Energy Harvesting on a 220-kV High-Voltage Overhead Power Line”, IEEE Transactions on Industrial Electronics, Vol. 58, No. 7, July 2011, pp. 2597-2604

Michael J. Moser

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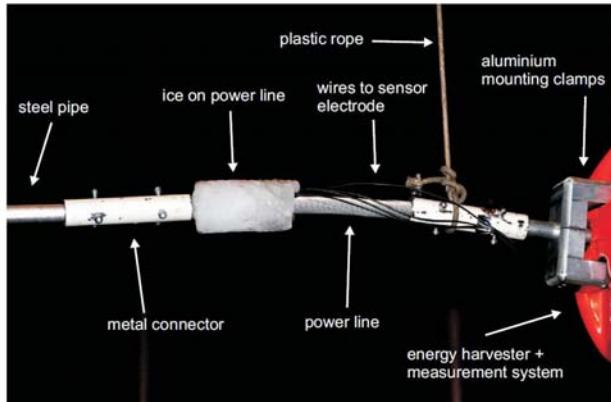
## HV Laboratory Test Setup



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## HV Laboratory Test Setup (cont'd)



Michael J. Moser

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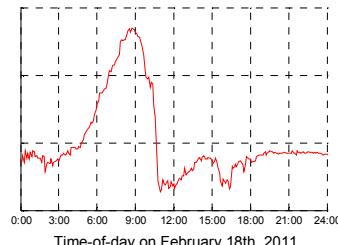
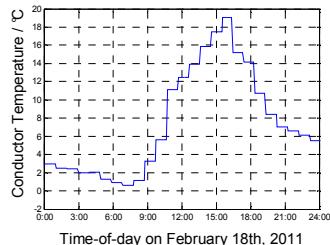
## Field Test on a 220 kV Line



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## Results



-> Conductor temperature is around 0°C for a short period of time

-> A thin layer of soft rime is forming @ 3 a.m. and melts again @ 9 a.m.

Michael J. Moser

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## Summary

- Approach is feasible, icing events were successfully detected.
- Evaluation of multiple capacitances allows estimation of the thickness of the ice layer.
- High sensitivity occurs for thin layers of ice – good for timely application of comparatively simple counter measures.
- Field Test until 05/2011
- Industrialization, first installations planned in winter 2011/12

Michael J. Moser

PhD Summit 2011, Linz, 30.6.2011



## Acknowledgment

Thank you for your valuable support:



- Herbert Lugschitz & Gerhard Bernhard



- Hubert Zangl, Thomas Bretterklieber & the Sensors&Instrumentation Working Group

# Sensor Integration in digital microfluidic systems

PhD Summit ARGE Sensorik  
Thomas Lederer



JOHANNES KEPLER  
UNIVERSITY LINZ | JKU

## Outline

- Microfluidics
- EWOD
- QCM
- Results (+Outlook)
- Impedance spectroscopy
- Results (+Outlook)

# Micro fluidics

## Microfluidics

Investigation of Properties as well as manipulations of small amounts of fluids (<nl)

## Digital Microfluidics

Electro wetting on Dielectrics (EWOD)

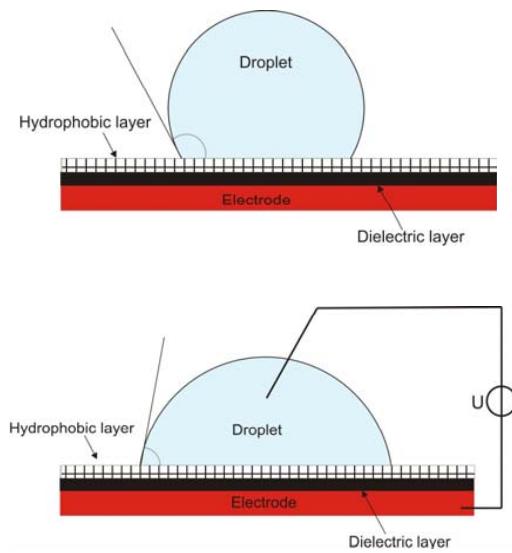
## Key Advantages

- short reaction times
- reduced consumption of reagents and sample materials
- high achievable level of automation

## Sensor Principles

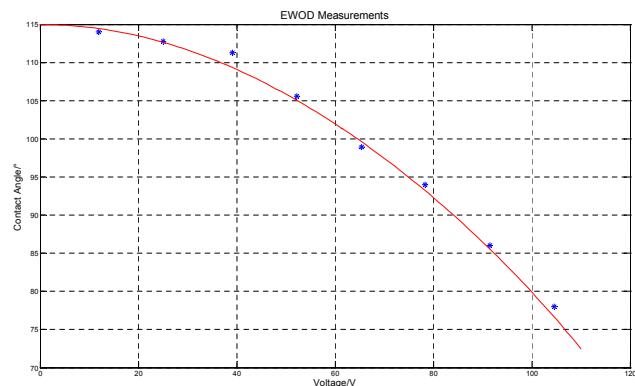
- Functionalized resonant sensor
- Impedance spectroscopy

## Electrowetting on Dielectrics (EWOD)



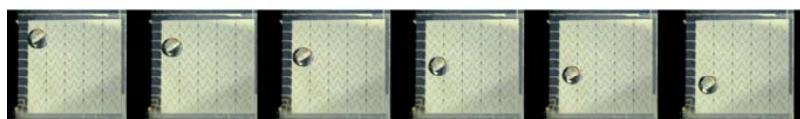
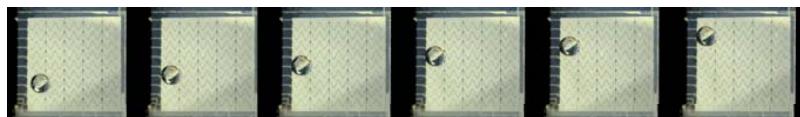
Lippmann-Young equation:

$$(\cos \theta) = \cos(\theta_0) + \frac{cV^2}{2\gamma_{LG}}$$

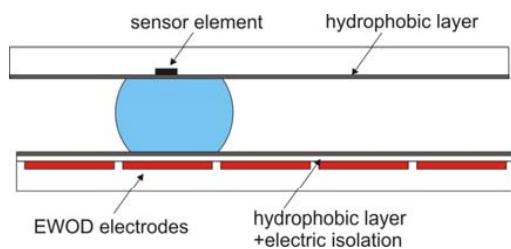
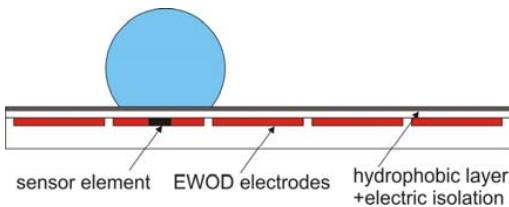


## EWOD Realisation

EWOD Translation



Sensor integration

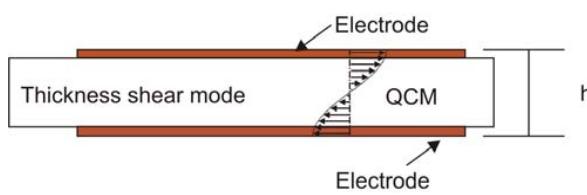


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Sensor Integration in digital microfluidic systems

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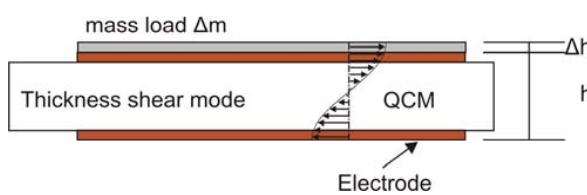
## Quartz Crystal Microbalance



Sauerbrey Equation:

$$\Delta f = -2f_0^2 \frac{\Delta m}{\sqrt{\rho \mu}}$$

Frequency shift dependent on the square of the fundamental resonance frequency  $f_0$



Resonance Condition:  $f_0 = \frac{\sqrt{\mu/\rho}}{2h}$  → Thin Resonators !

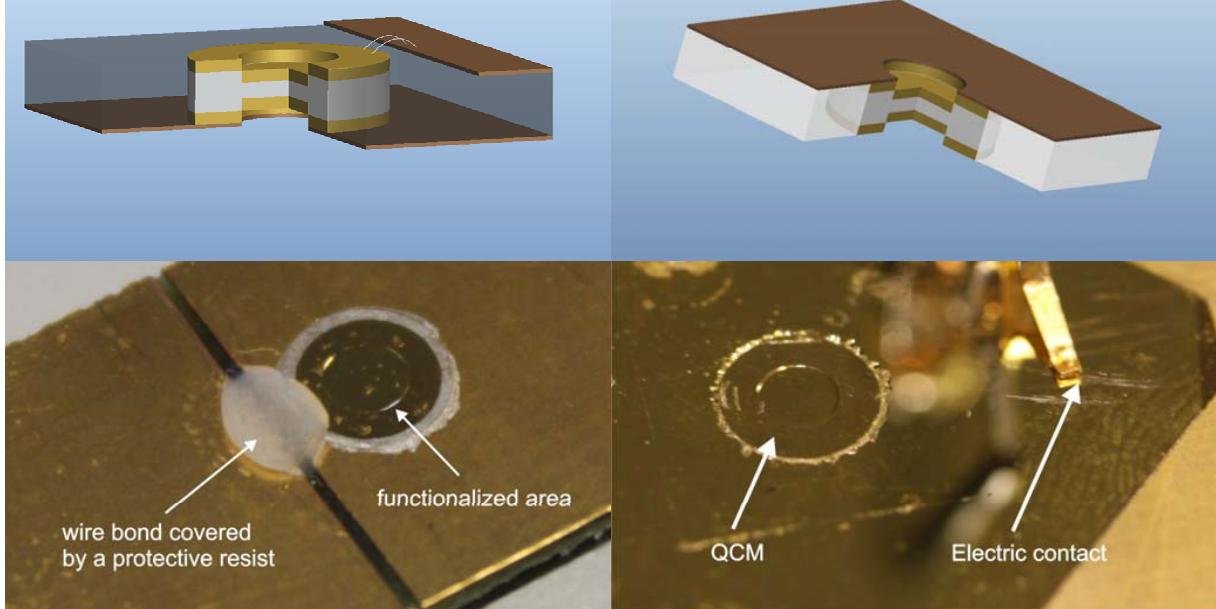


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Sensor Integration in digital microfluidic systems

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## QCM integration



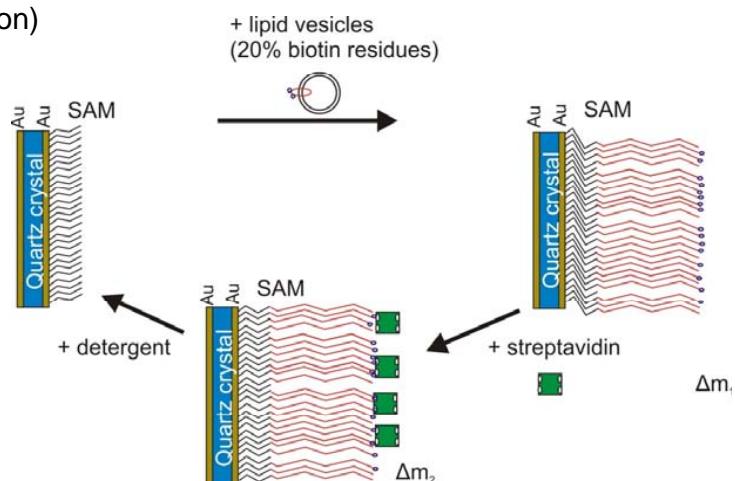
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Sensor Integration in digital microfluidic systems

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## Possible Applications

- density/viscosity
- mass deposition (sedimentation)
- binding of molecules (unspecific/ specific)

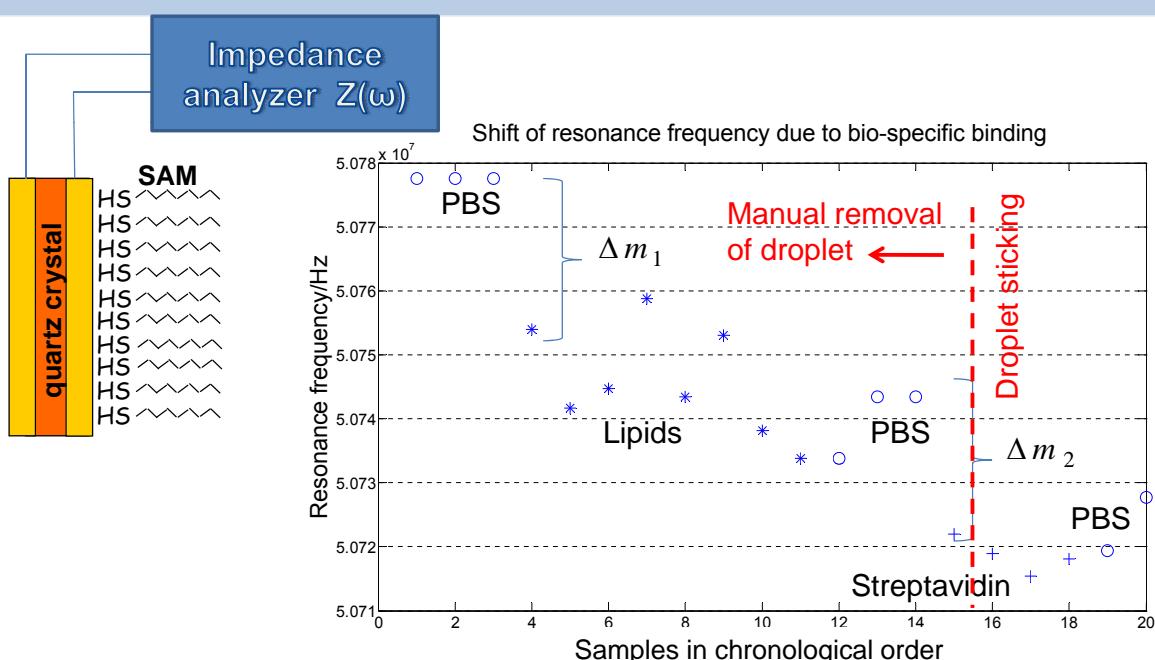


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Sensor Integration in digital microfluidic systems

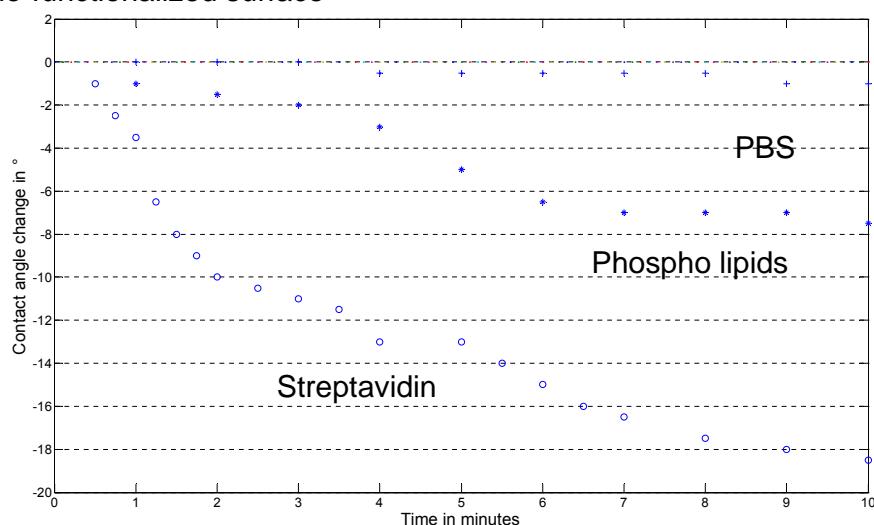
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# Detection of binding bio-molecules



# Optical measurement of the contact angle

→ Observed decrease of the contact angle due to specific binding on Bio-functionalized surface



## Discussion

- Detection of bio-molecules by measuring the shift of the resonance frequency
- Sticking problem due binding of the bio-molecules

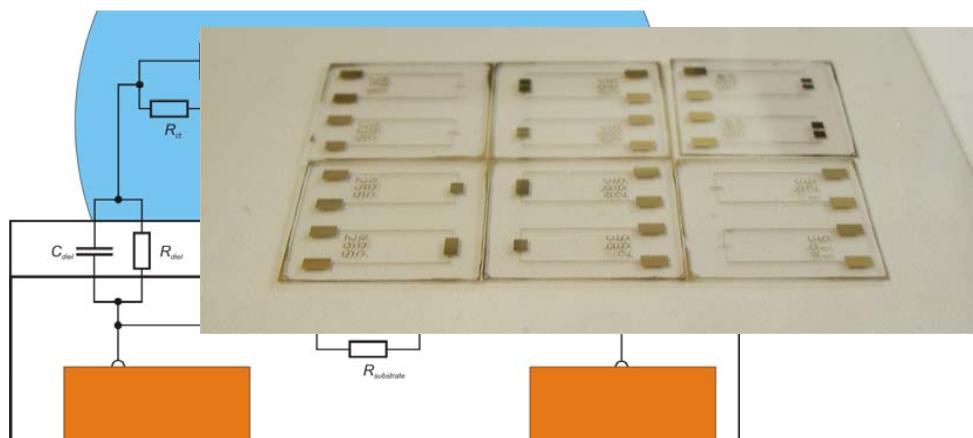
## Outlook

- Releasing the bio-molecules by washing with detergents
- Droplet pushing

## Impedance Spectroscopy

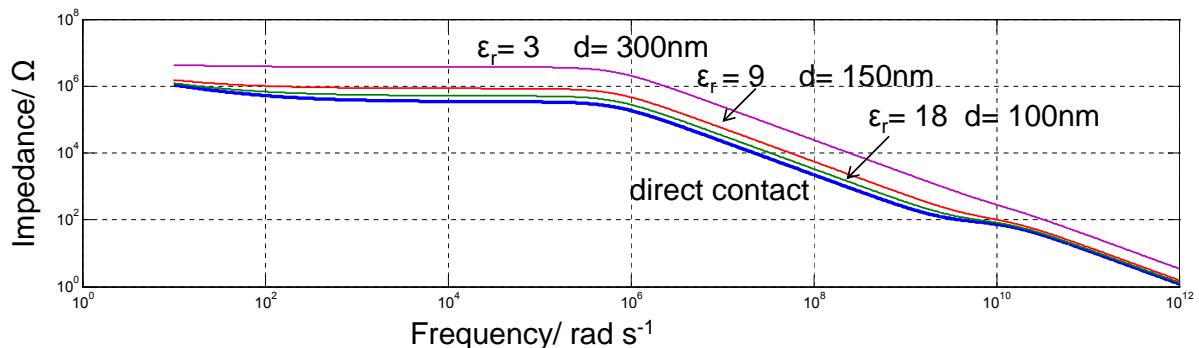
### Impedance function between two ports

$$Z(\omega) = Z'(\omega) + jZ''(\omega)$$

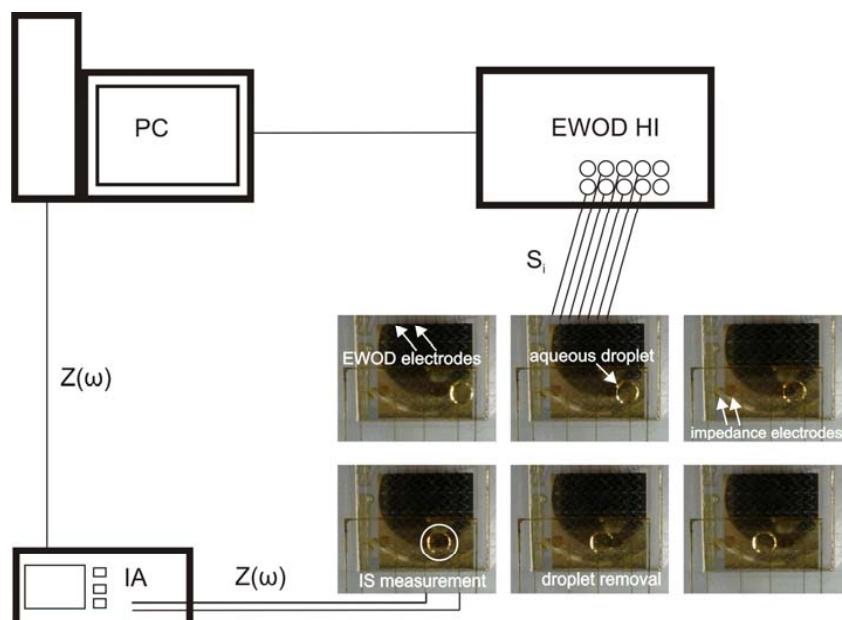


# Material Selection

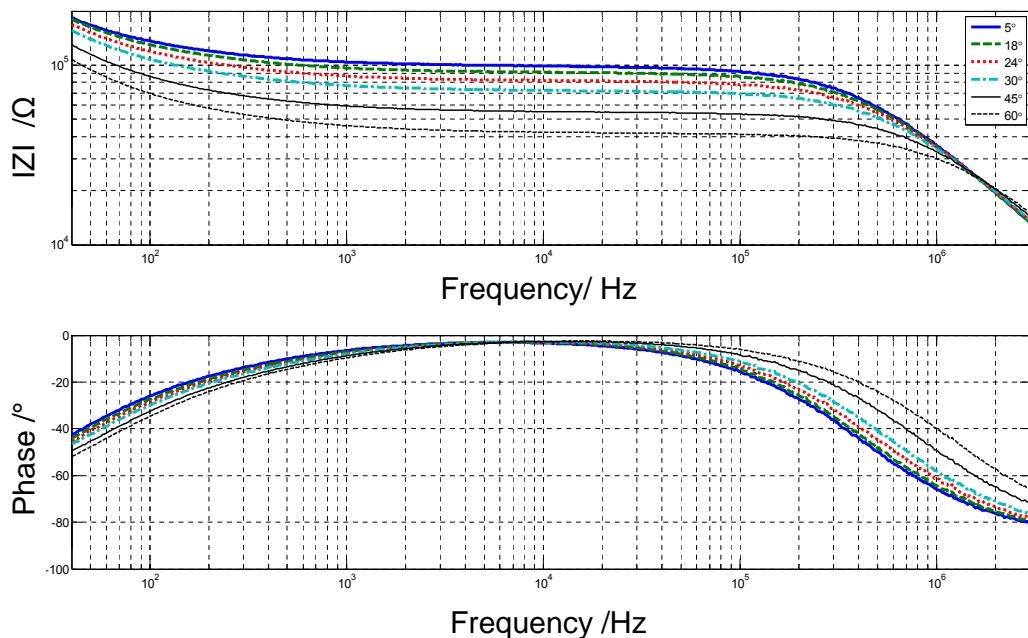
Bode plots of impedance of a DI-Water droplet onto dielectric materials



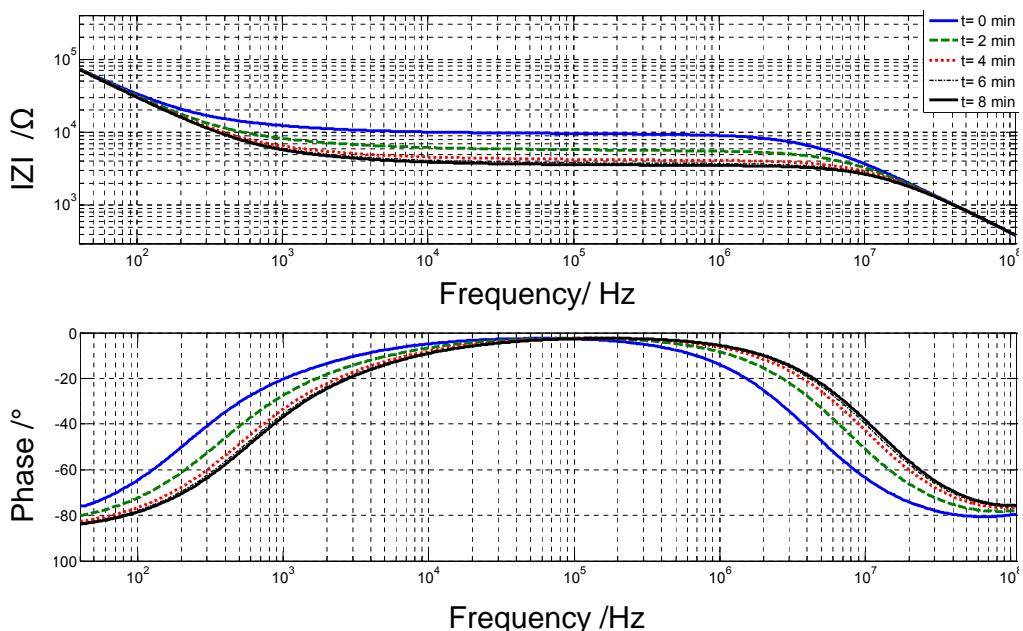
# Measurement sequence



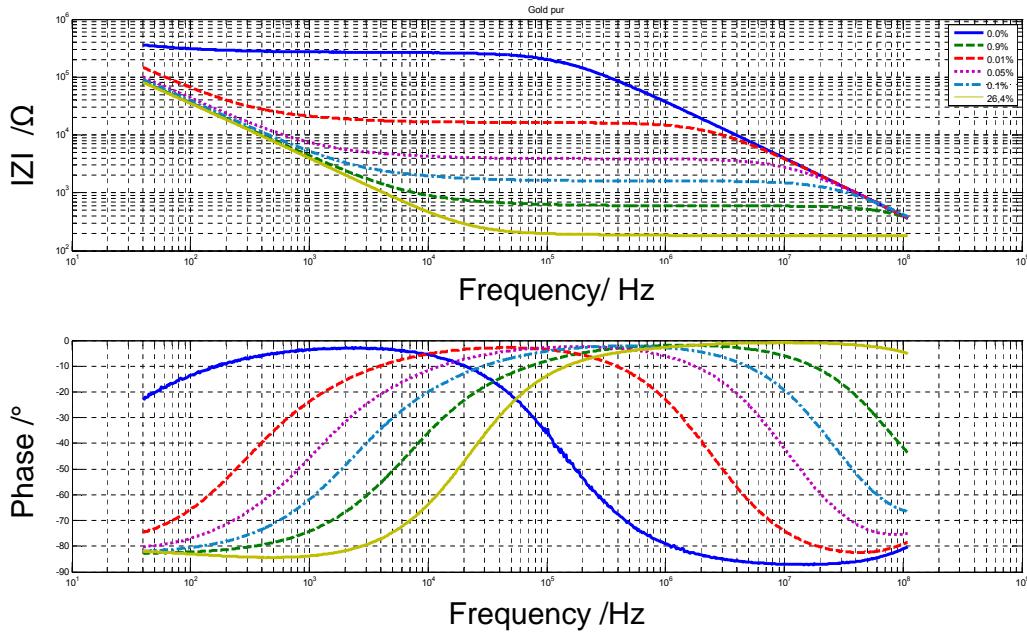
## Measurement (Temperature)



## Measurement (Sedimentation)



# Measurement (Ion concentration)



## Discussion

- All electric measurement of various chemical and physical parameters
- Suitable for online-measurements of chemical reactions

## Outlook

- Measurement on biologic samples
- Combination with RF-heating or with a dielectrophoretic concentration setup

## **Sensor Integration in digital microfluidic systems**

**Thank You for Your  
Attention**



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UNIVERSITY LINZ | JKU**



**Label-Free Cell Analysis:  
An Infrared Sensor for CH<sub>2</sub>-stretch Ratio  
Determination**

Sander van den Driesche  
Institute of Sensor and Actuator Systems  
Vienna University of Technology  
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ARGE Sensorik PhD Summit, 30. June 2011



**Overview**

- Motivation and objectives
- Sensor design and realisation
- Label-free tumour screening
- Conclusions

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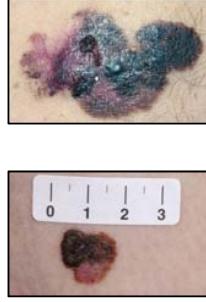
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WIEN** TECHNISCHE  
UNIVERSITÄT  
WIEN Vienna University of Technology

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**Motivation**

Tumour screening: Biopsy

- **Labelling and staining** methods based on **morphological interpretation**
- High number of **false positives** and **false negatives**
- **Early detection and accurate staging** of the primary tumour will **increase** the **overall survival** rate tremendously



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**Objectives**

- 1) to design a novel **tumour cell indicator** based on the cells **physical properties**
- 2) to design and realise a **sensor system**

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# Sensor design and realisation

The diagram illustrates the optical path of a sensor. Light from an LED (c) is collected by a plano convex lens (d). The beam passes through a narrow band-pass filter (e). At the point indicated by 'g', the beam is split by a beam splitter. One path continues through a sample (h) and two more lenses (f and i) to a photodiode (j). The other path from the beam splitter is shown as dashed lines.

S. van den Driesche, W. Witarski, S. Pastorekova, and M. J. Vellekoop,

*Meas. Sci. Technol.*, vol. 20, pp. 124015, 2009.

S. van den Driesche, W. Witarski, and M. J. Vellekoop,  
in *Proc of SPIE* vol. 7362, Dresden, Germany, May 2009, pp. 73 620Y–73 620Y–9.

S. van den Driesche, W. Witarski, C. Hafner, H. Kittler, and M. J. Vellekoop,  
in *Proc IEEE Sensors*, Christchurch, New-Zealand, Oct. 25–28, 2009, pp. 1562–1566.

S. van den Driesche and M. J. Vellekoop, Utility model, DE 20 2009 006 771.8, AT 11722(U1), 2009.

S. van den Driesche, C. Haiden, W. Witarski, and M. J. Vellekoop,  
in *Proc of SPIE* vol. 8066, Prague, Czech Republic, April 2011, pp. 80660E–80660E–8.

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## The CH<sub>2</sub>-stretches

Infrared absorbance spectra comparison of **normal** and **tumour** cells (colorectal, breast, oesophagus, blood, melanocytes, and brain) show **differences** in the wavelength region between **3 and 4 μm**

- **Functional** infrared absorbance **bands**:

Wavelength (μm)	Function
3.42	CH <sub>2</sub> -antisymmetric stretch
3.51	CH <sub>2</sub> -symmetric stretch

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## The CH<sub>2</sub>-stretch ratio

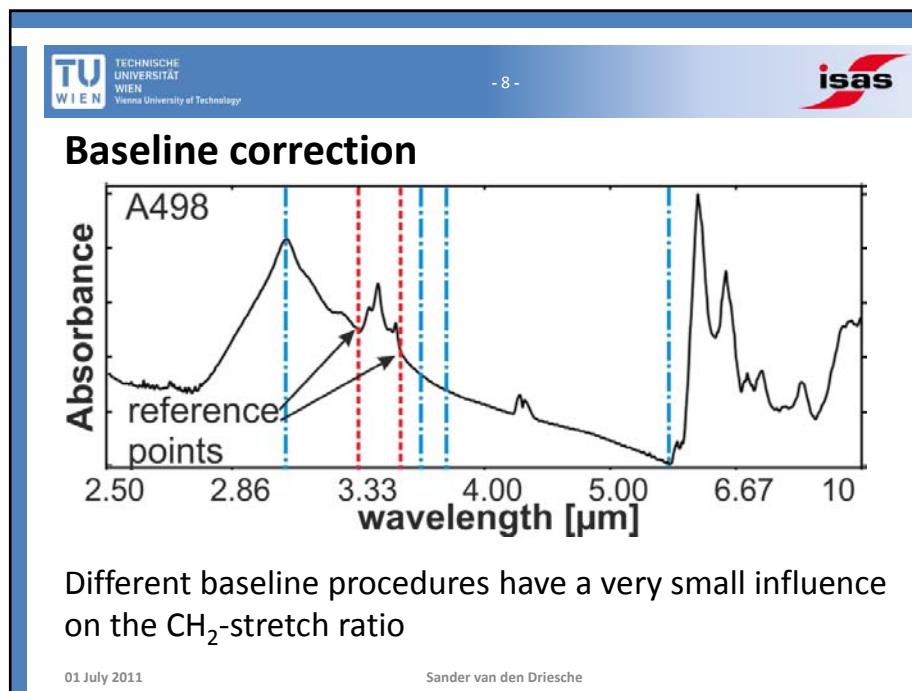
Record IR absorbance values at **specific functional wavelengths**

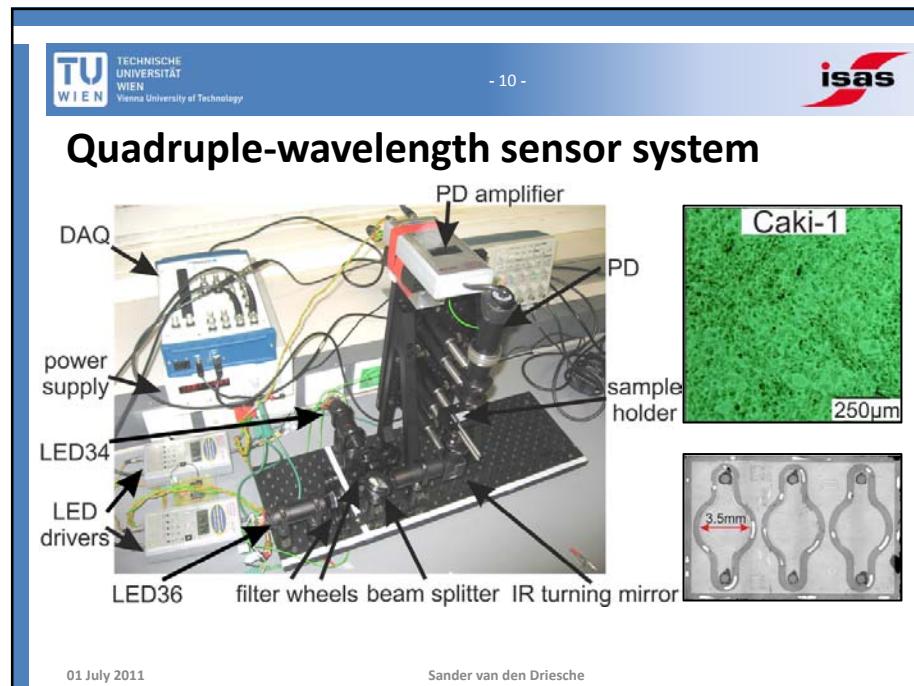
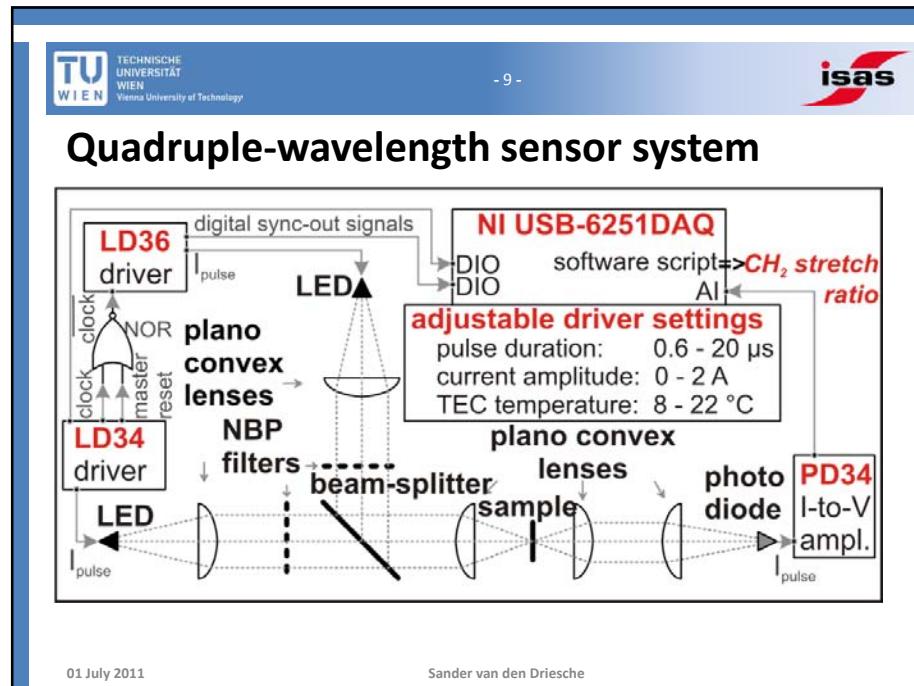
Cell-type discrimination by comparing **peak ratio's baseline correction** required due to **water content and sample thickness**

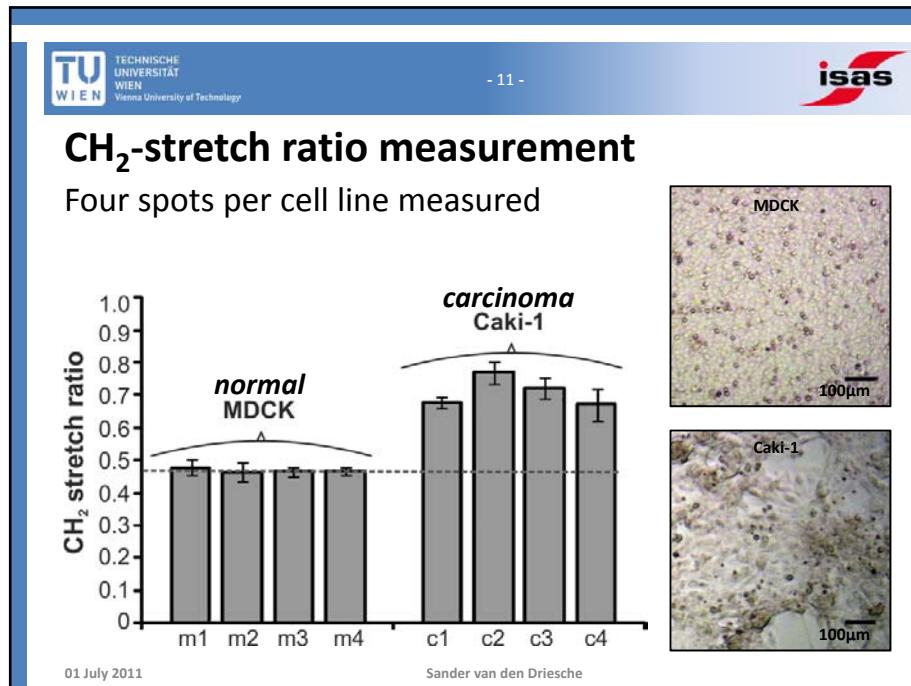
Absorbance [A.U.]

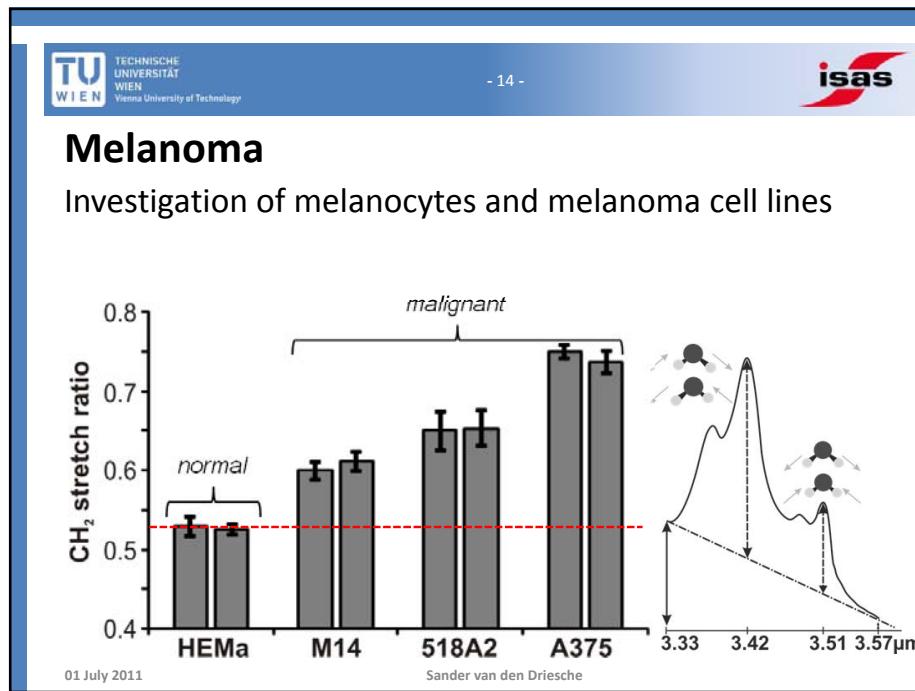
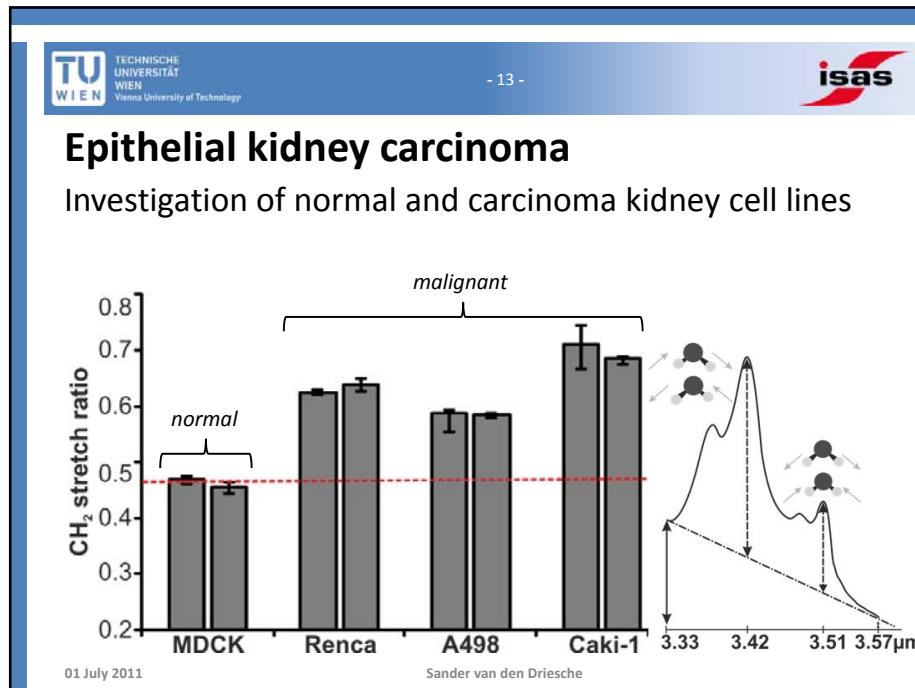
3.33      3.42      3.51      3.57  $\mu\text{m}$

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**Mechanism investigation**

Normal mammalian **plasma membranes** consist of about **20-25%** lipid mass **cholesterol**

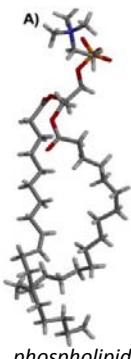
A **decreased** concentration of **membrane stabilizing cholesterol** per area has been found for **malignant breast cells** and **melanocytes** compared to their normal cells

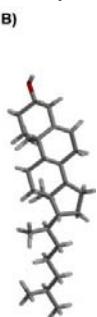
=> An **increase** in the **CH<sub>2</sub>-stretch ratio** of normal cells is expected when **reducing** the **cholesterol concentration**

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**Mechanism investigation**

Reducing the average plasma membrane cholesterol concentration yielded in a higher CH<sub>2</sub>-stretch ratio

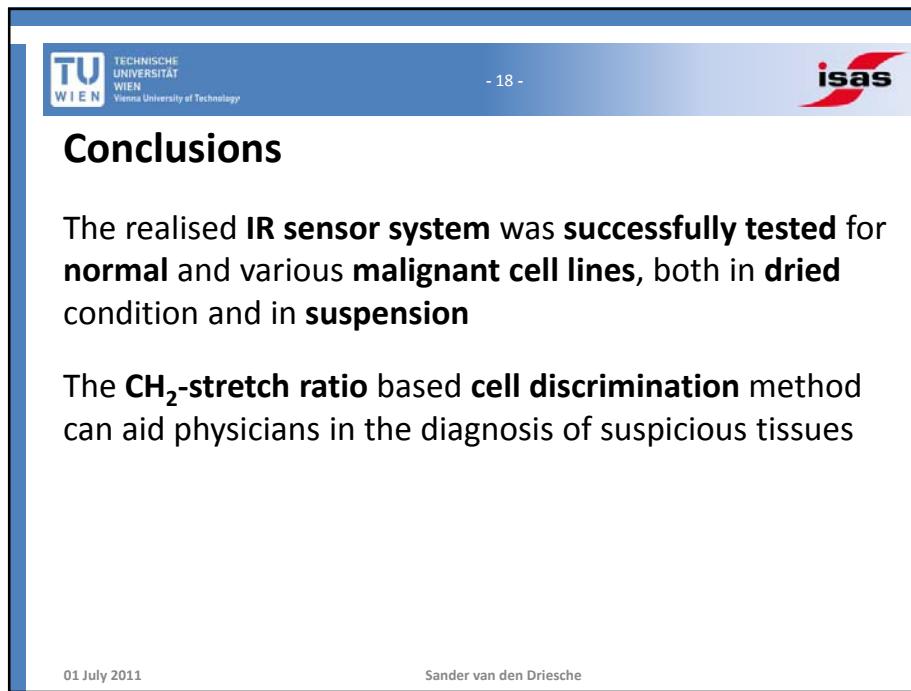
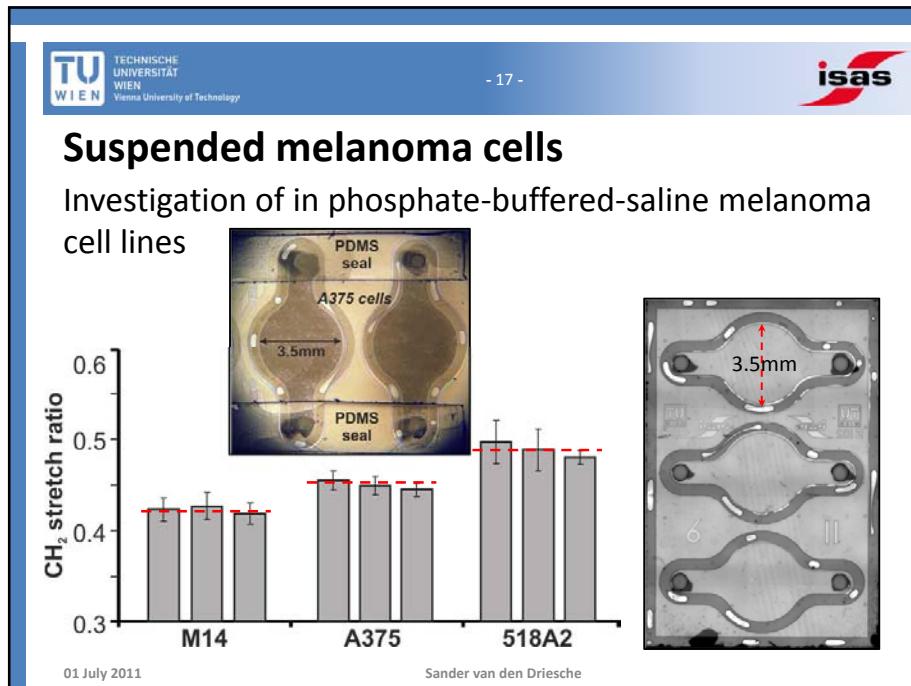
**A)**   
phospholipid  
Heller et al. 1993

**B)**   
cholesterol

**MDCK cells**

methyl- $\beta$ -cyclo dextrin	CH <sub>2</sub> stretch ratio
0 mM	~0.46
10 mM	~0.50
20 mM	~0.57

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## Acknowledgements

- Prof. Dr. Michael Vellekoop and Prof. Dr. Peter Verhaert
- Master students Dietmar Puchberger-Enengl, Vivek Rao, Christoph Haiden, and Helene Zirath
- Colleagues at the Institute of Sensor and Actuator Systems, TU Wien
- Group of S. Pastorekova, Institute of Virology, SAS Bratislava
- C. Hafner, Institute for Pathophysiology, Medical University of Vienna
- Group of B. Lendl, Analytical Biotechnology, TU Wien
- Colleagues of the CellCheck consortium
- The work was part of the EU Marie Curie Research Training Network, MRTN-CT-2006-035854, On-Chip Cell Handling and Analysis “CellCheck”

**Thank you for your attention!**

# Composition monitoring in a gas phase polymerization process

*Institute for Microelectronics und Microsensors*

*Johannes Sell, Alexander Niedermayer, Bernhard Jakoby*

*Borealis Polyolefine GmbH*

*Sebastian Babik, Christian Paulik*



## Contents

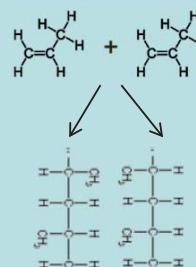
- Problem/Motivation
- Density measurement
- IR
- Conclusion

# Polymerization Process

## Cooperation of ACCM and Borealis

Polymerization: Bonding of monomers to polymers

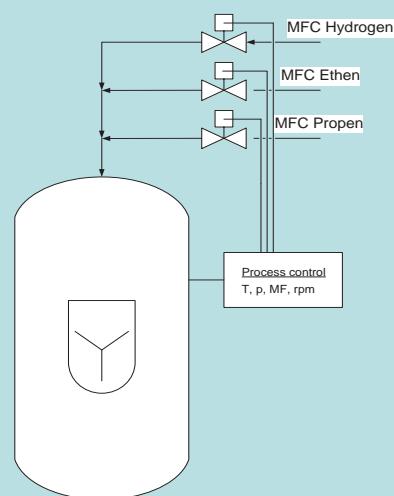
Monomers (e.g. propene)



Catalysts



Polymers



Typcial polymerization reactor

# Polymerization Process

## Problem

Different monomers are integrated into polymer chain with different probability.  
 => Concentration ratio changes during reaction

## Objective

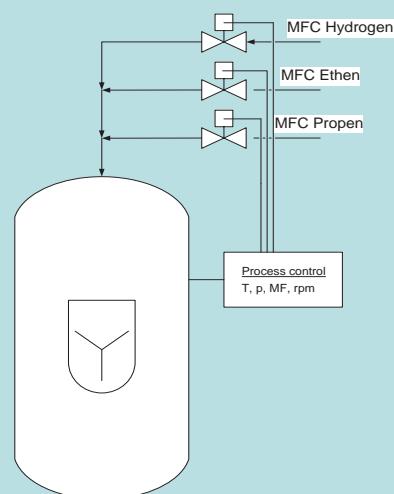
Monitoring of the gas composition during the process
 

- Measurement time: < a few seconds
- Integration into the polymerization reactor

## Approach

2 measurements to measure composition of a 3 component gas
 

- Density
- IR Absorption

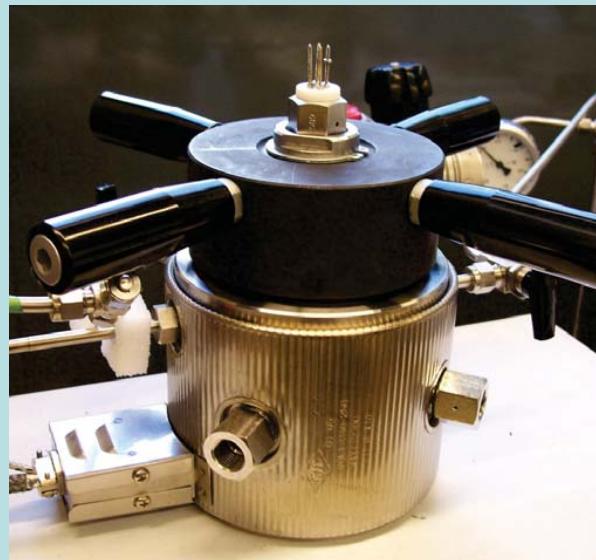


Typcial polymerization reactor

## Density measurement

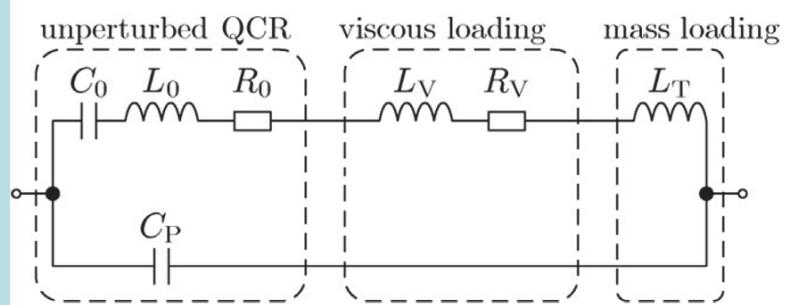
### Test system

- Pressure vessel
  - temperature
  - pressure
- Gases
  - propene
  - ethene
  - $\text{CF}_4$
  - $\text{N}_2$



## Density measurement

- Equivalent Circuit Model of a quartz tuning fork resonator [1]



$$Z_m = R_0 + j(\omega L_0 - 1/(\omega C_0))$$

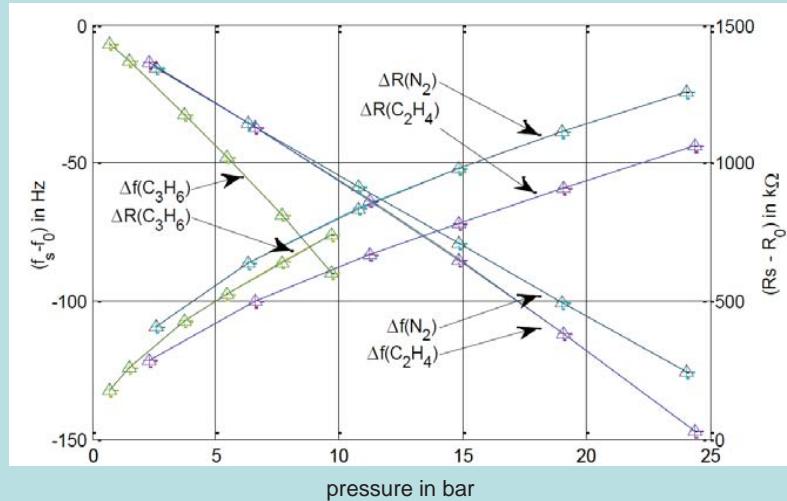
$$Z_V = B \sqrt{\rho \eta \omega}$$

$$Z_T = A \rho \omega$$

[1] L.F. Matsiev, *Proc. IEEE Ultrasonics Symposium (2000)*, 427-434

## Density measurement

- Measure frequency shift and motional resistance in dependence on pressure



## Density measurement – Pressure Dependence

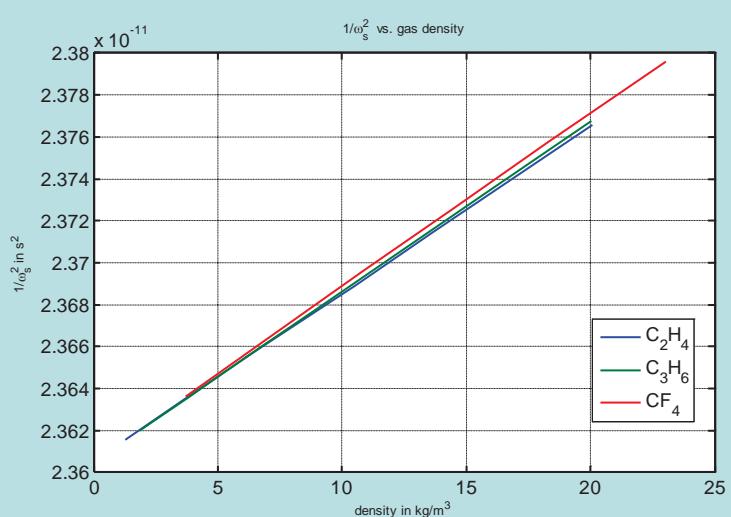
Remove viscosity dependence

$$L'C_0 = \frac{1}{\omega_s^2} = L_0 C_0 + A C_0 \rho + \frac{R - R_0}{\omega_s}$$

Measured resonance frequency of the motional branch

influence of viscous damping

$$\begin{aligned} \Rightarrow \frac{1}{\omega_{s,comp}^2} &= \frac{1}{\omega_s^2} - \frac{R - R_0}{\omega_s} \\ &= A C_0 \rho + \frac{1}{\omega_0^2} \end{aligned}$$



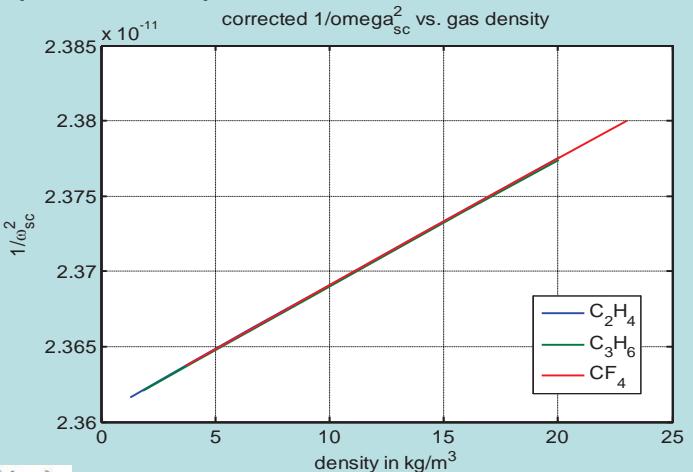
## Density measurement – Pressure Dependence

Consider additional pressure dependent impedance

$$\Rightarrow \frac{1}{\omega_{s,comp}^2} = AC_0\rho + \frac{1}{\omega_0^2}$$

$$= \frac{1}{\omega_s^2} - \frac{R - R_0}{\omega_s} - Dp/\omega_s$$

Modeled by additional impedance  $Z_p(p) = Dp$

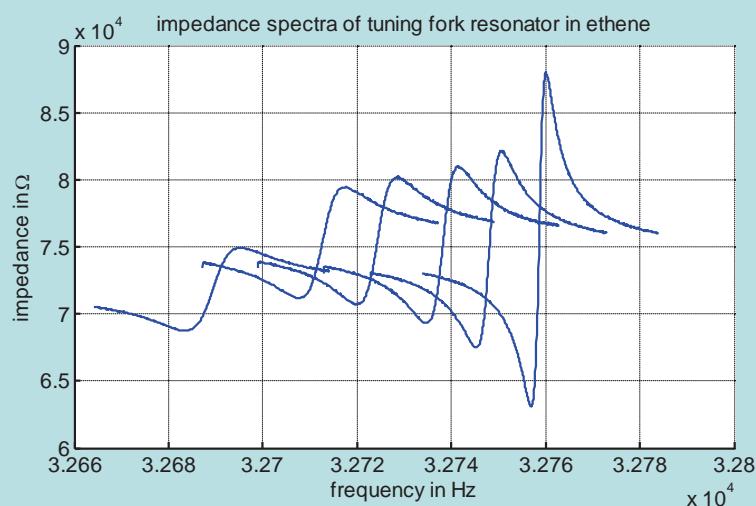


$$\rho = (1/(\omega_s C_1) - \omega_s L_1 - (Re(Z) - R_1 + Dp)) / (A\omega_s)$$

$$\eta = ((Re(Z) - R_1)/B)^2 / (\omega_s \rho),$$

By measurement of  $R_0$ ,  $f_{sm0}$  and  $p$ , density and viscosity can be calculated

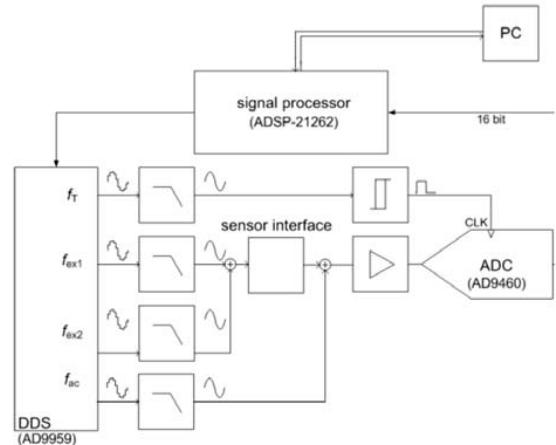
Determine  $f_s$  and  $R_1$  by fitting the model to impedance spectra



Long measurement time (about 1 min)

## Measurement system

Frequency tracking system, based on Impedance Analyzer [2]



**Fig. 2:** Schematic description of the measurement system

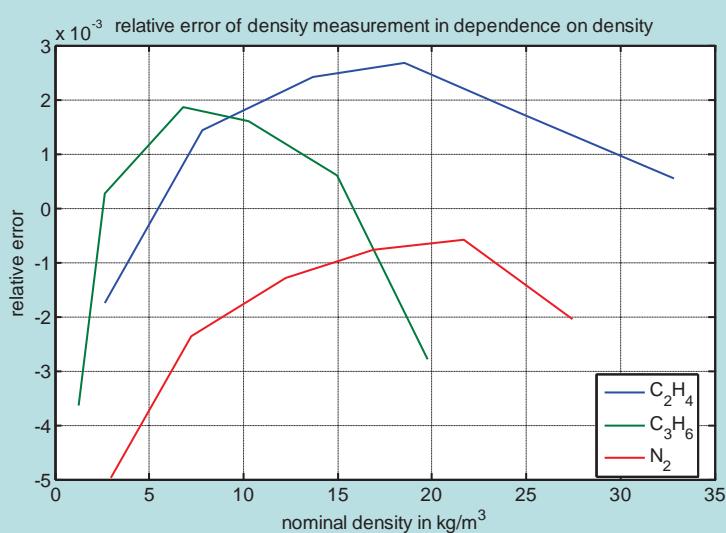
- Normal operation: Continuous measurement of  $R_1$  at  $f_s$   
 $\Rightarrow$  Fast and accurate measurement
- Main components:
  - Digital signal processor
  - Direct Digital Synthesizer
  - Analog-To-Digital Converter
  - Serial Connection to PC
- Compensation techniques:
  - digital
  - Analog

[2] A.O. Niedermayer, E.K. Reichel and B. Jakoby, "Yet Another Precision Impedance Analyzer (YAPIA) For Resonating Sensors", Eurosensors 2008

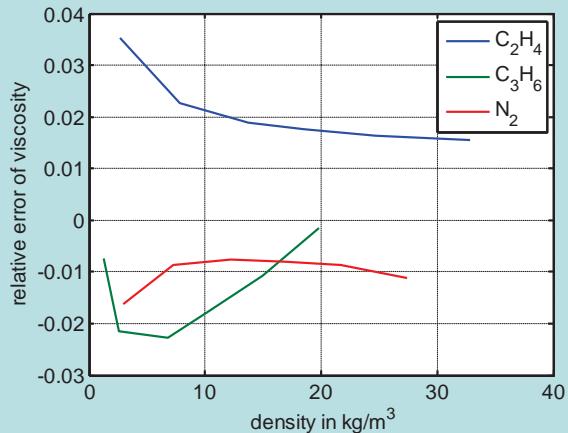
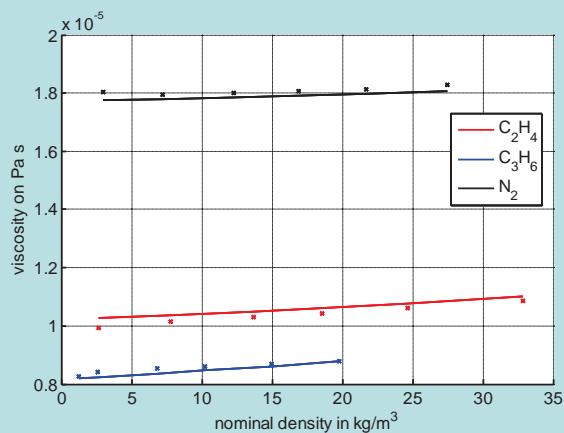


## Density measurement – Accuracy

Relative error in density measurement



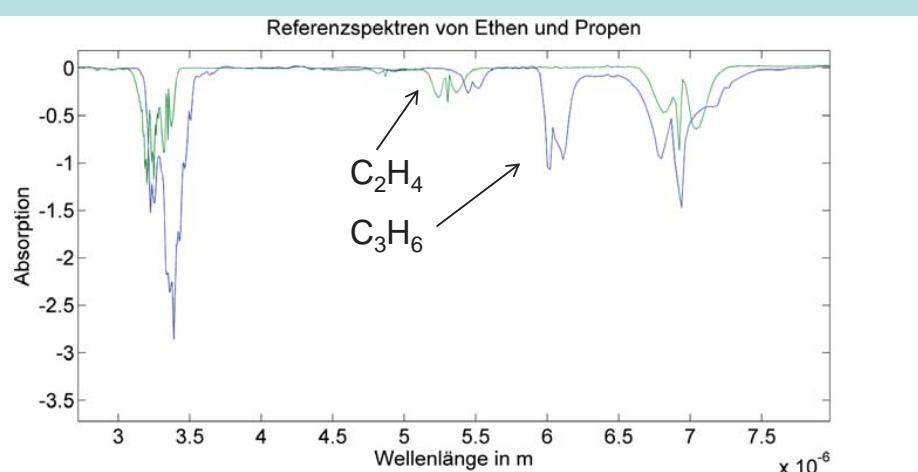
## Viscosity measurement



Accuracy is limited by reference data (viscosity:  $\approx 5\%$ , density  $0.05\%$ )

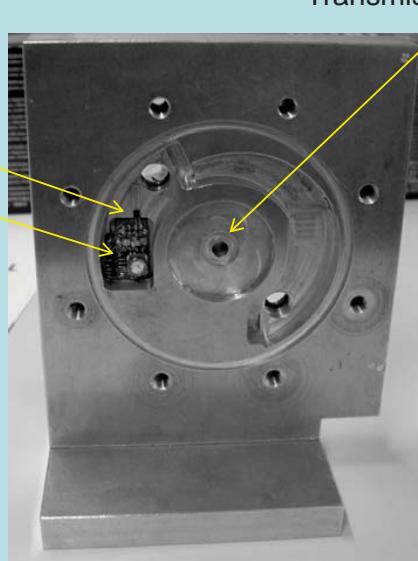
## IR

- IR absorption of ethene and propene

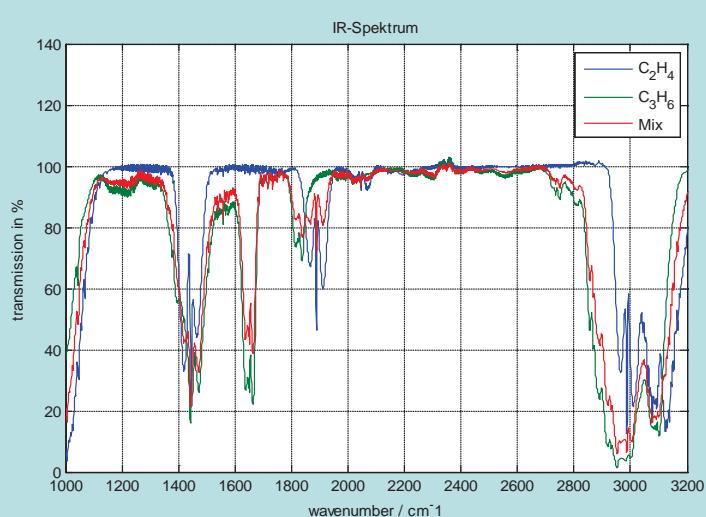


**IR****Measurements with FTIR Spectrometer****Measurement cell**

- Integrated T-sensor
- Pressure sensor
- $\text{CaF}_2$  window  
(pressure tested to 50 bar)

**Can concentration be measured**

- 1:1 mol sample provided by Borealis



$\text{C}_2\text{H}_4$ : 10.295 bar  
 $\text{C}_3\text{H}_6$ : 7.80 bar  
 Mix: ca. 9 bar

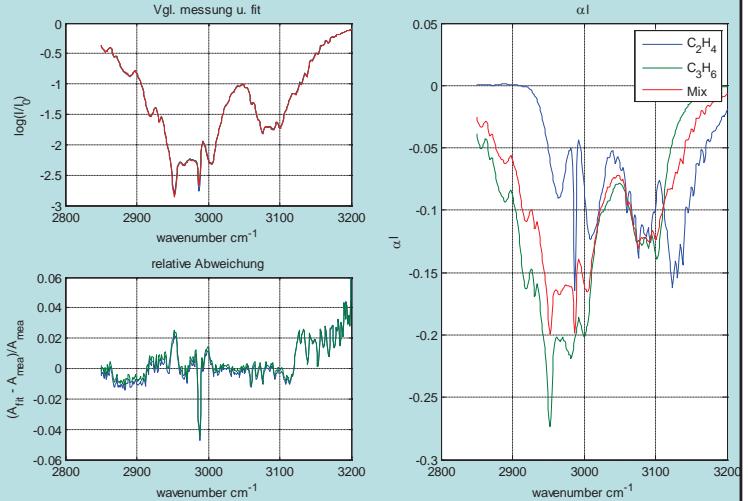
## Can concentration be measured

### Analysis

$$A(\nu) = \log\left(\frac{I(\nu)}{I_0(\nu)}\right) = \alpha_1(\nu)\rho_1 + \alpha_2(\nu)\rho_2$$

Solve:

$$l \begin{pmatrix} \alpha_{prop}(\nu_1) & \alpha_{eth}(\nu_1) \\ \vdots & \vdots \\ \alpha_{prop}(\nu_n) & \alpha_{eth}(\nu_n) \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} = \begin{pmatrix} A(\nu_1) \\ \vdots \\ A(\nu_n) \end{pmatrix}$$



mol-ratio: 1.000 : 1.343 (Ethen - Propen)

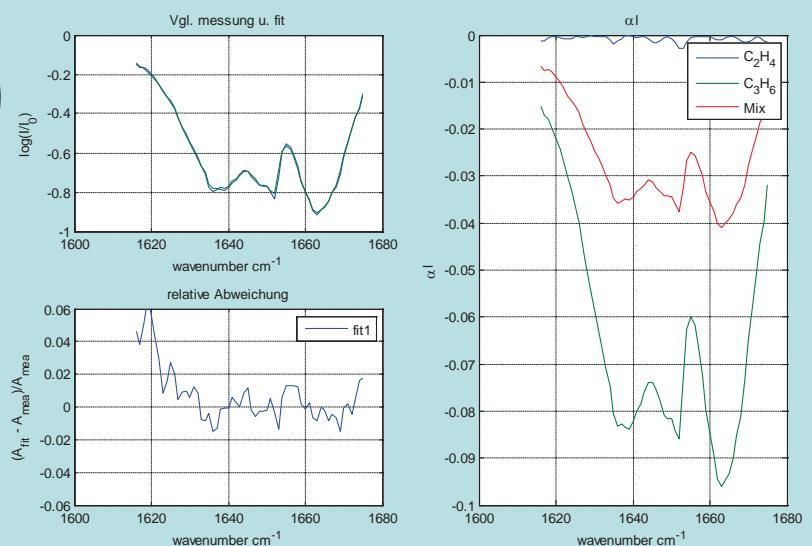
density:  $\rho_{eth}=4.640 \text{ kg/m}^3$ ,  $\rho_{prop}=9.348 \text{ kg/m}^3$

## Can concentration be measured

Band: 1620-1670 cm<sup>-1</sup>

- $$l \begin{pmatrix} \alpha_{prop}(\nu_1) \\ \vdots \\ \alpha_{prop}(\nu_n) \end{pmatrix} \rho_1 = \begin{pmatrix} A(\nu_1) \\ \vdots \\ A(\nu_n) \end{pmatrix}$$

$\rho_{prop}=9.438 \text{ kg/m}^3$



## GC validation (Reference Method)

Validation of concentration with gas chromatograph

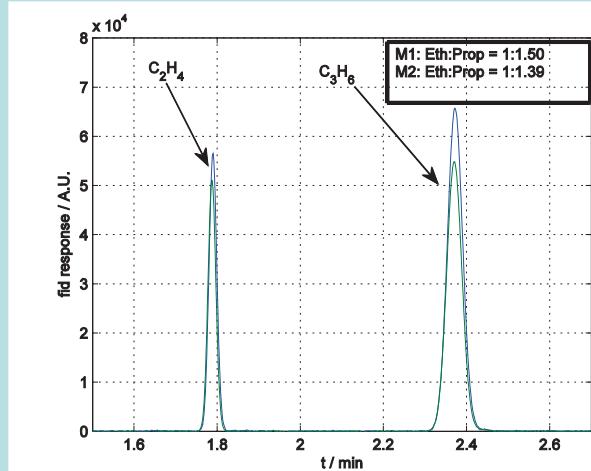
Obtained ratios:

1.51, 1.37, 1.35, 1.33

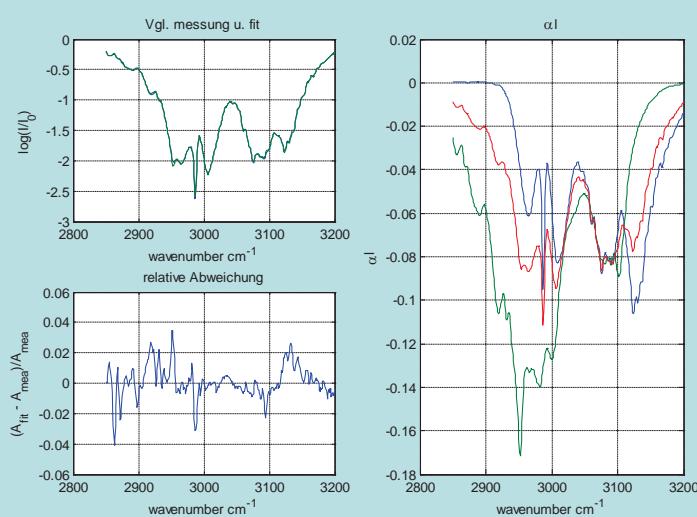
$$\Rightarrow \text{ratio} = (1.39 \pm 0.08):1$$

IR & GC measurement agree

Reference Method is not very accurate

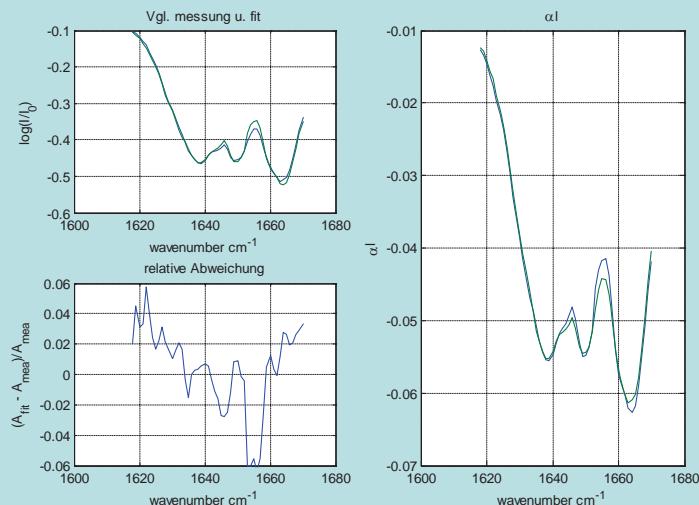


- 2<sup>nd</sup> Mixture



mol-ratio: 2.69:1(Ethene: Propene)  
density:  $\rho_{\text{eth}} = 15.184 \text{ kg/m}^3$   
 $\rho_{\text{prop}} = 8.479 \text{ kg/m}^3$

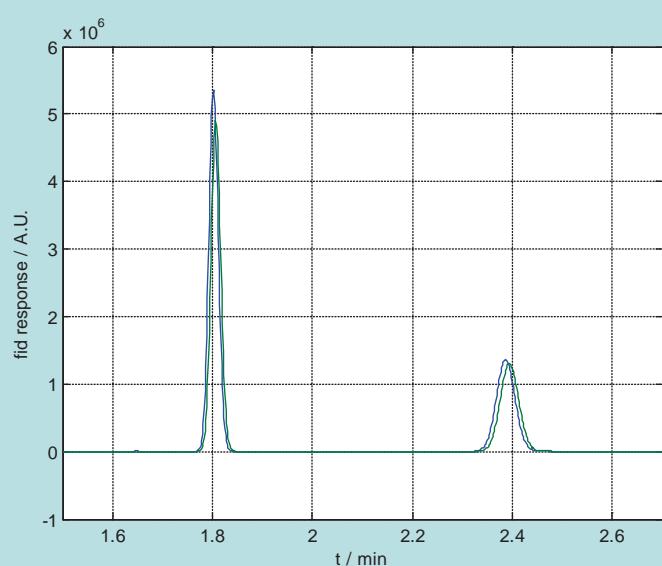
- 2<sup>nd</sup> Mixture



$$\rho_{\text{prop}} = 8.361 \text{ kg/m}^3$$

- GC measurement

- M1:  $r=3.05$
- M2:  $r= 2.96$



## Questions

- Is GC accurate?
  - Measurement of more samples necessary for accurate value
- Is absorption coefficient proportional to total pressure? Does it depend on the partial pressures of the gas components?
  - Measurement of mixtures with exactly known concentration ratios.
  - due to limited accuracy of GC measurement many iterations are necessary
- Are specific wavenumbers suitable for concentration measurement without FTIR?
  - See above
  - PLS regression

## Conclusion

- Density measurement with quartz tuning forks
  - continuous monitoring
  - accuracy:  $\sim 0.075 \text{ kg/m}^3$  ( $\sim 0.5 \%$ )
  - Waiting for integration into polymerization reactor
- IR measurement
  - direct concentration of propene and/or ethene
  - More work needed....

# Accelerated Statistical Inversion and Bayesian Calibration for Electrical Tomography

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30. 6. 2011

## Outline

- Inverse Problems.
  - What are Inverse Problems
  - Statistical Inversion.
  - Model Errors.
- Computational methods.
  - Fast Computational Methods.
  - Approximation Techniques.
- Case Studies
  - Shape Reconstructions.
  - Gibbs Sampling.
  - Different Calibration Approaches

## Inverse Problems

Determine  $\mathbf{x}$  from

$$\tilde{\mathbf{d}} = P(\mathbf{x}) + \mathbf{v}, \quad (1)$$

Forward map (model)  $F : \mathbf{x} \mapsto \mathbf{y}$ .

$$\mathbf{y} = F(\mathbf{x}) \quad (2)$$

$$F(\mathbf{x}) = P(\mathbf{x}) \quad \forall \mathbf{x}, \quad (3)$$

Where does the name come from:

$$\mathbf{x} = F^{-1}(\tilde{\mathbf{d}}), \quad (4)$$

Does not work as inverse problems are ill posed. → Use Regularization terms or Prior knowledge to stabilize  $F^{-1}(\cdot)$

$$\mathcal{F}^{-1}(\tilde{\mathbf{d}}). \quad (5)$$

## Statistical Inversion

Bayes Law:

$$\pi(\mathbf{x}|\tilde{\mathbf{d}}) = \frac{\pi(\tilde{\mathbf{d}}|\mathbf{x})\pi(\mathbf{x})}{\pi(\tilde{\mathbf{d}})} \propto \pi(\tilde{\mathbf{d}}|\mathbf{x})\pi(\mathbf{x}). \quad (6)$$

- The approach is applicable to any forward problem.
- No derivatives have to be computed.
- Available prior knowledge can be incorporated in a natural way.
- Information about the measurement noise can be added in the same natural way.
- The result is a probability density function. Hence, complete information about the uncertainty of the result is available.

## Statistical Inversion 2

Meaningful point estimates:

$$\mathbf{x}_{ML} = \arg \max \pi(\tilde{\mathbf{d}}|\mathbf{x}), \quad (7)$$

$$\mathbf{x}_{MAP} = \arg \max \pi(\mathbf{x}|\tilde{\mathbf{d}}). \quad (8)$$

... can be formulated as optimization problem.

$$\mathbf{x}_{CM} = \int \mathbf{x} \pi(\mathbf{x}|\tilde{\mathbf{d}}) d\mathbf{x}, \quad (9)$$

→ high dimensional integral.

- Analytic solution is often not possible.
- Also not suitable for quadrature techniques.

Solution: Monte Carlo integration → support points are generated from the density itself.

## Metropolis Hastings Algorithm

- 1 Pick the actual state  $\mathbf{x} = \mathbf{X}_n$  from the Markov chain.
- 2 With proposal density  $q(\mathbf{x}, \mathbf{x}')$  generate a new state  $\mathbf{x}'$ .
- 3 Compute the likelihood ratio  $\alpha = \min \left[ 1, \frac{\pi(\mathbf{x}'|\tilde{\mathbf{d}})q(\mathbf{x}',\mathbf{x})}{\pi(\mathbf{x}|\tilde{\mathbf{d}})q(\mathbf{x},\mathbf{x}')} \right]$ .
- 4 With probability  $\alpha$  accept  $\mathbf{x}'$  and  $\mathbf{X}_{n+1} = \mathbf{x}'$ , otherwise reject  $\mathbf{x}'$  and set  $\mathbf{X}_{n+1} = \mathbf{x}$ .

- Slow as every proposal requires an evaluation of the forward map.
- Proposals can be rejected.
- Samples are highly correlated (large IACT  $\tau_{int}$ ).
- Problem with multi modal distributions.

Speedup possible with Delayed Acceptance MH (DAMH) algorithm ( $F^*(\mathbf{x})$ ).

## Gibbs Sampler

- 1 Pick the actual state  $\mathbf{x} = \mathbf{X}_n$  from the Markov chain.
- 2 For every element  $i$  of the vector  $\mathbf{x}$ :
  - 1 Set  $x_i$  of  $\mathbf{x}$  as independent variable, while all other elements are fixed.
  - 2 Calculate  $\Phi_i(t) = \int_{-\infty}^t \pi(\mathbf{x}) dx_i$ .
  - 3 Draw  $u \sim \mathcal{U}([0, 1])$  and set the  $i$ -th component of  $\mathbf{x}$  as  $x_i = \Phi_i^{-1}(u)$ .
- 3 Set  $\mathbf{X}_{n+1} = \mathbf{x}$ .
  - Every proposal is accepted.
  - Evaluation of the conditional distribution is expensive.

## Calibration and Model Errors

Useful approach to test the inversion algorithm

$$\mathcal{F}^{-1}(F(\mathbf{x}) + \mathbf{v}). \quad (10)$$

... is called "Inverse Crime". Fine if everything also works directly with real data ... but sometimes it completely fails!

Reason

$$F(\mathbf{x}) \approx P(\mathbf{x}). \quad (11)$$

- Absolute imaging
- Differential imaging

# Calibration of Computer Models 1

Approach:

$$P(\phi) \approx \rho F(\mathbf{x}) + \mathbf{c}. \quad (12)$$

Hyperparameter  $\xi = \{\rho, \mathbf{c}\}$ .

$$\pi(\mathbf{x}, \xi | \tilde{\mathbf{d}}, \mathbf{d}_c) = \pi(\tilde{\mathbf{d}}, \mathbf{d}_c | \mathbf{x}, \mathbf{x}_c, \xi) \pi(\mathbf{x}) \pi(\xi), \quad (13)$$

Product rule:

$$\pi(\mathbf{x}, \xi | \tilde{\mathbf{d}}, \mathbf{d}_c) = \pi(\mathbf{x} | \xi, \tilde{\mathbf{d}}, \mathbf{d}_c) \pi(\xi | \tilde{\mathbf{d}}, \mathbf{d}_c) \quad (14)$$

$\rightarrow \xi$  depends on the data!

# Calibration of Computer Models 2

How to use calibration information

- Empirical Bayes: fix  $\xi$

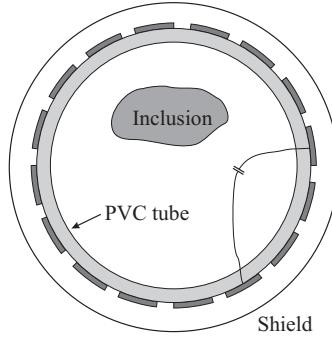
$$\xi = \arg \min_{\xi=\{\rho, \mathbf{c}\}} \|\rho F(\mathbf{x}_c) + \mathbf{c} - \mathbf{d}_c\|_2^2 \quad (15)$$

- Mutual inference: treat also  $\xi$  as random variable.
- Bayesian Forward map:

$$\mathcal{Y} = \tilde{F}(\mathbf{x}) + \mathcal{D}(\cdot). \quad (16)$$

Say  $\tilde{F}(\mathbf{x})$  is the best available forward map and build an inadequacy function  $\mathcal{D}(\cdot)$  to incorporate error knowledge from calibration measurements.

## Electrical Capacitance Tomography



PDE:

$$\nabla \cdot (\epsilon_0 \epsilon_r \nabla V) = 0, \quad (17)$$

BC:

$$V_{\partial\Omega} = 0, \quad (18)$$

$$V_{\Gamma_j} = V_{\Gamma_j}, \quad (19)$$

$$V_{\Gamma_i} = 0 \quad \forall i \neq j, \quad (20)$$

Gauss law:

$$C_{i,j} = -\frac{1}{V_{\Gamma_j}} \oint_{\Gamma_j} \epsilon_0 \epsilon_r \nabla V_i \cdot \vec{n} d\Gamma. \quad (21)$$

Gives a  $N_{elec} \times N_{elec}$  matrix.

- $\Omega$ : whole domain
- $\Omega_{ROI}$ : interior of the pipe.
- $\partial\Omega_{ROI}$ : interior of the pipe.

## Standard Computations: $F : \mathcal{E} \mapsto \mathcal{C}$

Finite element system:

$$\mathbf{K} = \sum_{i=1}^{N_e} \epsilon_i \mathbf{K}_{e,i}, \quad (22)$$

With BC:

$$\hat{\mathbf{K}} \mathbf{v} = \mathbf{r}. \quad (23)$$

Charge method:

$$Q_{elec} = \sum_{n_{elec}} (\mathbf{K} \mathbf{v})_{n_{elec}}, \quad (24)$$

Derivatives:

$$dC_{i,j} = \gamma_j^T \left[ \left[ \frac{\partial \mathbf{r}}{\partial \epsilon_k} \right] - \left[ \frac{\partial \hat{\mathbf{K}}}{\partial \epsilon_k} \right] \mathbf{v}_i \right] d\epsilon_k, \quad (25)$$

## Solution with Greens Functions

PDE:  $Lu = f$  solve by  $u = L^{-1}f$  or  $u = Gf$

- Jacobian operation  $J : \varepsilon \mapsto Q$ :

$$dQ = -G_Q^T \hat{K}_{d\varepsilon} G_Q \quad (26)$$

$$dQ = -G_Q^T \left[ \sum_I^p W_I d\varepsilon W_I^T \right] G_Q. \quad (27)$$

- Jacobian transpose operation  $J^T : Q \mapsto \varepsilon$

$$J^T q = - \left( \sum_{I=1}^p (G_Q^T W_I)^T \otimes (Q G_Q^T W_I) \right), \quad (28)$$

- Low rank updates

Neumayer and Fox 2011 Fast Forward Map Framework for Electrical Capacitance Tomography, submitted to IEEE Transactions

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## Low Rank Updates

How is  $Q$  effected when a low number of elements are updated?

Purpose: line search, conditional sampling

Woodbury Formula:

$$B^{-1} = (A + LU)^{-1} = A^{-1} - \underbrace{A^{-1} L (I + U A^{-1} L)^{-1} U A^{-1}}_{\text{update term}}, \quad (29)$$

How can we use this:

$$B = \hat{K}_{new} = \hat{K}_{old} + \gamma \sum_{I=1}^p W_I \Delta \varepsilon W_I^T = \hat{K}_{old} + \gamma L U \quad (30)$$

With  $G_Q$  to replace  $A^{-1} = \hat{K}_{old}^{-1}$

$$\Delta Q = -\gamma G_Q^T L (I + \gamma U_{:,C} G_{C,C} L_{C,:})^{-1} U G_Q, \quad (31)$$

Neumayer and Fox 2011, to be published.

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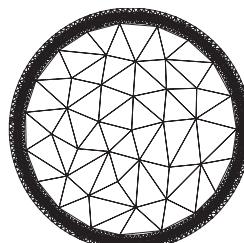
# A Speed Comparison

Operation/Method	$t_{mesh1}$	$t_{mesh2}$
	ms	ms
Forward problem standard	96	640
Forward problem new	4.8	26
Standard material update	35.5	230
Fast material update	0.039	2
Matrix inversion	3.3	19
Jacobian by AVM	360	> 2000
Jacobian op. $J : \varepsilon \mapsto Q$	0.48	3.9
Jacobian transp. op. $J^T : Q \mapsto \varepsilon$	3.3	15.5
Exact low rank update (1 elem.)	3.5	16.3
$WSW^T$ Woodbury (1 elem.)	0.66	4.2
Exact low rank update (20 elem.)	11.6	55.4
$WSW^T$ Woodbury (20 elem.)	2.7	14.1
Exact update 1 elem $\times$ 20	5.6	18
$WSW^T$ Woodbury 1 elem $\times$ 20	1.1	3
Domain d. by Schur c.	23.8	66
Schur c. with Cho.	2.9	8
Woodb. for Schur c. with Chol.	0.895	17.1

# Approximation Techniques $F^*(x)$

- First order approximation.

$$F(\mathbf{x} + \Delta\mathbf{x}) \approx F(\mathbf{x}) + \frac{\partial F(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x}} \Delta\mathbf{x}, \quad (32)$$



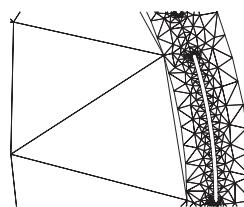
- Polynomial approximation.

$$F(\mathbf{x}) \approx P\tilde{\mathbf{x}}, \quad (33)$$

Adaptive version

$$\mathbf{p}_{k+1} = \mathbf{p}_{k+1} + \mu(F(\mathbf{x}) - \mathbf{p}_k^T \tilde{\mathbf{x}}) \tilde{\mathbf{x}}, \quad (34)$$

- Reduced physical model



# Adaptive Error Learning within DAMH

How can the evaluation of  $F(\cdot)$  be used:

$$\mathbf{e}_n = F(\cdot) - F^*(\cdot) \quad (35)$$

$$\mu_{\mathbf{e},n} = \frac{1}{n} ((n-1)\mu_{\mathbf{e},n-1} + \mathbf{e}_n), \quad (36)$$

$$\mathbf{C}_{\mathbf{e},n} = \mathbf{C}_{\mathbf{e},n-1} + \mathbf{e}_n \mathbf{e}_n^T, \quad (37)$$

$$\Sigma_{\mathbf{e},n} = \frac{1}{n-1} ((n-1)\mathbf{C}_{\mathbf{e},n} - n\mu_{\mathbf{e},n}\mu_{\mathbf{e},n}^T). \quad (38)$$

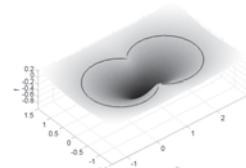
Likelihood function:

$$\pi_{\mathbf{x}^*}(\mathbf{x}|\tilde{\mathbf{d}}) = \exp \left\{ -\frac{1}{2} (\mathbf{y}^* + \mu_{\mathbf{e},n} - \tilde{\mathbf{d}})^T (\Sigma_{\mathbf{v}} + \Sigma_{\mathbf{e},n})^{-1} (\mathbf{y}^* + \mu_{\mathbf{e},n} - \tilde{\mathbf{d}}) \right\}. \quad (39)$$

# RBF Shape Model

Contour description by

$$f(\mathbf{z}) = \sum_j^N \lambda_j \phi(||\mathbf{z} - \mathbf{x}_j||) + P(\mathbf{z}), \quad (40)$$



Thin plate RBF:

$$\phi(r) = r^2 \cdot \log(r), \quad (41)$$

Prior:

$$\pi(\mathbf{x}) = \exp \left( -\frac{1}{2\sigma_{pr}^2} \frac{c(\mathbf{x})}{\sqrt{\pi \Gamma(\mathbf{x})}} \right) I(\mathbf{x}), \quad (42)$$

Moves:



(a) Translation.



(b) Rotation.

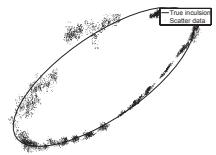


(c) Scale.

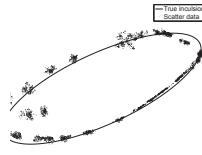


(d) Corner move.

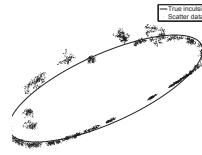
## Some DAMH Results



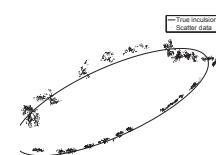
(e) Standard MH,  $\varepsilon_r = 3.5.$



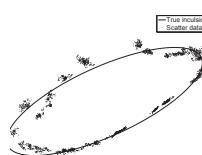
(f) Jacobian,  $\varepsilon_r = 3.5$



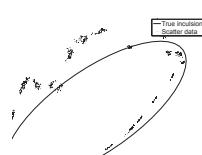
(g) Affine map,  $\varepsilon_r = 3.5.$



(h) Adapt. affine map,  $\varepsilon_r = 3.5.$



(i) Red. model,  $\varepsilon_r = 3.5.$



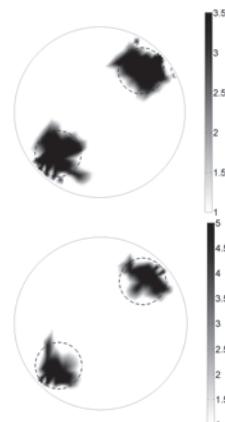
(j) Standard MH,  $\varepsilon_r = 80.$

## Gibbs Sampler for ECT

$$\pi(\mathbf{x}|\tilde{\mathbf{d}}) \propto \exp\left(-\frac{1}{2}\mathbf{e}^T \boldsymbol{\Sigma}_v^{-1} \mathbf{e}\right) \exp\left(-\frac{1}{2}\alpha \mathbf{x}^T \mathbf{L}^T \mathbf{L} \mathbf{x}\right) I(\mathbf{x}) \quad (43)$$

- Bimodal Distributions
- Arbitrary Distributions: requires some support points of the conditional distribution.

→ low rank updates mandatory for efficient sampling.



IACT:  $\tau_{int} = 1 !$

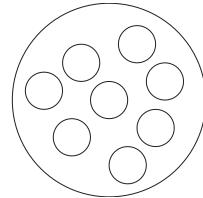
# Incorporation of Calibration Information

Observations:

- Low level representations cover most calibration effects.
- Shape determination suffers for inclusions with high permittivities.

How to find a better set of calibration parameters  $\xi$ ?

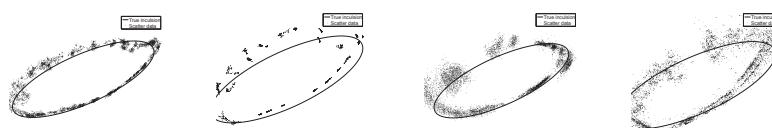
Or is there another way to incorporate calibration information?



# Mutual Inference Approaches

$$\begin{aligned} \pi(\tilde{\mathbf{d}}, \mathbf{d}_c^{(N)} | \mathbf{x}, \xi, \mathbf{x}_c^{(N)}) &\propto \exp \left\{ -\frac{1}{2} (\rho \mathbf{y} + \mathbf{c} - \tilde{\mathbf{d}})^T \Sigma_v^{-1} (\rho \mathbf{y} + \mathbf{c} - \tilde{\mathbf{d}}) \right. \\ &\quad \left. - \frac{1}{2} \sum_{i=1}^{N_c} (\rho \mathbf{y}_{c,i} + \mathbf{c} - \mathbf{d}_{c,i})^T \Sigma_c^{-1} (\rho \mathbf{y}_{c,i} + \mathbf{c} - \mathbf{d}_{c,i}) \right\}. \end{aligned} \quad (44)$$

Implementation: sample from  $\xi$  with a Gibbs sampler.



(k)  $\epsilon_r = 3.5$ .

(l)  $\epsilon_r = 80$ .

(m)  $\epsilon_r = 3.5$ .

(n)  $\epsilon_r = 80$ .

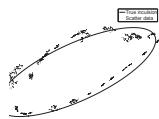
Decreased IACT but the gain in quality is comparatively low.

## Bayesian Forward Map

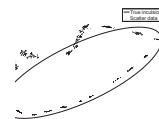
Use calibration measurements to build

$$\mathcal{Y} = \tilde{F}(\mathbf{x}) + \mathcal{GP}_{\mathcal{D}_e}(\cdot). \quad (45)$$

$$\begin{bmatrix} \mathbf{e}_c \\ \mathbf{e} \end{bmatrix} = \mathcal{N} \left( \mathbf{0}, \begin{bmatrix} \Sigma(\mathbf{x}_{c,r}, \mathbf{x}_{c,r}) & \Sigma(\mathbf{x}_{c,r}, \mathbf{x}_r) \\ \Sigma(\mathbf{x}_r, \mathbf{x}_{c,r}) & \Sigma(\mathbf{x}_r, \mathbf{x}_r) \end{bmatrix} \right), \quad (46)$$



(o) No Bayesian Forward Map (Extreme high IACT).



(p) With Bayesian Forward Map (Low IACT).

Neumayer and Fox 2011 to be published

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Thank you for your attention!

# Yet another precision impedance analyzer

## Readout electronics for resonating sensors

Alexander O. Niedermayer

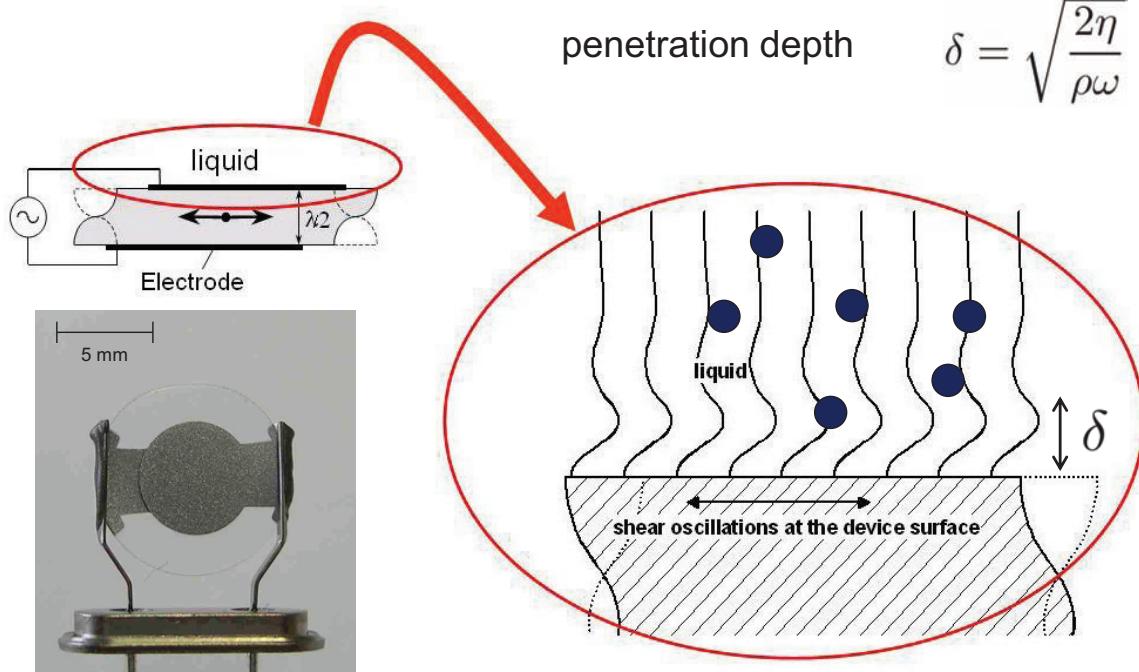
Institute for Microelectronics and Microsensors,  
Johannes Kepler University, Linz

Institute for  
Microelectronics and  
Microsensors

ACCM

JKU  
JOHANNES KEPLER  
UNIVERSITY LINZ

## Modeling

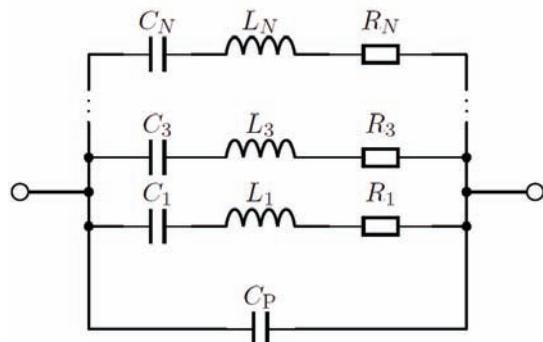


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# Modeling



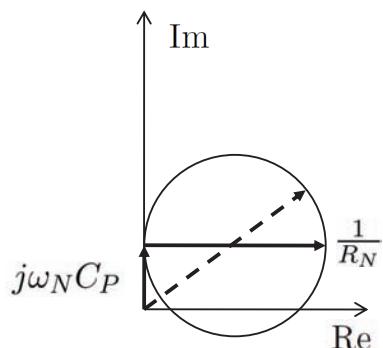
motional branch resistance  
of harmonic number  $N$ :

$$R_N = \text{unloaded resonator} + \text{viscous loading} = R_{11} \cdot N^2 + R_{12} \cdot N$$

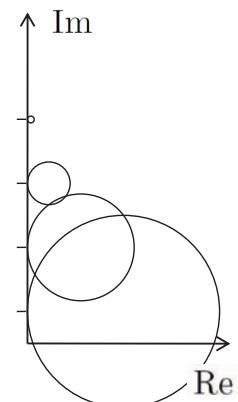
unloaded  
resonator

viscous  
loading

sensor admittance



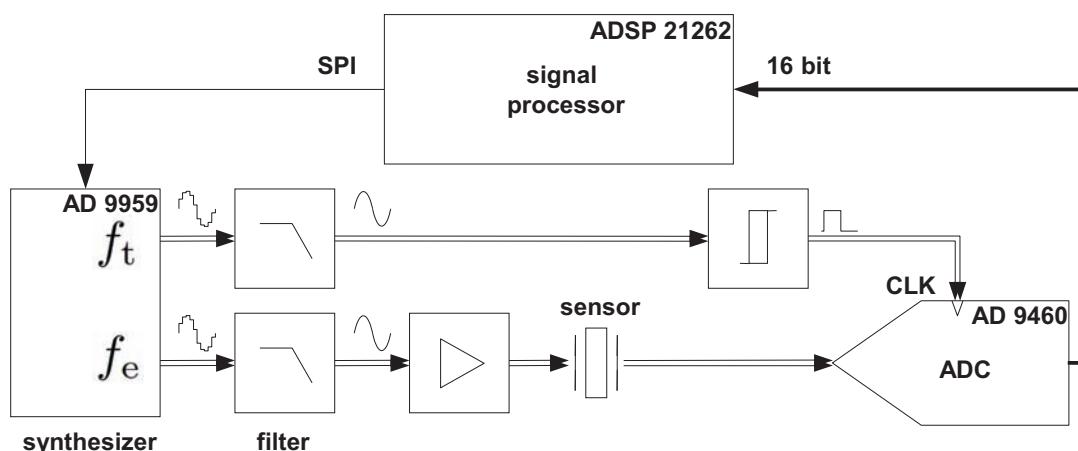
[S. Martin '94]



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## Circuit Concept



Synchronous subsampling

$$f_t = f_e \cdot \frac{n}{n-m}$$

$n$  samples per  $m$  periods

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# Demodulation

$$Y(f) = \sum_{k=0}^{N-1} \left( x[k] \cdot \cos\left(\frac{2\pi f k}{N}\right) + j x[k] \cdot \sin\left(\frac{2\pi f k}{N}\right) \right)$$

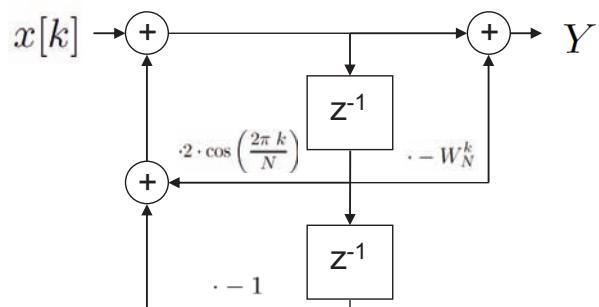
~~$\cdot \cos\left(\frac{2\pi f k}{N}\right)$~~

Synchronous sampling

$$f_t = f_e \cdot \frac{n}{n-m}$$

$n$  samples per  $m$  periods

Goertzel Algorithm

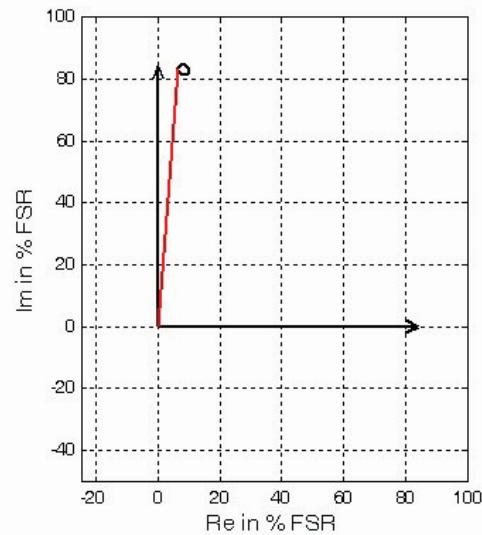
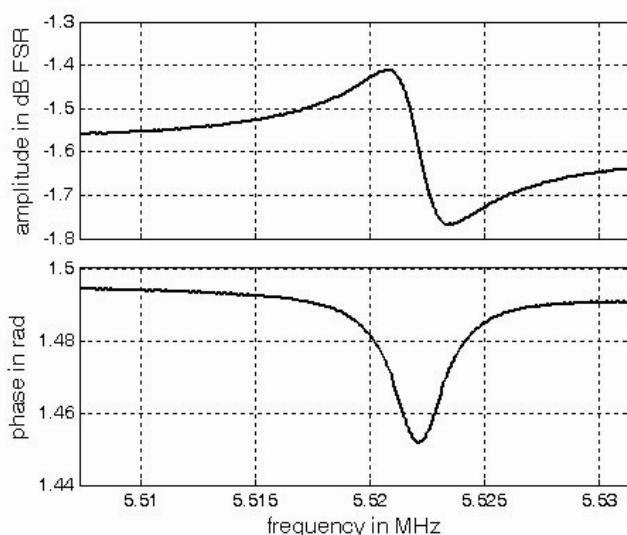


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## Sensor admittance

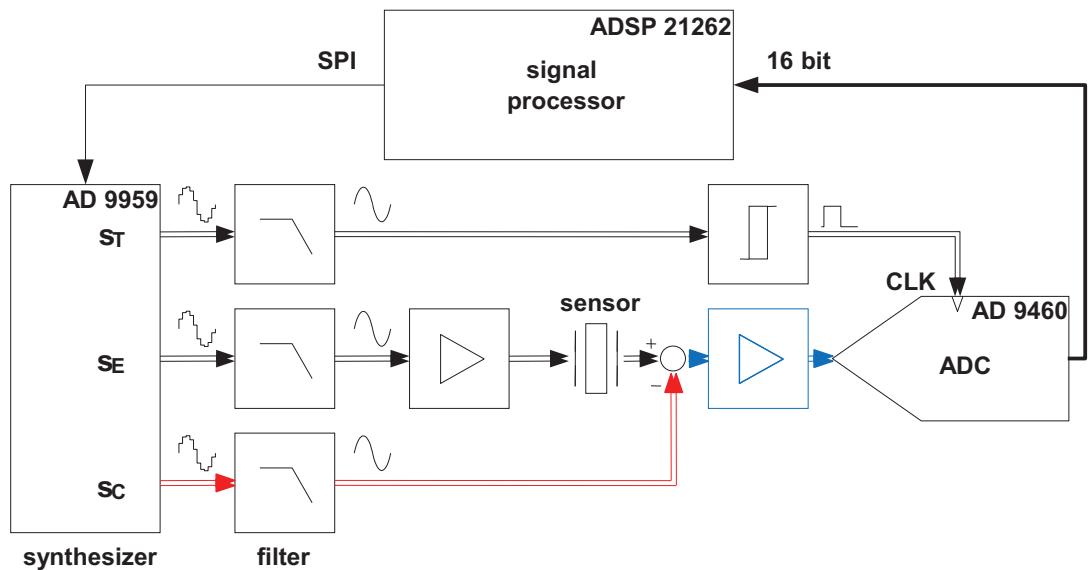
AT-cut QCR,  $f_1 = 1.8432$  MHz,  $N=3$ , in Isopropanol



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# Circuit Concept

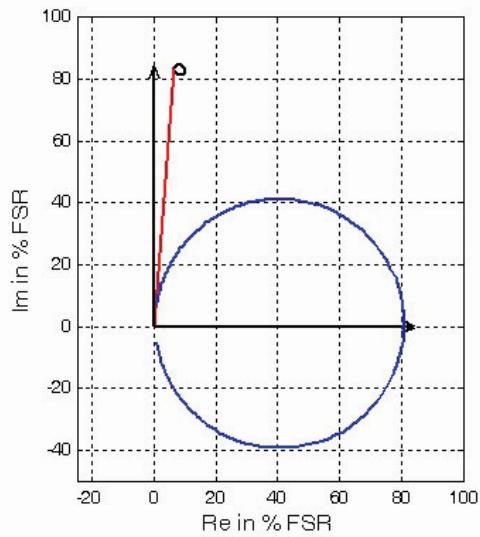
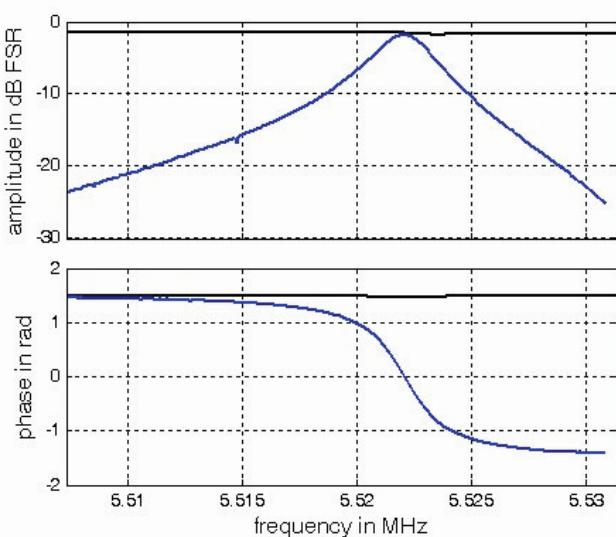


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## Sensor admittance

AT-cut QCR,  $f_1 = 1.8432$  MHz,  $N=3$ , in Isopropanol,  $t = 12$  s

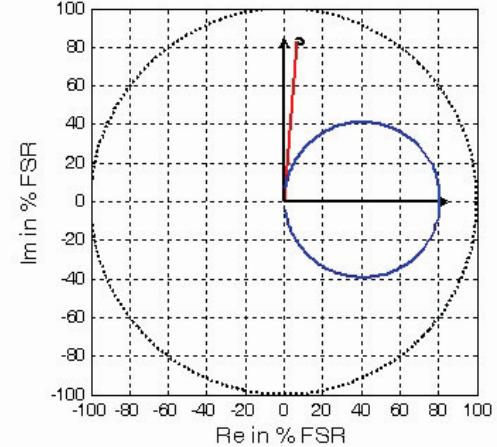
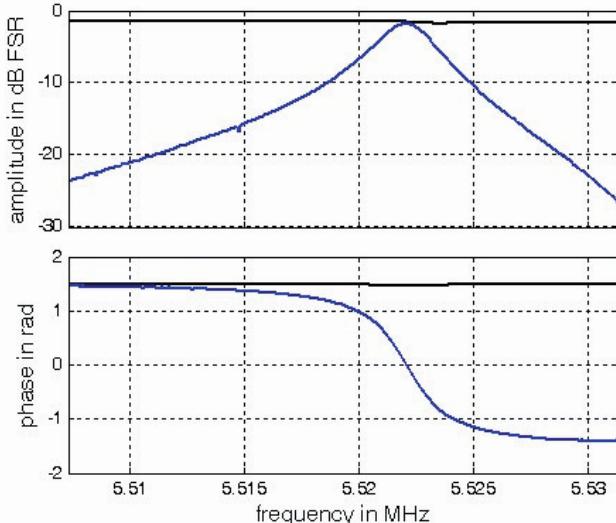


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# Applying compensation signal

AT-cut QCR,  $f_1 = 1.8432$  MHz,  $N=3$ , in Isopropanol,  $t = 12$  s



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## Conclusion

- phase resolution is very important
- wide frequency range (subsampling)
- handle higher harmonics
- various types of resonating sensors
- very compact design



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