

Microwave characterisation and modelling of materials in European initiatives

from a personal and a Polish SME perspective

Malgorzata Celuch

QWED Sp. z o.o., Poland

IEEE Ukrainian Microwave Week

Session 3: Plenary Session, 17 November 2022



to my Father,
MSc in engineering with PhD in economics,
Sybirak - survivor of Soviet deportation to Siberia

with an appeal for a stronger response
to Russia's invasion of Ukraine
to prevent Siberia happening to my children



Outline

1. About myself and my company QWED: how European initiatives support our research
2. Electromagnetic & Multiphysics Modelling: in Microwave Engineering and at QWED
3. Materials Characterisation: why it is needed in Microwave Engineering and how QWED contributes
4. Exploring the synergies between Computational Modelling and Material Measurements
5. Calling for YOUR participation and Collaboration: examples of EU initiatives



NMBP: Nanotechnologies, Advanced Materials, Biotechnology and Advanced Manufacturing and Processing

Marie Skłodowska-Curie Actions



**European Materials
Characterisation Council**



I unexpectedly ended up as Ph.D. in Electronic Engineering
(but remaining a mathematician and globetrotter by passion)



Please join our Women in Engineering Meeting,
UkrMW, Thursday afternoon

15:00-17:00 Session **WIE**: 2nd Ukrainian Microwave Week: Women in Engineering meeting

CHAIR: [Malgorzata Celuch](#) (QWED Sp. z o.o., Poland)

LOCATION: [Plenary Zoom Room](#)

QWED business started 1997

based on research at the Warsaw University of Technology

celebrating 25 years

Founders: A.Wieckowski, M.Sypniewski, M.Celuch, W.Gwarek



Prof. Jerzy Buzek awarding QWED team in 1998
Prime Minister of Poland 1997-2002
President of the European Parliament 2009-2012



Dr. Malgorzata Celuch
President since 2017, VP 1997-2017

- 35 y experience in mathematical, 25 y in management
- Awards for excellence from e.g. Prime Minister of Poland, Rector of WarsawUnivTech



Janusz Rudnicki, MS,
VP for IT

- 22 years of experience in simulation software development



Dr. Marzena Olszewska-Placha,
VP for R&D

- 15 y of experience in simulation-based MHz to THz design and consultancy
- 4 y experience in research management



Dr. Andrzej Więckowski
Senior in CAD

- 48 years of experience in computer-aided electronic engineering and engineering software development



Prof. Wojciech Gwarek,
President 1997-2017

- 22 years of experience in simulation software development



Dr. Maciej Sypniewski
Senior in CAE

- 35 years of experience in engineering software development and GHz measurements



10

employees

7

consultants

50%

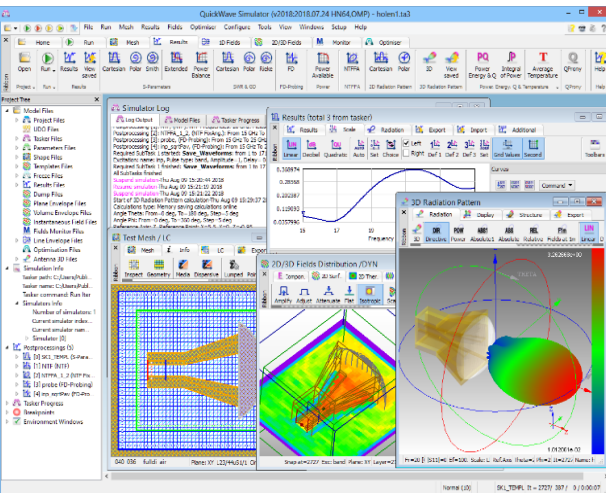
female





25 years in a Nutshell

R&D projects



Electromagnetic simulation & design software, 3D & BOR 2D tools

based on 300+ publications by:
prof.W.Gwarek, IEEE Fellow, DML, Pioneer Award
dr.M.Celuch, President of QWED

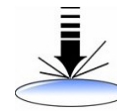


PREZES RADY MINISTRÓW

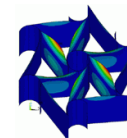
przyznaje III nagrodę
za wybitne krajowe osiągnięcie naukowo-techniczne

mpolowi Politechniki Warszawskiej w składzie:
dr inż. Małgorzata CELUCH-MARCUSIAK, dr inż. Marek STYPIEWSKI,
dr inż. Andrzej WIECZORSKI
pod kierownictwem: prof. dr hab. inż. Włodzisław GWAREK

Jerzy Bock
Prezes Rady Ministrów



FP6 SOCOT – development and validation of an optimal methodology for overlay control in semiconductor industry, for the 32 nm technology node and beyond.



FP6 CHISMALCOMB – development, modelling, and applications of chiral materials → EM validation of mixing rules



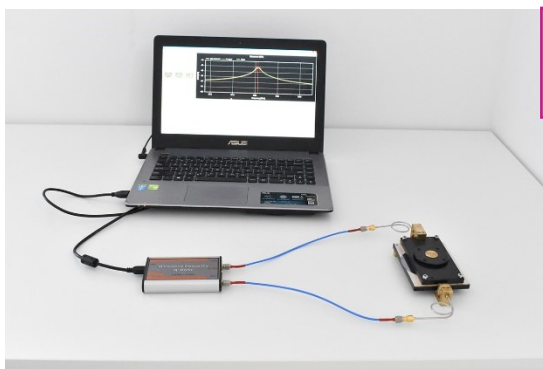
Eureka E! 2602 MICRODEFROST MODEL – innovative software-based product development tool for simulating and optimising heating and defrosting processes in microwave ovens



FP7 HIRF SE (High Intensity Radiated Field Synthetic Environment) - numerical modelling framework for aeronautic industry

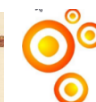


Eureka FOODWASTE – developing new microwave treatment system for high water content waste



Instruments for precise material measurements

based on 300+ publications
by prof.J.Krupka, IEEE Fellow



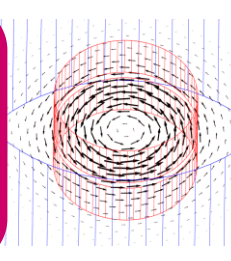
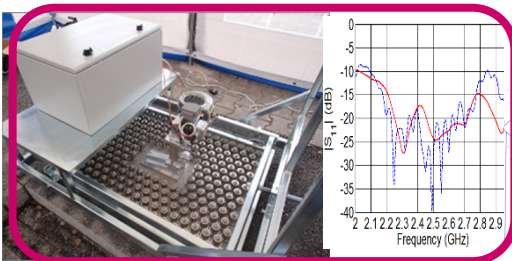
ERA-NET MNT NACOPAN – applications and modelling of nano-conductive polymer composites



NGAM2 – designing an industrial device for thermal bonding of bituminous surfaces with the aid of microwave heating



MMAMA (Microwave Microscopy for Advanced and Efficient Materials Analysis and Production) – EM modelling & characterisation for the development of high efficiency solar cells



Consultancy & design services based on EM expertise & tools

team of 10+engineers, 4 PhDs, 2 Profs
key areas: MW power appliances,
customised resonators, antennas & feeds



NanoBat - developing a novel nanotechnology toolbox for quality testing of Li-ion and beyond Lithium batteries with the potential to redefine battery production in Europe and worldwide.



ULTCC6G_EPac – development & application of novel ceramics for 5G & beyond
I4BAGS – modelling & characterisation of ion-implanted battery & graphene-enabled devices

Electromagnetics and Computational EM Modelling

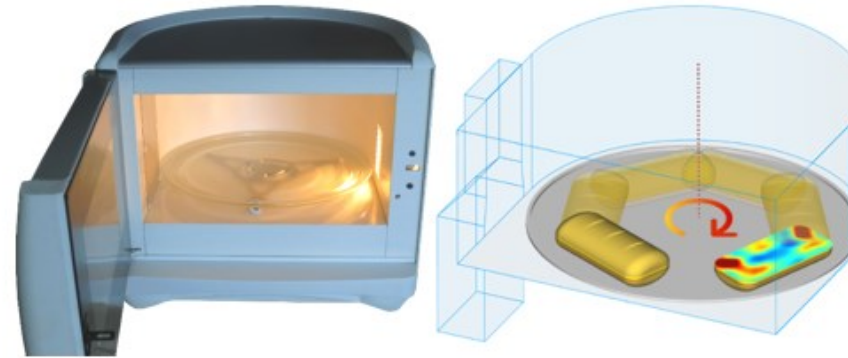
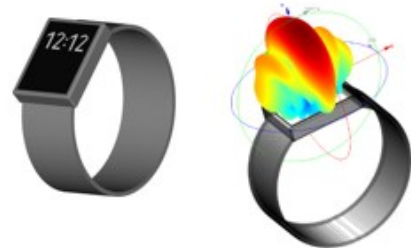
Electromagnetics (EM) = physics governed by Maxwell equations

Frequency ranges: DC – static (f=0), microwaves (MW) – ca. GHz range (cm to mm), mmWaves (e.g. 5G), light (nm)..

Electromagnetic modelling, Computational Electromagnetics (CEM)

= solving Maxwell equations with boundary & initial conditions subject to material constitutive relations

$$\begin{aligned}\nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{H} &= \frac{\partial \vec{D}}{\partial t} + \vec{J} \\ \nabla \cdot \vec{D} &= \rho \\ \nabla \cdot \vec{B} &= 0 \\ \nabla \cdot \vec{J} &= -\frac{\partial \rho}{\partial t}\end{aligned}$$



general:

$$\vec{D}, \vec{B}, \vec{J} = F(\vec{E}, \vec{H})$$

typical:

$$\vec{D} = \underline{\underline{\epsilon}} \cdot \vec{E}$$

$$\vec{B} = \underline{\underline{\mu}} \cdot \vec{H}$$

$$\vec{J} = \underline{\underline{\sigma}} \cdot \vec{E}$$

Two perspectives of EM modelling (continuum, physics-based)	
EM wave propagation in space (also in-between boundaries)	EM field interaction with materials
1990s: radars, radio & TV, electronic circuits	MW ovens
today: telecommunications (5G), RFID (ski-pass), IoT (wearable sensors)	biomedical (diagnostics – breast cancer, treatment – hyperthermia) MW chemistry, wood drying, plastics curing, rock comminution



Computational Electromagnetics in Microwave Technology

Until 1980s:

- heuristic equations (experimental models; today: data based?)
- lumped circuit approximations (**0-dimensional**: dimensions $\ll$ wavelength)
- **1D** approximations (transmission lines, long lines, telegraphists equations, Smith chart)

In 1980-1990s:

- academic research on solving Maxwell eqs.

dimensionality in space	fields in space	fields in time
2D	modal expansions (method of moment, mode matching...)	monochromatic (frequency-domain approach FD)
3D	discretisation (FEM , FD , FV, TLM, SpN,..)	arbitrary (time-domain approach TD)

- commercial software packages implemented in industry
- QWED follows **FDTD** approach based on original works of W.Gwarek & M.Celuch

Engineers question in 1990s: will EM software help me?

Engineers question today: can I trust EM software (to fully replace hardware prototyping)?



Origins of QWED Computer Modelling

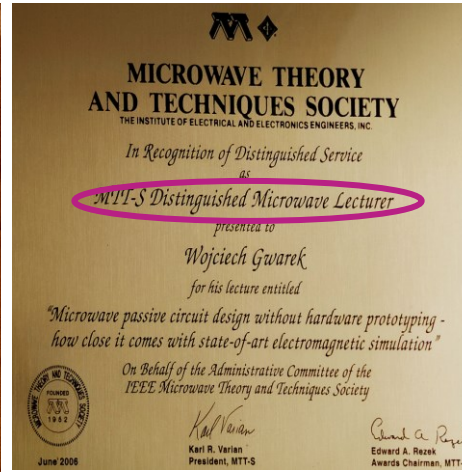
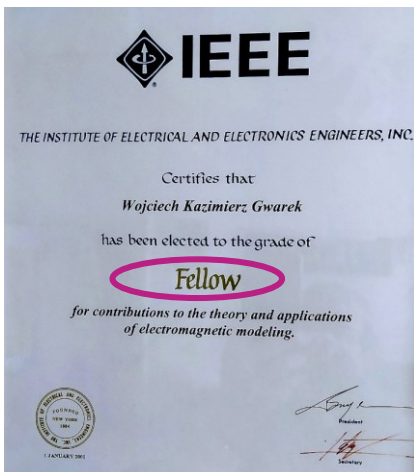
since 1980s...

IEEE- awarded research of **Prof. Wojciech Gwarek**
on 2D FDTD modelling (with novel conformal meshing)

Fellow,

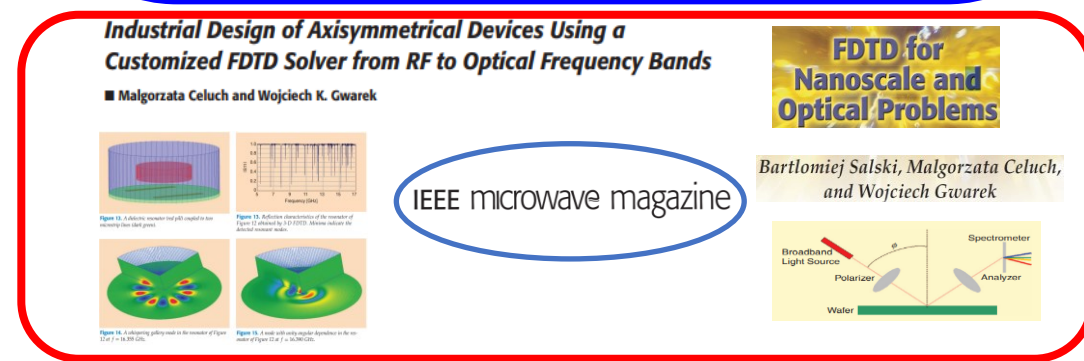
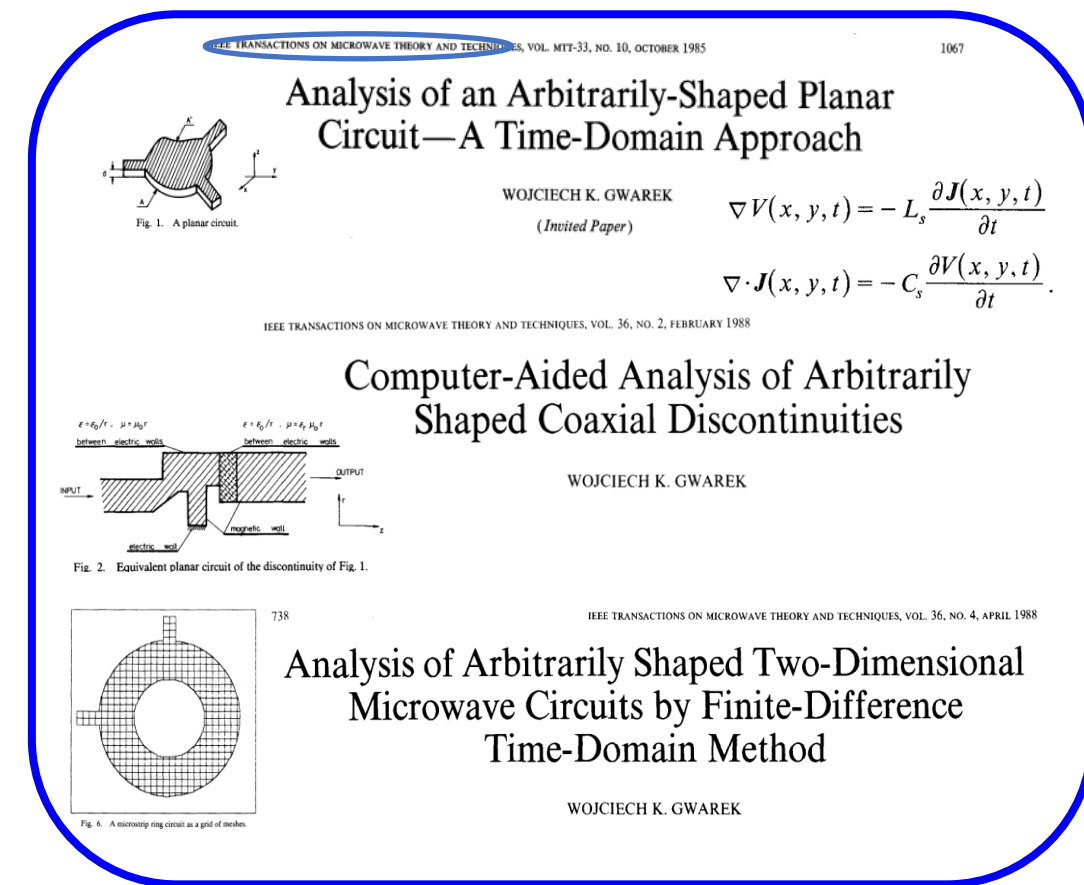
Pioneer Award,

DML

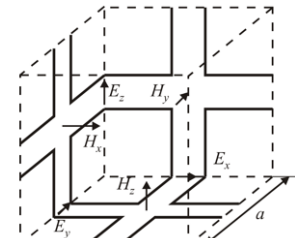


... by early 2000s:

QWED commercialises & continues the development
licences for **QuickWave-3D** by QWED used worldwide
industrial applications from RF to optical bands

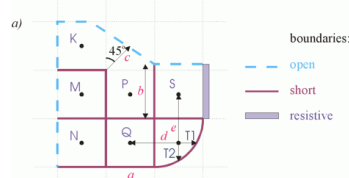


my contributions around 1990s:

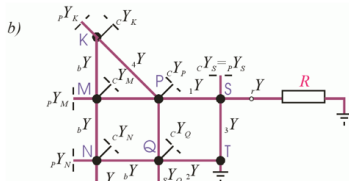


nodes: FDTD discretisation of Maxwell eqs.
connecting lines & stubs: TLM discretisation of Huygens principle

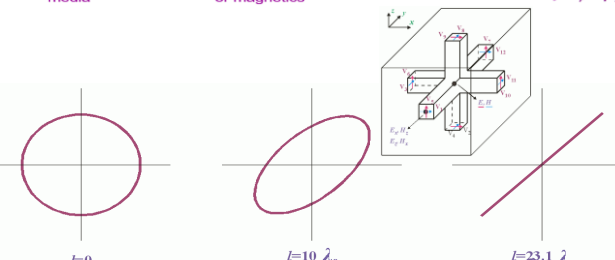
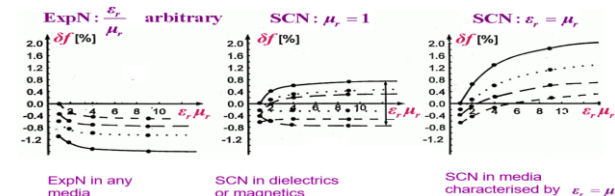
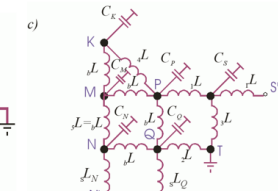
a) generalized gridding of a microwave structure



b) generalized TLM model



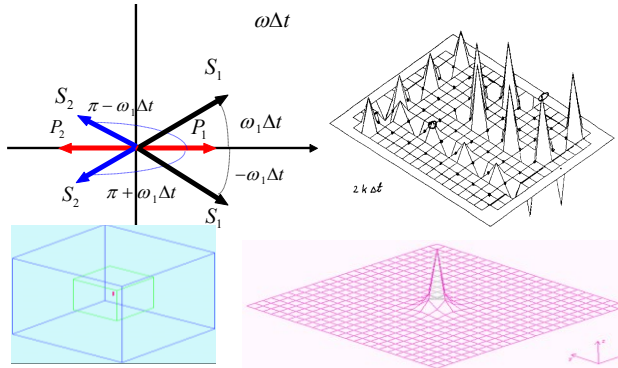
c) generalized FDTD model



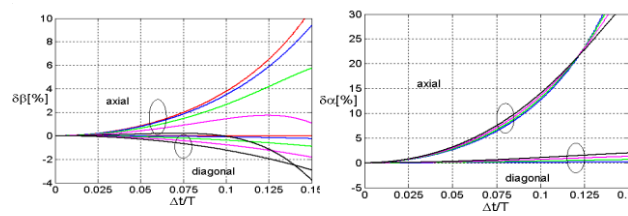
Generalised dispersion relations Theory of P- and S-eigenmodes

$$P(\omega\Delta t) S(\omega\Delta t, \beta_x a, \beta_y a, \beta_z a) = 0$$

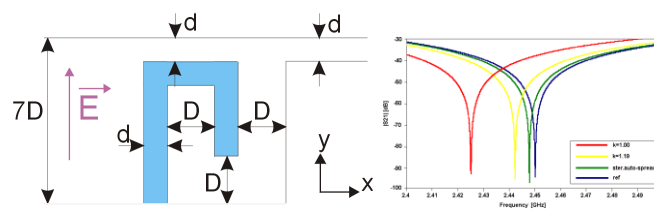
$$\omega_{ph}^2 [-\omega_{ph}^2 \mu \epsilon + \beta_{xph}^2 + \beta_{yph}^2 + \beta_{zph}^2] = 0$$



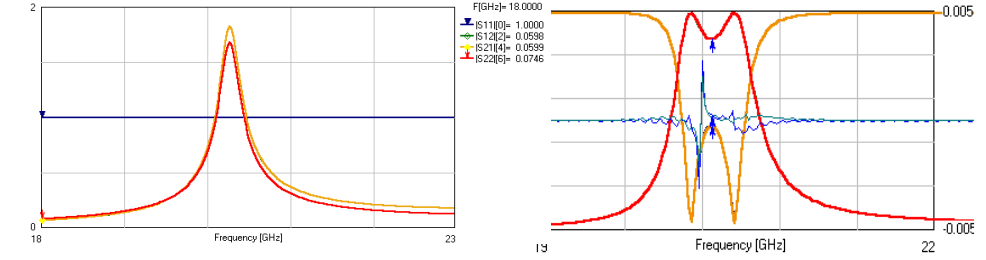
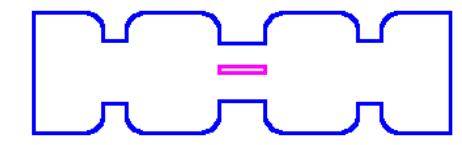
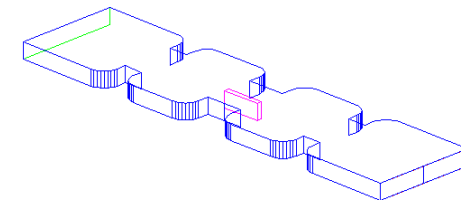
Dispersion in lossy media



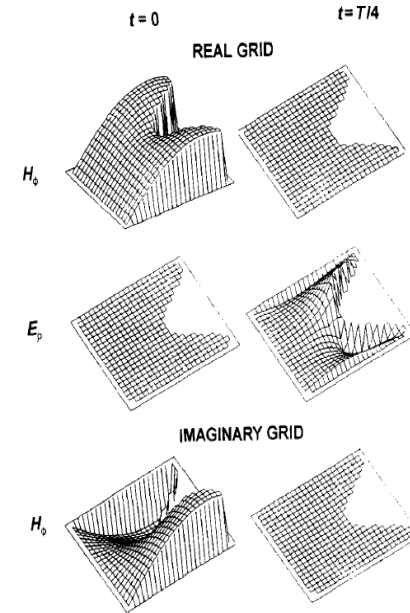
Field singularities



Generalised extraction of S-parameters in multi-modal transmission lines (incl. evanescent modes)



Periodic & vector 2D FDTD and TLM in real & complex form



Classification of time-domain methods

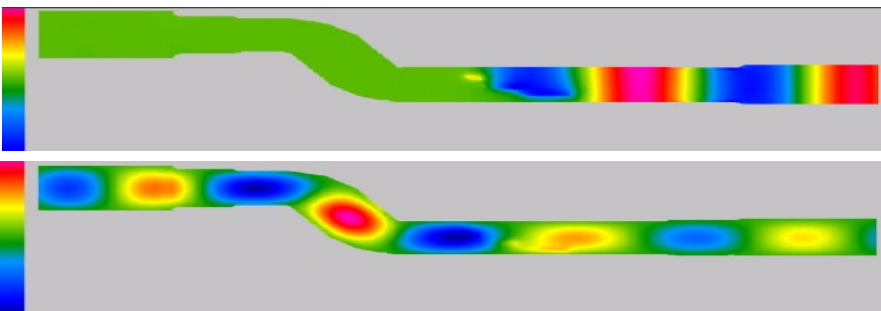
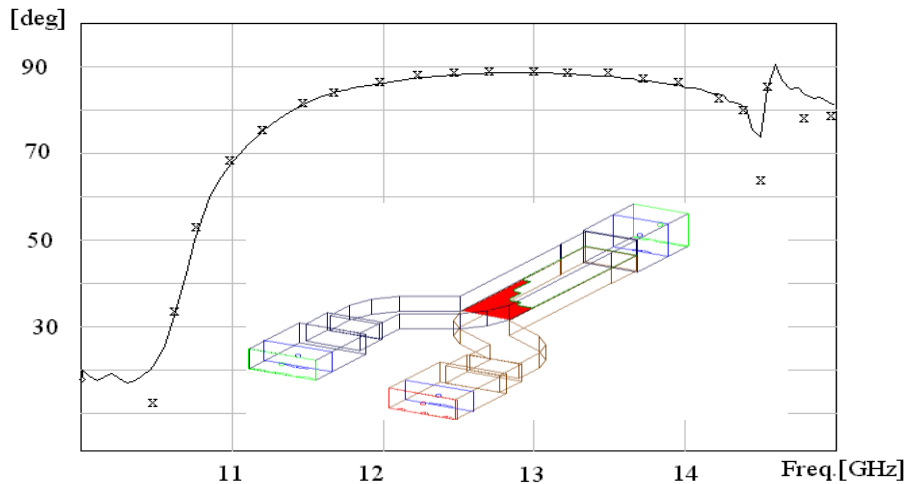
PROBLEM	ELECTROMAGNETIC	STEP 1: SPACE-DISCRETE MODELS OF FIELDS			STEP 2: PROCESS MODELLING		FINAL MODEL
		TYPE OF DISCRETIZATION	DISTRIBUTION BETWEEN NODES	ELECTROMAGNETIC EQUATIONS	FOR EXPLICIT TIME-INTEGRATION		
E-H node	expanded node (ExpN)	stair-case	finite differencing and averaging by trapezoidal rule	Maxwell curl eqs.		ExpN FDTD 1966 [11]	
				Integral form of Maxwell curl eqs.		SpN 1984 [108]	
				Huygens principle		2D FDTD modified cells 1985 [5]	
		linear or mixed		wave eq.		nonorthogonal ExpN FDTD 1983 [18]	
				Integral form of Maxwell curl eqs.		ExpN TLM 1971 [48]	
				generalized wave eq.		wave-FDTD 1994 [38]	
condensed node (SCN)	E-H node	stair-case		Maxwell curl eqs.		FETD 1990 [114]	
				Integral form of Maxwell curl eqs.		FETD 1988 [113]	
				conservation of Maxwell curl eqs.		FETD 1987 [112]	
	linear or mixed			Maxwell curl eqs.		MFV 1988 [111]	
				Integral form of Maxwell curl eqs.		2DV wave-FDTD 1993 [41]	
				generalized wave eq.		SCN TLM 1987 [63]	
OTHER MODELS OF FIELDS IN SPACE	entire (sub)domain expansion	stair-case		Lax-Wendroff averaging		SCN FDTD 1992 [132]	
				conservation of Maxwell curl eqs.		alpha - SCN 1994 [82]	
				Maxwell curl eqs.		FVTD 1989 [116]	
				Maxwell curl eqs.		MMTD 1991 [122]	

QuickWave original applications in cosmic research & satellite telecommunication

Septum polariser by SES

design & measurements: Saab Ericsson Space
modelling: QWED, 1997

below: differential phase-shift

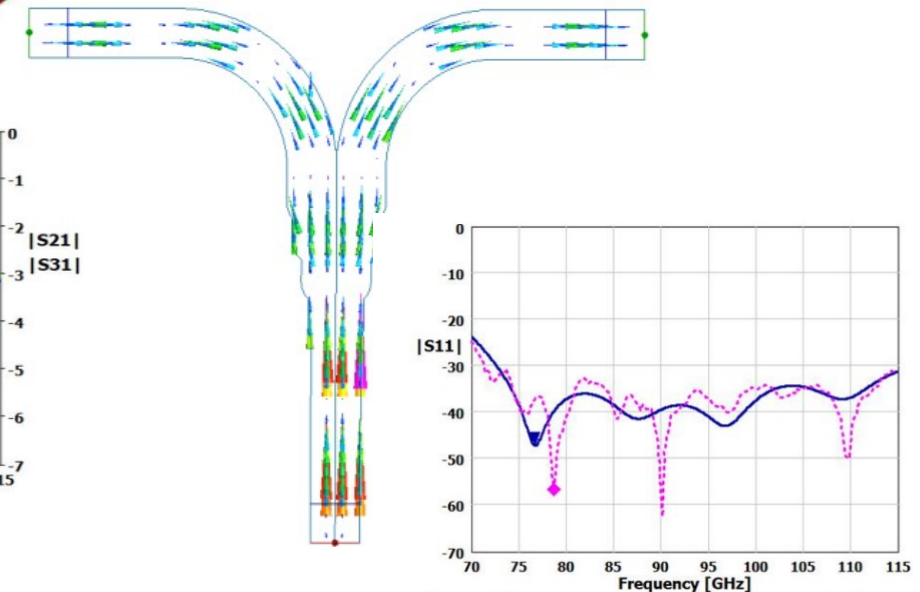
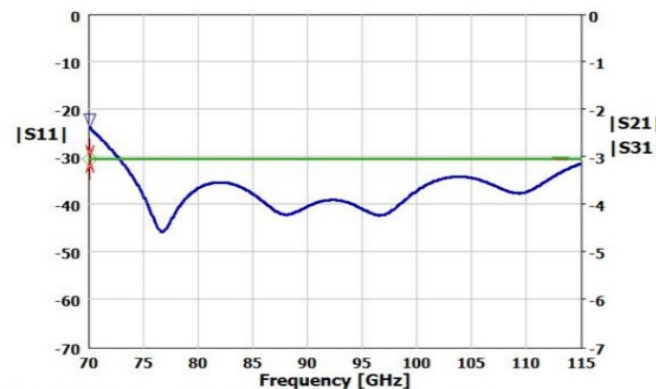
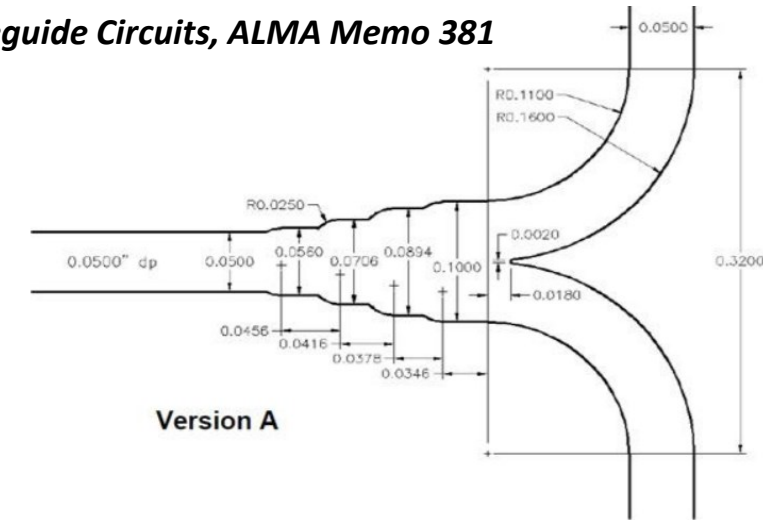
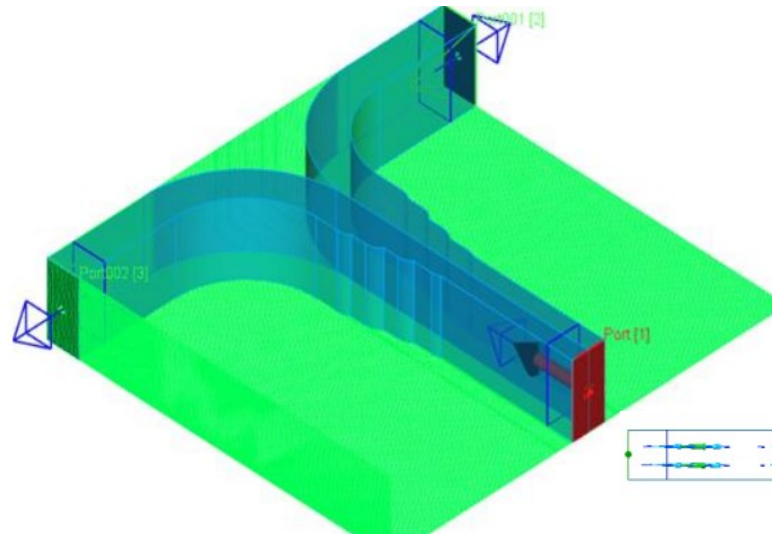


propagation of two polarisations
at centre frequency



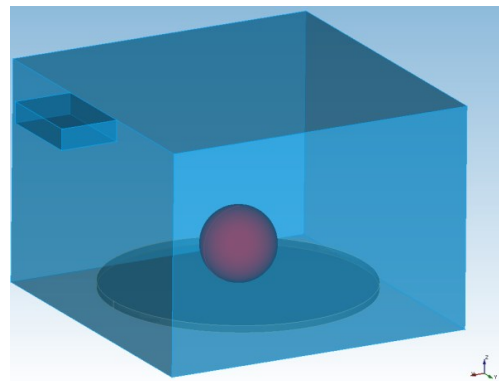
E-plane Y-junction by NRAO

after A. R. Kerr, Elements for E-Plane Split-Block Waveguide Circuits, ALMA Memo 381

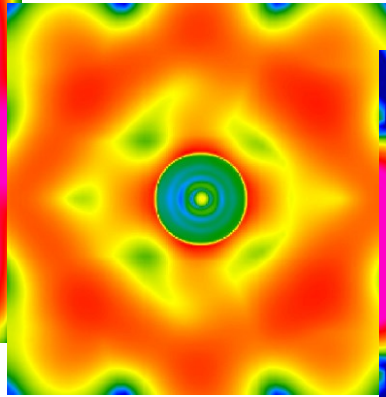
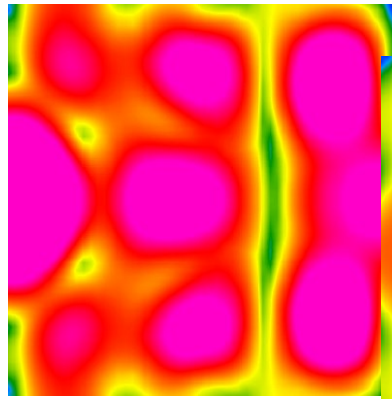


QuickWave modelling EM field interaction with tissues (for food processing & medical applicators)

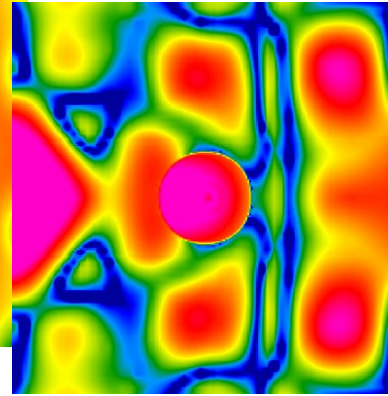
Separation of incident and diffracted fields (*option implemented per request of P.O.Risman, Malardalen University*)



E-field in an empty cavity

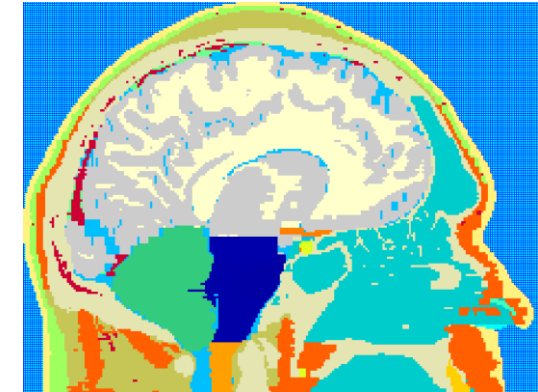


E-field in a loaded cavity

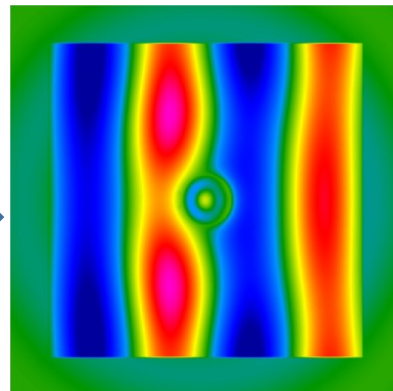
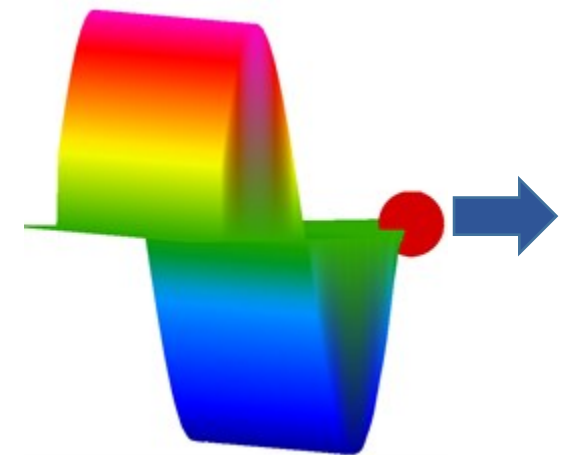


Scattered near-field in cavity

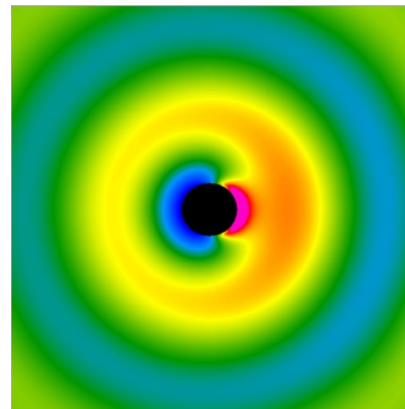
Detection of inhomogeneities in tissues



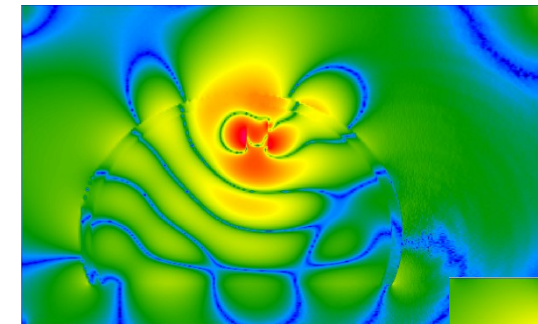
AustinMan model*
converted to
QuickWave EM
software for
Mälardalen
University, Sweden



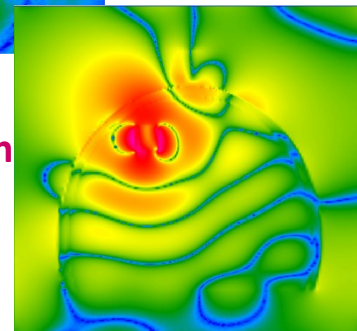
Total field
Focusing by the load
"exploding egg effect"



Diffracted field reveals
cause of focusing:
circumferential resonance



- ✓ Tumours & haemorrhages detection
- ✓ Optimisation of multiantenna tomographic systems

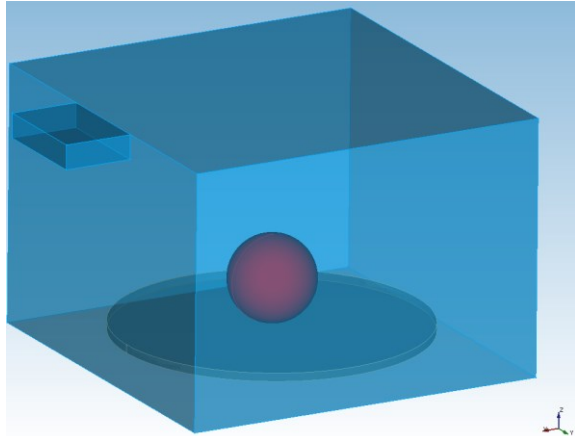


QWED

Illustration & cross-verification of QuickWave Multiphysics Regimes in Elsevier Book

Simple microwave heating benchmarks
& microwave heating phenomena studies*

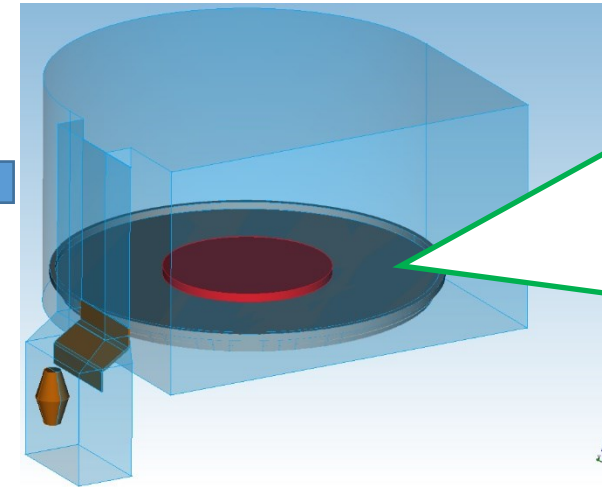
Design & analysis of real-life microwave oven cavities, incl.
complicated cavity shapes and advanced feeding system*



- heat transfer & load dynamics
- Load rotation & arbitrary movement during heating
- Source parameters tuning – regime for solid state sources
- Temperature dependence of material parameters

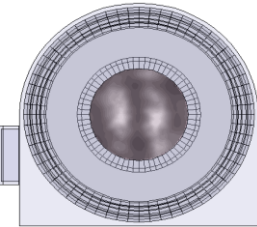
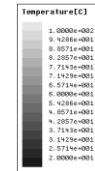
Freezing to file
the state of the
simulation

De-freezing on
arbitrary computer
& at convenient
time

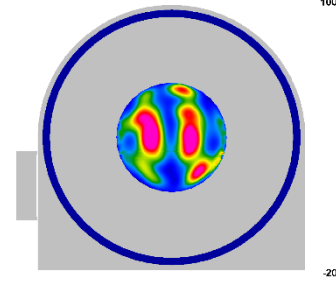


Courtesy of Whirlpool Inc. – Whirlpool MAX oven

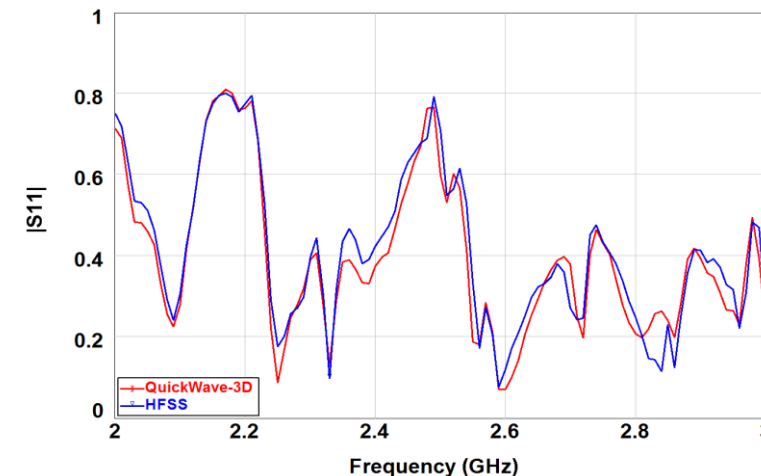
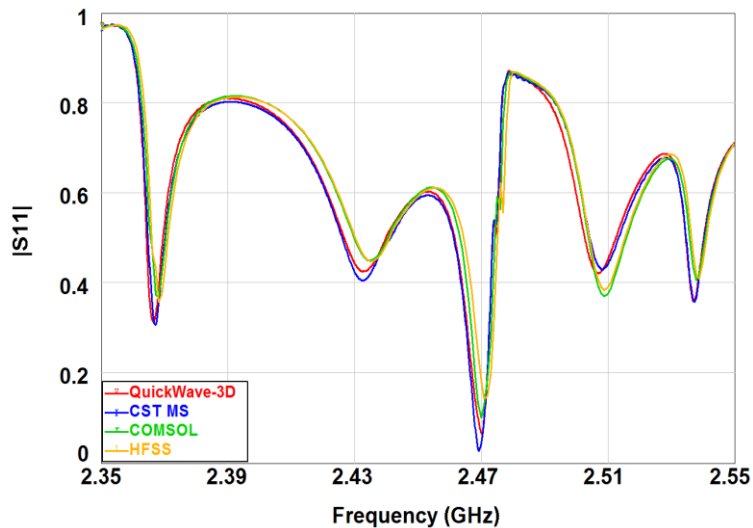
HFSS v11



QuickWave 3D & BHM

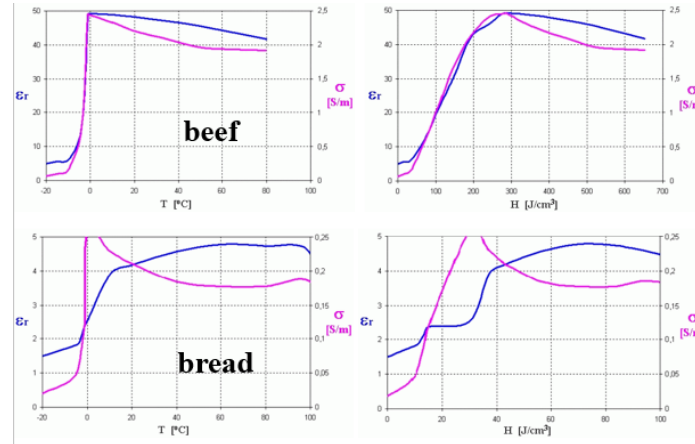
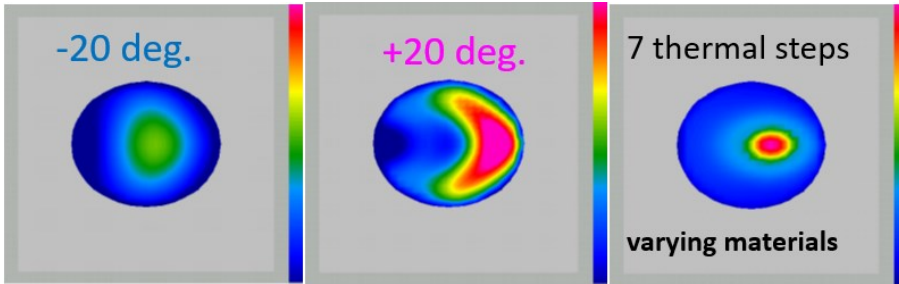


With QuickWave EM
computation as fast as
1 min 18s on a **low-cost
video card** – supporting
all graphic cards **with
OpenCL**



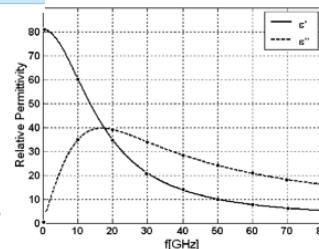
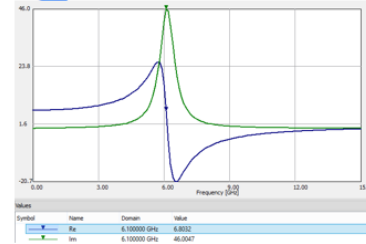
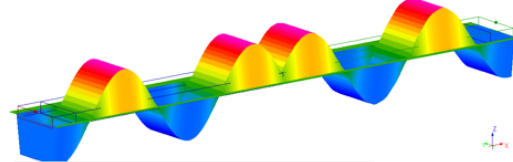
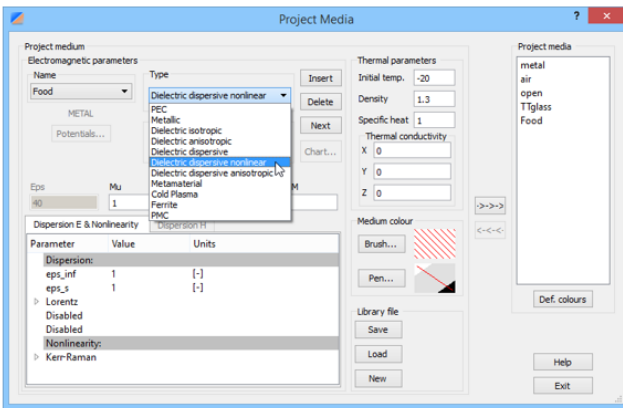
* M.Celuch, P.Kopyt & M. Olszewska-Placha in eds. M. Lorence, P. S. Pesheck, U. Erle, *Development of packaging and products for use in microwave ovens*, 2nd Ed. Elsevier 2020.

Materials' Characteristics in Microwave Engineering Design: REPRESENTATION



#Raw beef draft media file for QW-BHM module (00-09-06 POR)
 #Measurements & refinements by Per O Rismann, Microtrans AB, Sweden
 #Modified by QWED, Poland
 # DATA FROM -20 C to +80 C, dH/dV in J/cm3 reversedEnth/Temp column

Temperature # Data deg C	Enthalpy J/cm3	EPa	SIGa S/m	SpecHeat	Density	Ka
-20	0	4.9	0.064	2.21	1.06	0.0069
-15	14.0	5.5	0.093	2.21	1.06	0.0069
-10	34.4	6.1	0.153	2.21	1.06	0.0069
-5	71.4	12.3	0.573	2.21	1.06	0.0069
-3	110.4	22.0	1.118	2.21	1.06	0.0069
-2.2	144.4	30	1.636	2.21	1.06	0.0069
-1.6	192.4	42	2.113	2.21	1.06	0.0069
-1.3	240.4	46	2.385	2.21	1.06	0.0069
-1.1	274.4	48.9	2.426	2.21	1.06	0.0069
-1.0	288.4	49.2	2.440	2.21	1.06	0.0069
10	327.9	48.9	2.317	2.21	1.06	0.0069
20	382.9	48.2	2.194	2.21	1.06	0.0069
35	450.4	46.9	2.072	2.21	1.06	0.0069
50	517.9	45.5	1.949	2.21	1.06	0.0069
65	585.4	43.6	1.922	2.21	1.06	0.0069
80	652.9	41.7	1.908	2.21	1.06	0.0069



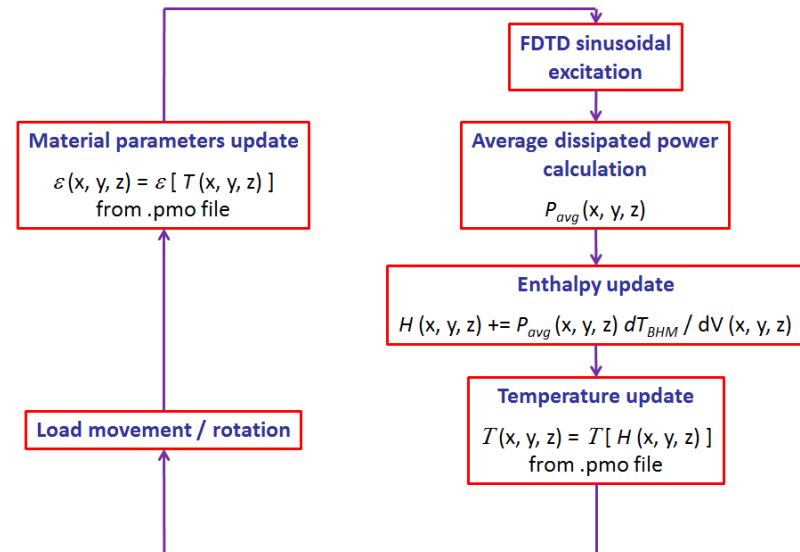
material parameters from equations

Drude: $\epsilon_r(\omega) = \epsilon_\infty + \frac{(2\pi f_p)^2}{(j\omega 2\pi\nu_c - \omega^2)}$

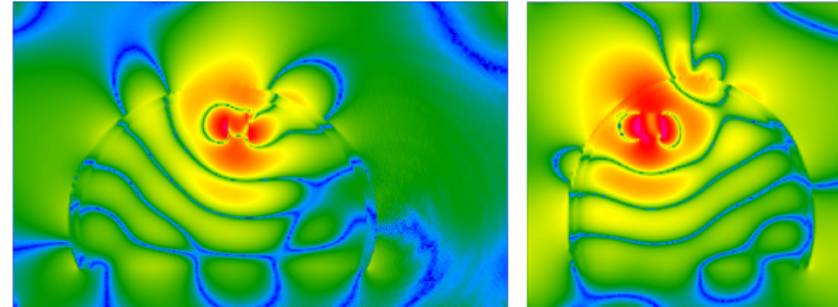
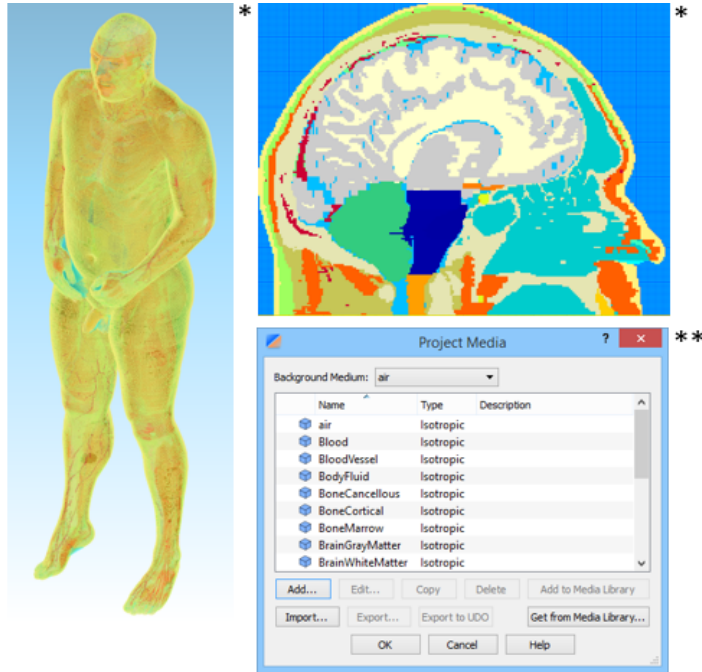
Debye: $\epsilon_r(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{(1 + j\omega\tau)}$

Lorentz: $\epsilon_r(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty (2\pi f_p)^2}{((2\pi f_p)^2 + j\omega 2\pi\nu_c - \omega^2)}$

text-files for a coupled EM-thermal process



Materials' Characteristics in Microwave Engineering Design: SOURCE of DATA

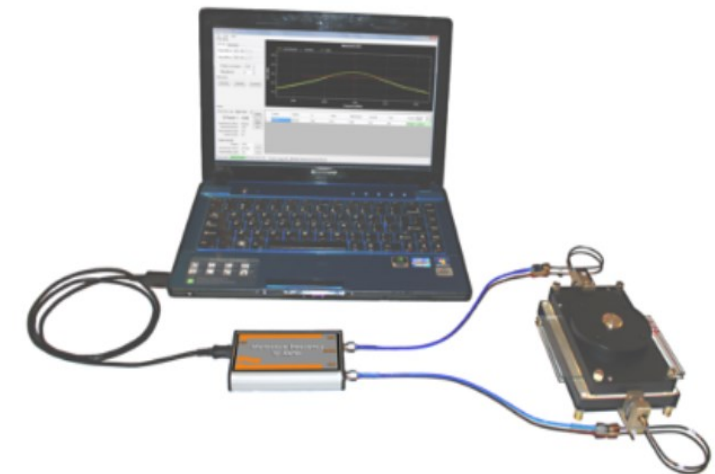


Detection of inhomogeneities in human tissues, e.g. tumours, haemorrhages

Design and development of diagnostic devices

Macroscopic parameters of tissues taken from a public database

Own (proprietary) measurements



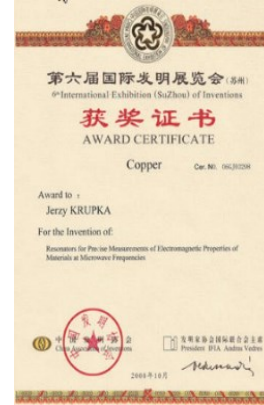
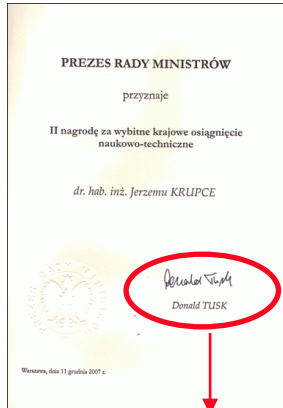
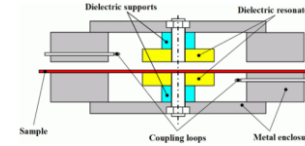
* AustinMan model (<https://sites.utexas.edu/austinmanaustinwomanmodels/>) converted to **QuickWave EM** software for Mälardalen University, Sweden

**D. Andreuccetti, R. Fossi, and C. Petrucci: An Internet resource for calculation of the dielectric properties of body tissues in the frequency range 10 Hz – 10 GHz. IFAC-CNR, Florence (Italy), 1997. Based on data published by C. Gabriel et al. In 1996. [Online]. Available: <http://niremf.ifac.cnr.it/tissprop/>

Origins of QWED Material Measurements

since 1980s...

awarded research of **Prof. Jerzy Krupka** (IEEE Fellow)
on dielectric resonators (best known: Split-Post Dielectric Resonator)



Agilent Both
IEEE IMS 2006, San Francisco, CA



MMA-2010, Warsaw PL
co-organised by QWED & Warsaw Univ.Tech.

... by early 2000s:

QWED commercialises the SPDRs
endorsement by Agilent / Keysight
publication of standard IEC 61189-2-721:2015

Popular Dielectric Resonators by QWED

SPDRs for laminar dielectric materials
typical units: 1.1 GHz -15 GHz



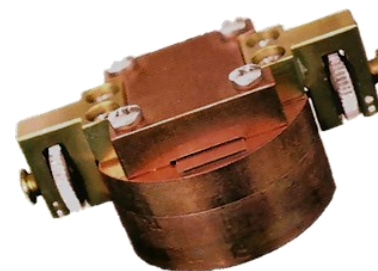
5 GHz SiPDR for resistive sheets



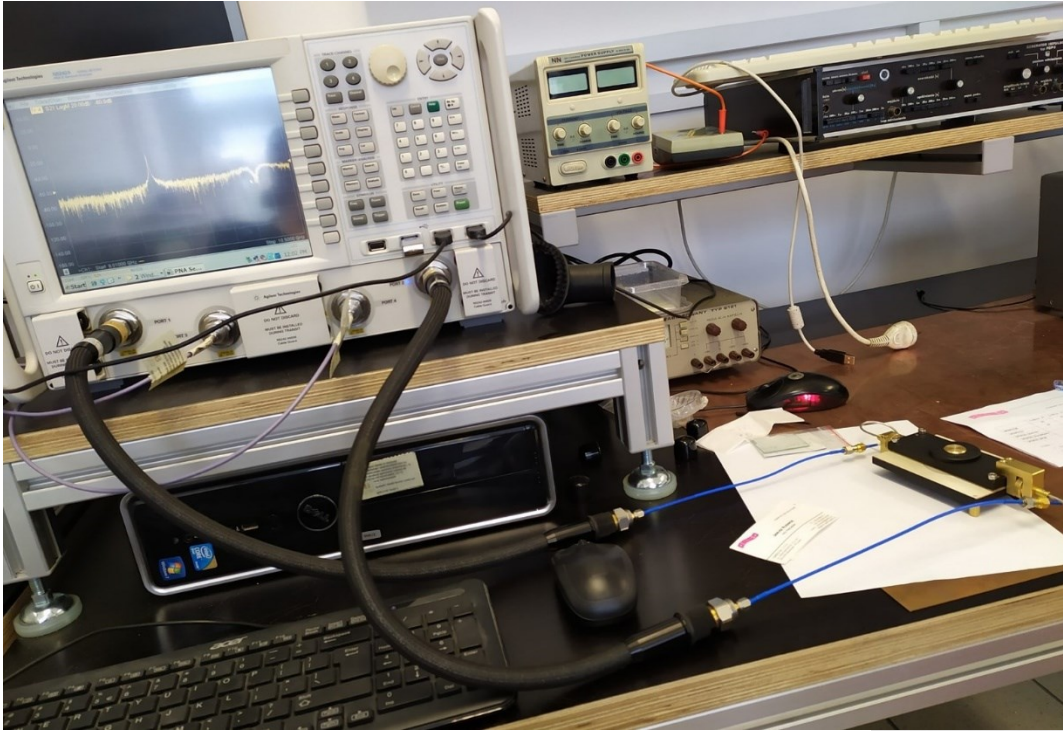
TE_{01δ} cavities, typically 1 – 10 GHz
for bulk low-loss dielectrics



modified SiPDR for graphene

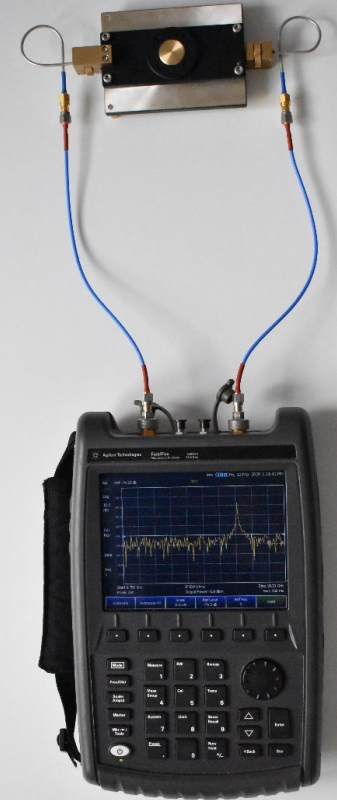
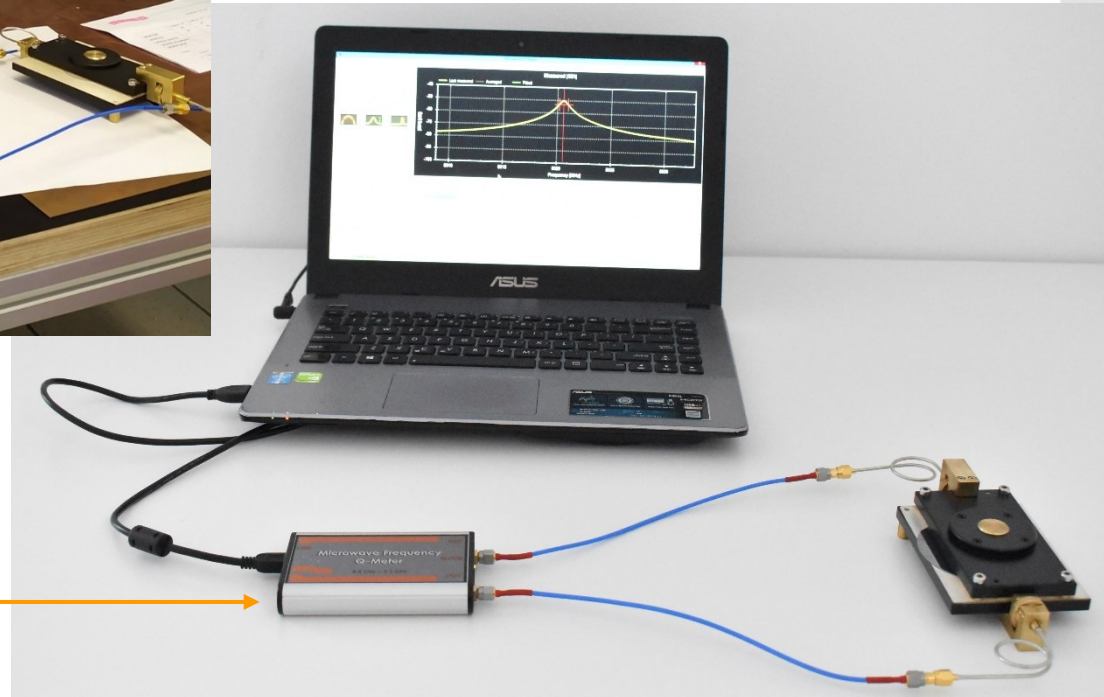


Resonators Operating in Different Setups

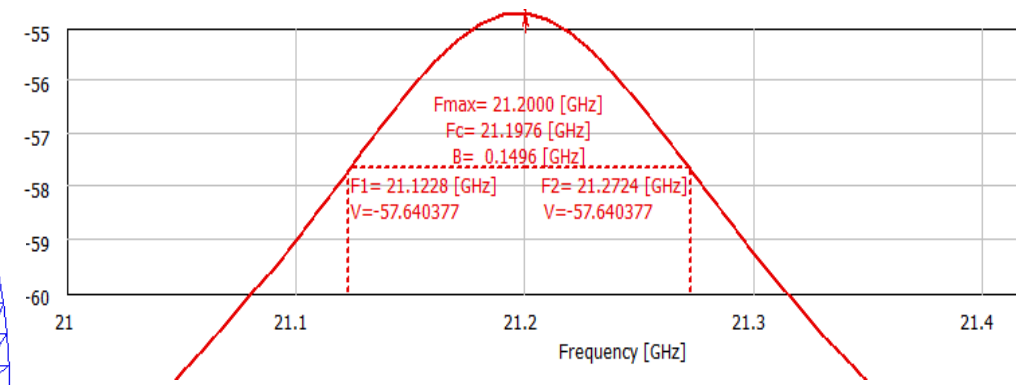
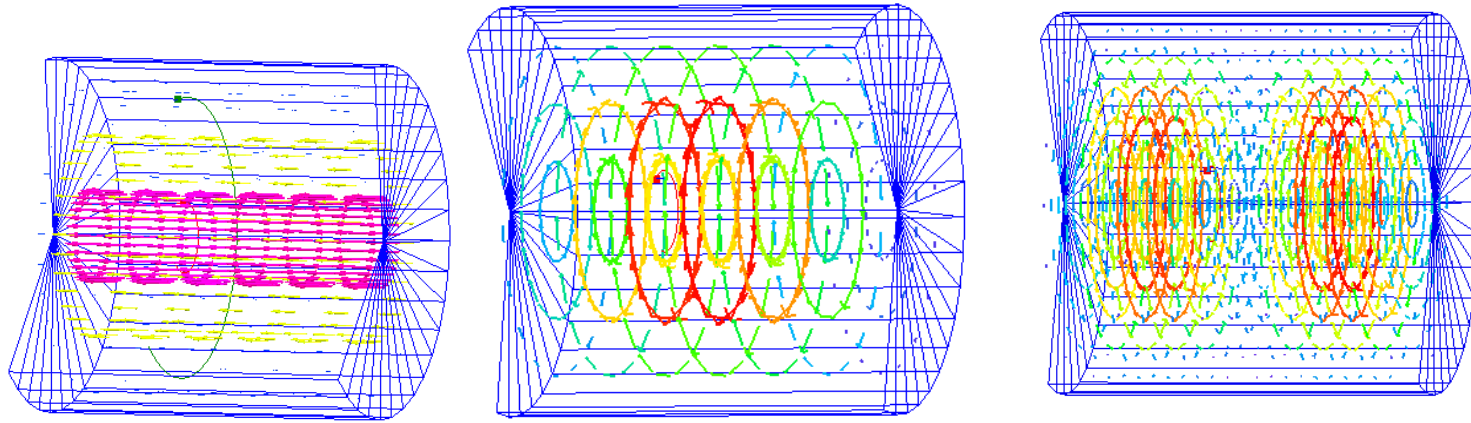


also for home-office!

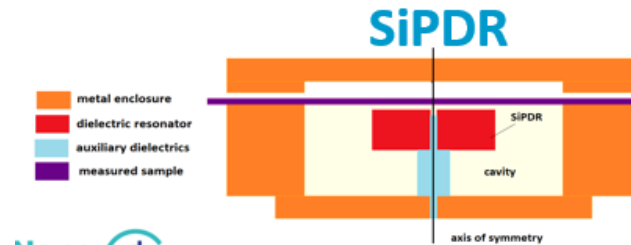
QWED Microwave Frequency Q-Meter
units for 5 GHz and 10 GHz



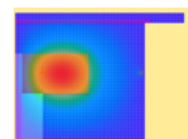
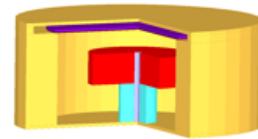
Where Modelling and Measurements Meet: Enhanced Design & Calibration of Resonators



Tutorial examples on
NanoBat Open Platform
<https://qwed.eu/nanobat.html>

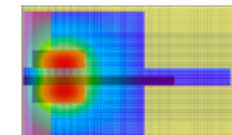
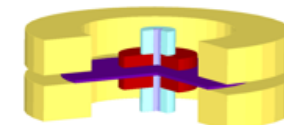
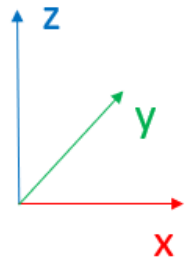
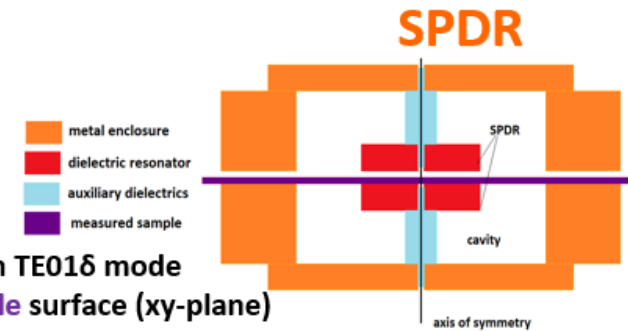


two configurations used with TE016 mode
E-field tangential (parallel) to **sample** surface (xy-plane)



E-field distribution
in the half cross-section

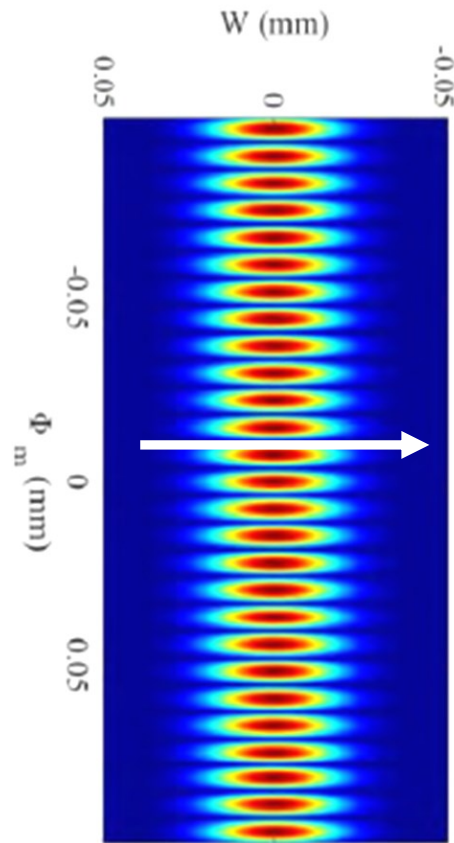
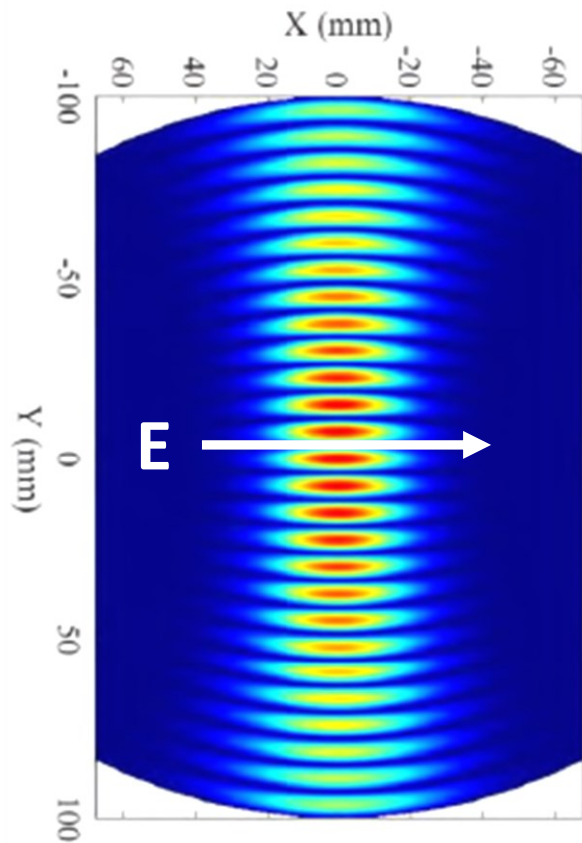
sample between the **single post dielectric** and the **ground plane**



E-field distribution
in the half cross-section

sample half-way between the **two dielectric posts** (in the "split" of the "post")

New: Fabry-Perot Open Resonator 20 – 110 GHz



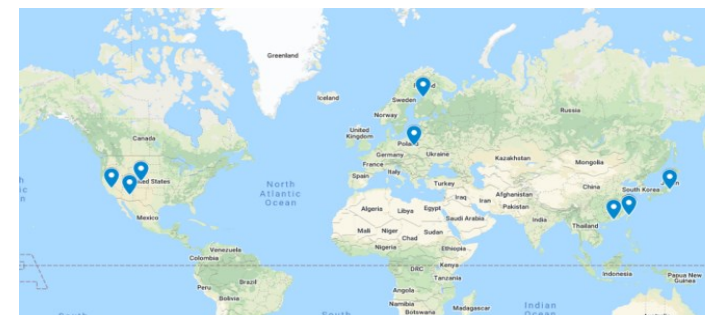
continuing the successful collaboration with Warsaw Univ. Tech. (Profs. J.Krupka, B.Salski, P.Kopyt)

Validation in iNEMI Round Robin - STRATEGY

Our project:



- | | | |
|--|--|---|
| <ul style="list-style-type: none"> 3M AGC-Nelco Ajinomoto USA AT&S Centro Ricerche FIAT-FCA Dell Dupont EMD Electronics (Co-Chair) Flex | <ul style="list-style-type: none"> Georgia Tech Showa Denko Materials IBIDEN Co Ltd IBM Intel Isola ITRI (Co-Chair) Keysight (Co-Chair) MacDermid-Alpha | <ul style="list-style-type: none"> Mosaic Microsystems NIST Nokia Panasonic QWED Shengyi Technology Company Sheldahl Unimicron Technology Corp Zestron |
|--|--|---|



Sample Material Requirements

- Stable, Low loss
- Low moisture absorption / temperature dependency
- Isotropic
- Good mechanical & handling properties

1st Project Stage

- Precision Teflon
- Cyclo Olefin Polymer

2nd Project Stage

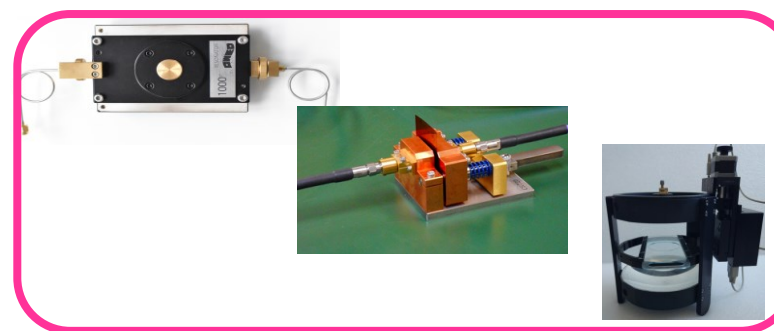
- Rexolite
- Fused Silica

Industrial

- Automotive

Techniques Included

- Split Post Dielectric Resonator
- Split Cavity Resonator
- Fabry-Perot
- Balanced Circular Disk Resonator

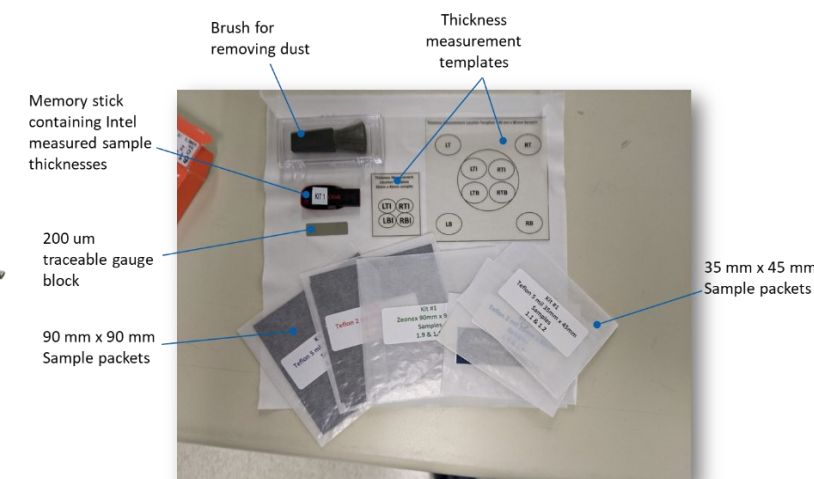
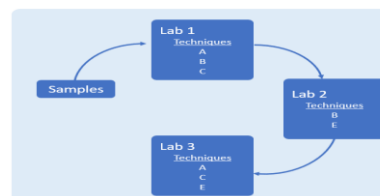


→ Frequency Span : 10GHz – 100GHz with overlaps

10 Sample Kits Created

- Sample sizes 35 mm x 45 mm, 90 mm x 90 mm
- circulated between 10 labs

10 Laboratory Round Robin



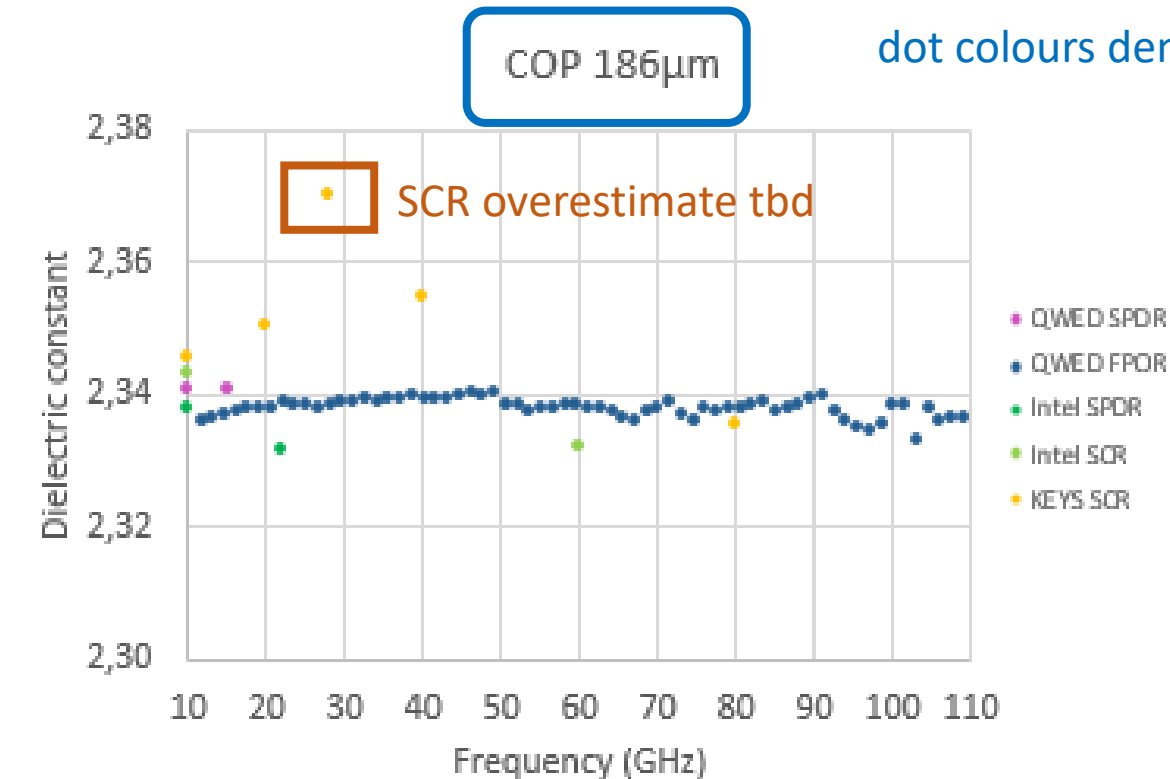
Validation in iNEMI Round Robin – EXAMPLE RESULTS

3 labs, 3 techniques, 14 laboratory setups

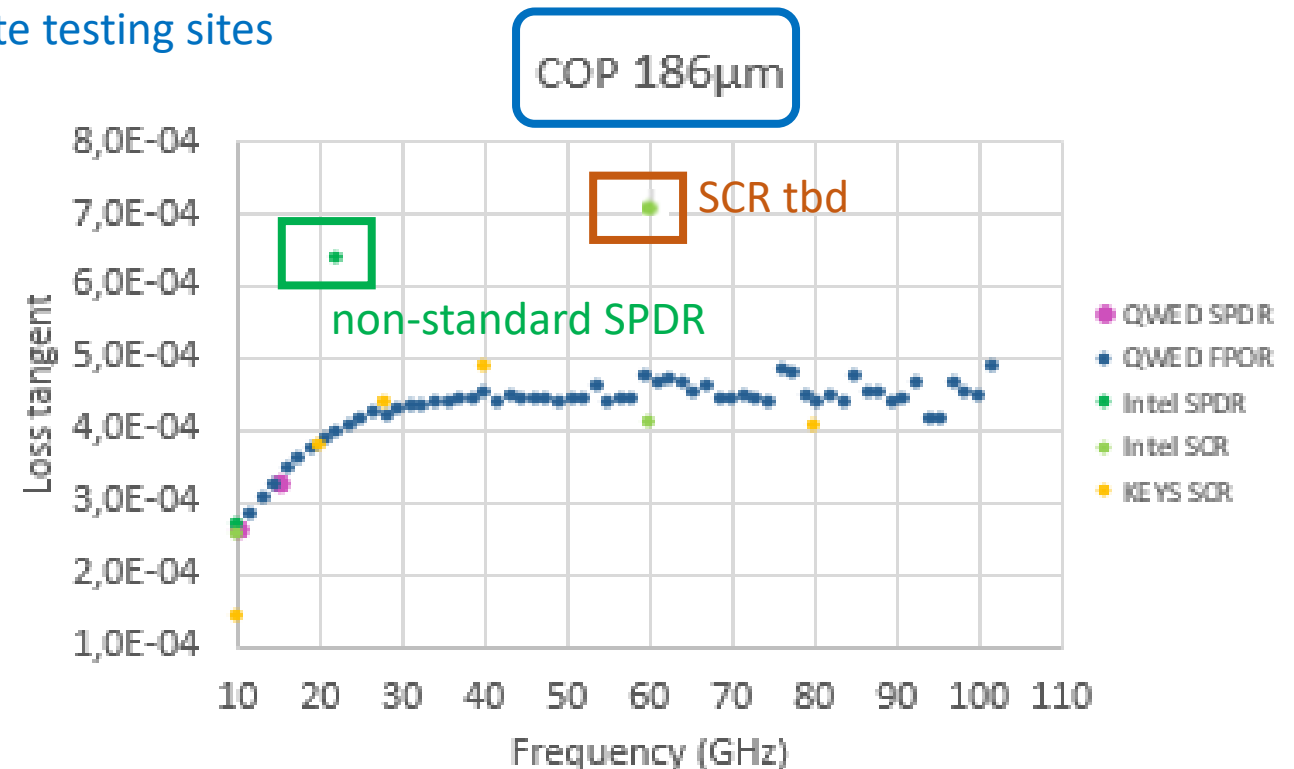
Intel - SCR at 10 / 60 GHz and SPDR at 10/ 20 GHz,

Keysight - SCR at 10 / 20 / 28 / 40 / 80 GHz

QWED - SPDR at 10/ 15 GHz and FPOR over 10-110GHz.

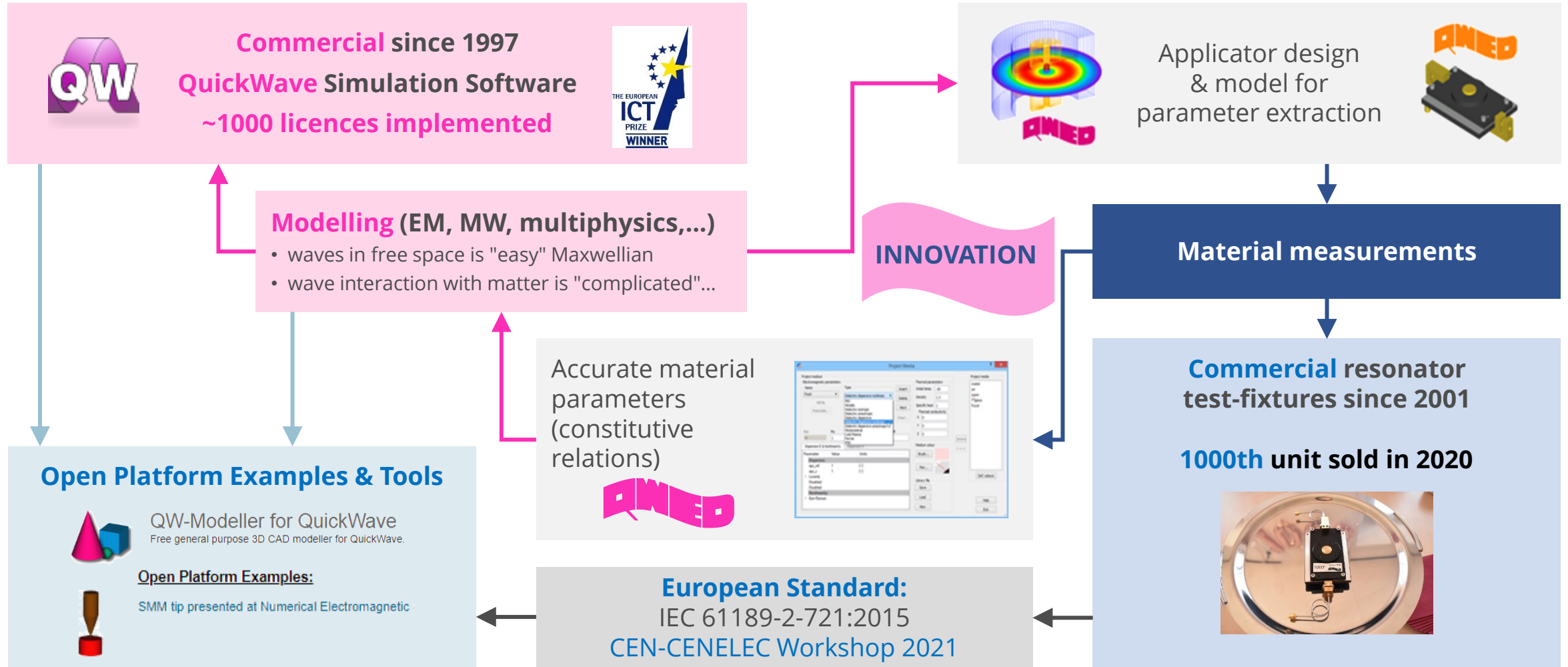


Dk spread < 1% (within $\pm 0.5\%$ from average)
(< 2% incl. outliers)



> 40GHz 2x increase in Df compared to 10GHz

Exploring Synergies between Computer Modelling and Material Measurements



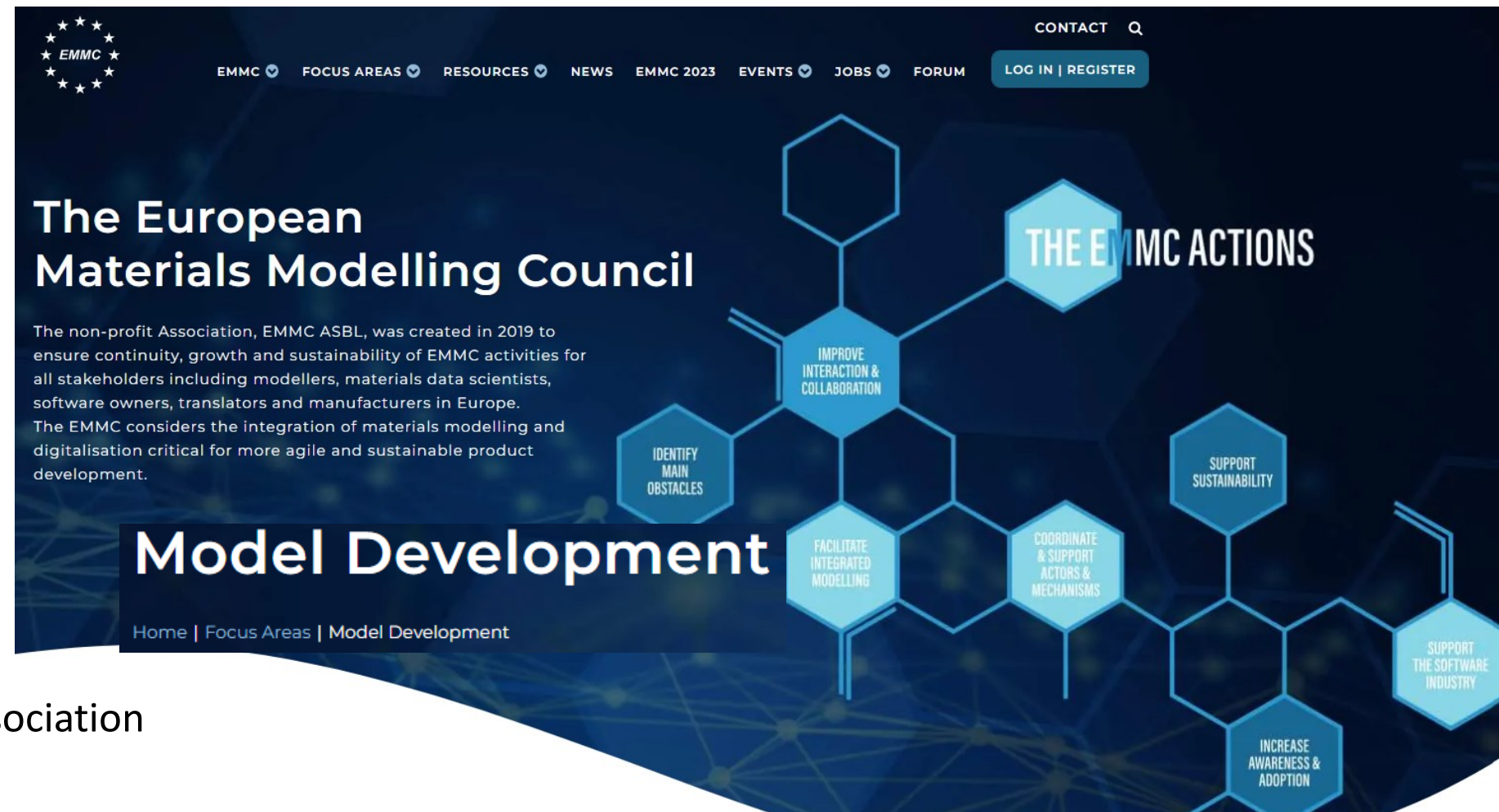
EU Initiatives - EMMC

<https://emmc.eu/>

2104: created
2016-2019: H2020 EMMC-CSA
→ EMMC ASBL not-for-profit association

EMMC considers the integration of **materials modelling & digitalisation** **critical** for more agile and sustainable **materials & product development**.

New and improved materials and the use of existing materials in **new applications** are a **key factor** for the success and **sustainability** of **European** industry and society in general.



Focus Areas



Model Development

Everything that has to do with the capabilities and qualities of the materials models and the modelling workflows: development, validation and application.

[Read more](#)



Digitalisation & Interoperability

Topics include the semantic foundation (from terminology to ontology), standardised documentation and cross-domain interoperability platforms.

[Read more](#)



Software

Successful materials modelling software uses the best algorithms, it is numerically robust, carefully validated, well documented, easy to use, and continuously maintained during decades.

[Read more](#)



Impact in Industry

This Focus Area is concerned with all aspects that play a role in the impactful use of materials modelling in industry, including People, relevant research and business Processes, Models use and simulations, and Data Infrastructures and Analysis.

[Read more](#)



Policy

The RoadMap recognises the importance of making advances in materials modelling and digitalisation of materials sciences to support the competitiveness of European industry.

[Read more](#)

EMCC Focus Areas

Model Development

[Home](#) | [Focus Areas](#) | [Model Development](#)

Objectives

- Promote the use of materials modelling in industry
- Promote actions and activities to enhance the capabilities of materials modelling

Leading Team

Chair: [Kersti Hermansson](#) (*Uppsala University, Sweden*)

Co-chairs: [Malgorzata Celuch](#) (*QWED, Poland*) [Maria Alfredsson](#) (*University of Kent, UK*)

Task Groups

TG 1.1 - Linking and Coupling
Computational Chemistry to
Electromagnetics



EU Initiatives - EMCC

<http://characterisation.eu/>

2014
European Materials Characterisation Cluster

2016
European Materials Characterisation Council

initiative, not a legal body



European Materials Characterisation Council (EMCC)

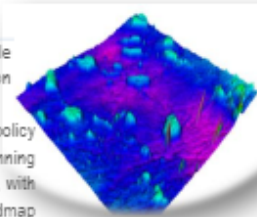
Scope

Characterisation is a central pillar across the spectrum from research development via engineering and upscaling to production and product quality control. A survey of 100 FP7 projects carried out in 2014 under the umbrella of the Engineering & Upscaling Cluster clearly demonstrated the central role of characterisation. Over 90% of projects apply characterisation methods and 50% of projects include characterisation developments. Characterisation was ranked by far the highest in terms of importance of engineering and upscaling with an average across all projects of 9/10, compared to averages of below 7/10 for modelling and standardisation for example. A lot of these projects however have a weak link to the impact required by the EC, with little tangible output in relation to commercial exploitation or reliable recommendations to regulation. There is therefore the need to set up a European Materials Characterisation Council (EMCC) in order to support commercialization and regulation through the provision of characterisation tools.



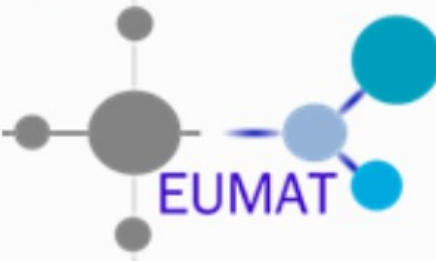
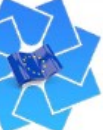
Objectives

- To support establishing a community of European stakeholders in the process of developing and improving characterisation tools in order to bring the development of nanomaterials and advanced materials in Europe into end products more successfully.
- To gather the needs and requirements of that community for characterisation tools and supporting actions.
- To provide a forum for discussion, problem solving and planning R&I activities in Europe.
- To establish the formation of standard methodologies on nanocharacterization in Europe, and create a common background.
- To create a platform for nanocharacterization, with the attempt to act with Open Research Data.
- To link nanometrology with in-situ monitoring and industrial needs.
- To provide a suitable background for regulation and nanosafety.
- To support EC policy development, underpinning the relevant EC priorities, with a stakeholder driven roadmap for characterisation techniques for engineering and upscaling of nanomaterials and advanced materials in Europe. This activity is to support the strengthening of Europe's industrial capacity and competitiveness and thus contributes to the main objectives of the LEIT-NMBP programme.



Stakeholders

- Materials manufacturers and integrators
- Manufactures of analytical instruments
- Standardisation bodies and metrology institutes
- Materials scientists divided into sub-groups according to the main specific expertise (microscopy, spectroscopy, surface and interface characterisation techniques, etc.)







Typical materials model descriptions ...

- By **phenomena (application)**:
 - "I have a mikro-kinetics model."
- By **scale** of the phenomena:
 - "I have a mesoscale model."
- By name of the **software (code)**
 - "I use the Uppsala model"
- By **solver**:
 - "I have a FE model"



The European Materials Modelling Council

Materials Modelling – Characterisation Solutions Proposed by EU Initiatives

- Communication tool: capture and convey application of modelling and characterisation
 - To wider audience of scientists and engineers
 - Complex characterisation or modelling process shown "in a nutshell", visible "at a glance"
- Standard documentation
- Potential to use in Data Management and as Supplementary Material in Publications: standardised form means better quality control
- Widely agreed terminology and classification a first step to digitalisation



2015: EMMC works on MODA

MODA - Description & use cases

Modelling Data

In a CEN Workshop Agreement, CWA 17284 "Materials modelling - terminology, classification and metadata", several stakeholders formally agreed on:

Terminology used to describe materials modelling

<https://emmc.eu/moda/>

2018: EMMC CEN/CWA 17284

CEN

WORKSHOP

AGREEMENT

CWA 17284

April 2018

ICS 01.040.35; 35.240.50

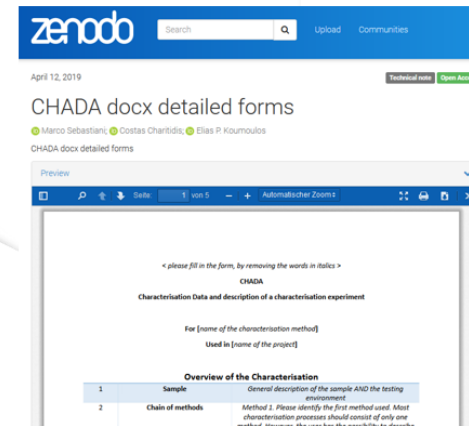
English version

Materials modelling - Terminology, classification and metadata

https://emmc.info/wp-content/uploads/2018/05/CWA_17284.pdf



2019: EMCC works on CHADA



<https://zenodo.org/record/2637419#YbMXUyYxm9I>

2021: CEN/WS 'OYSTER on Materials characterisation - Terminology, classification and metadata'

The Workshop and the related CWA provide standardised terminology that will improve future exchanges among experts in the entire area of materials characterisation, facilitate the exchange with industrial end-users and experimentalists and reduce the barrier to utilising advanced materials characterisation.

The common language is expected to foster dialogue and mutual understanding between industrial end-users, equipment manufacturers, and academic researchers. Standardisation of terminology and classification has been identified as critical to collaboration in and dissemination of European research projects. In particular, standards will facilitate interoperability between methods and databases. The standardization is relevant for an integrated technological development and brings benefits for industrial end-users due to simplified and much more efficient communication in the field of materials characterisation. The classification helps data interpreters by translating industrial problems into problems that can be analysed with characterisation methods. It assists workflow development where several methods can interoperate in addressing a specific end-user question.

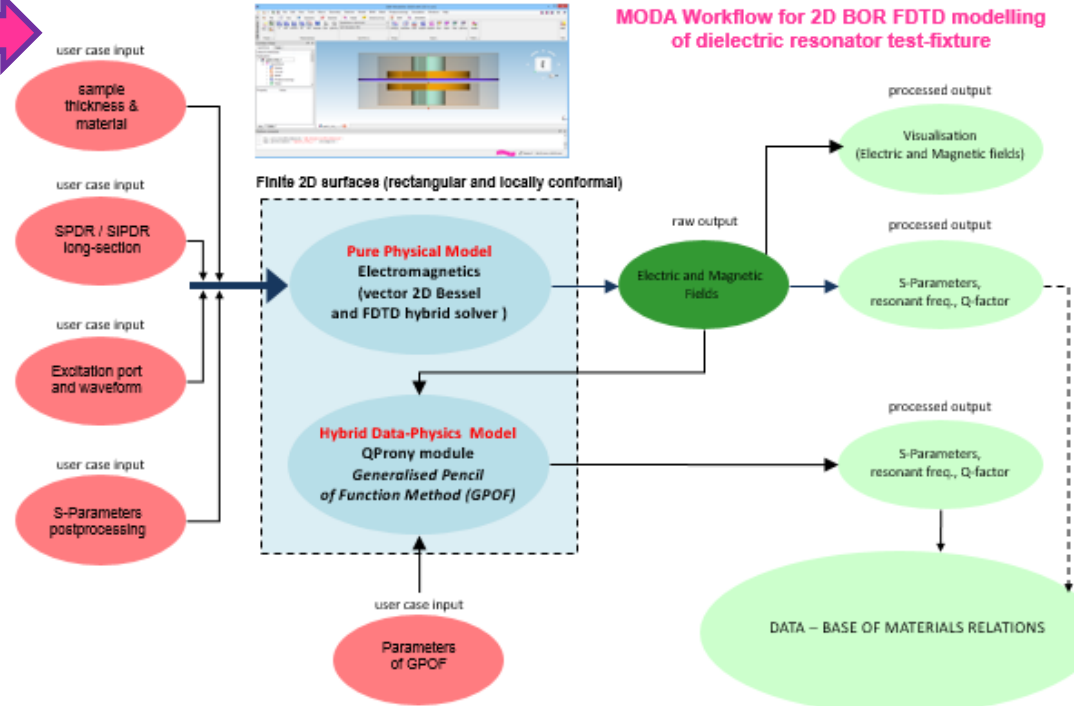
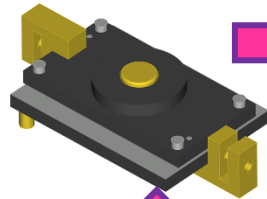
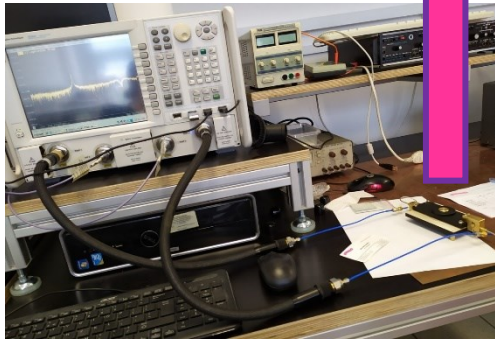
- Draft CWA 'Materials characterisation - Terminology, classification, and metadata' (pdf)
- Commenting form (word)
- Project Plan (pdf)

<https://www.cencenelec.eu/news-and-events/news/2021/workshop/2021-06-23-cen-ws-oyster-materials-characterisation/>

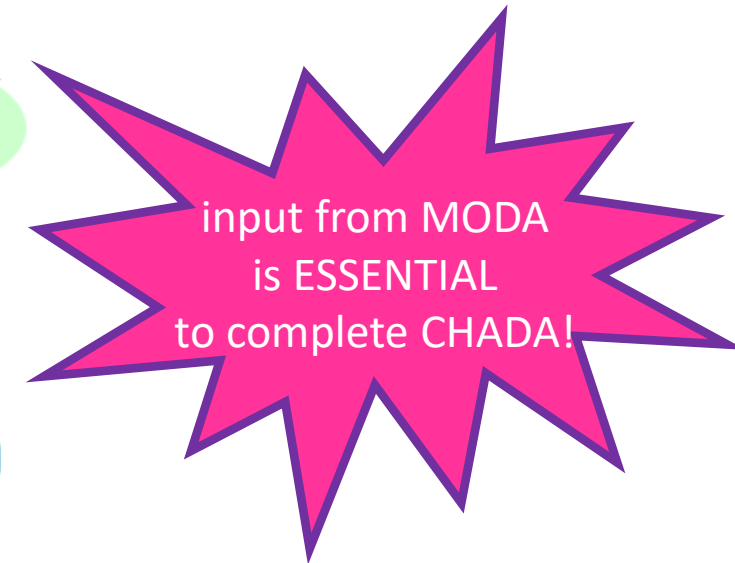
Twinned MODA + CHADA Example by QWED



MODA

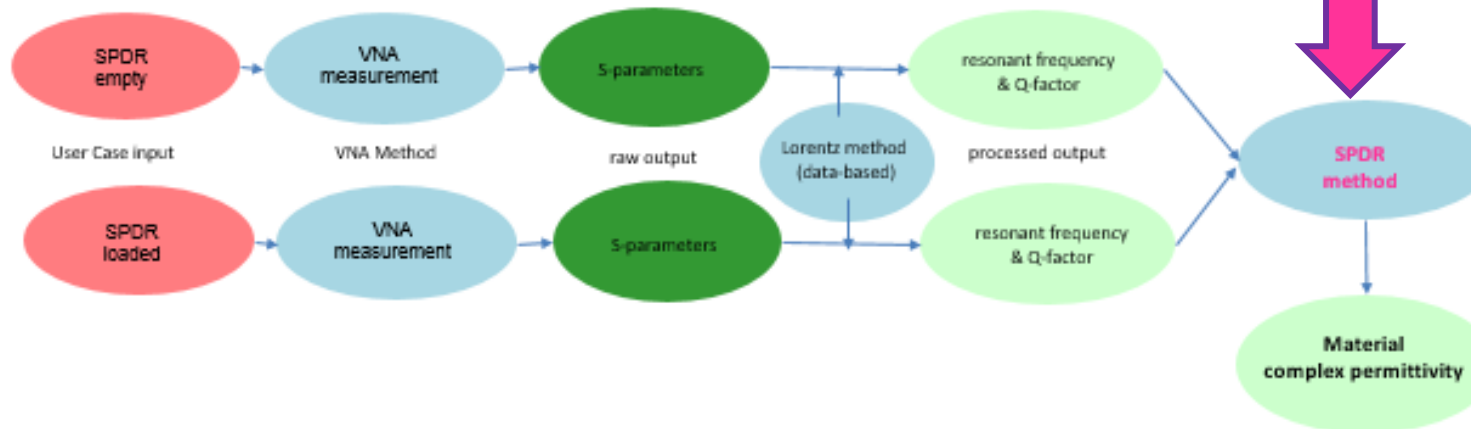


...more physics behind...

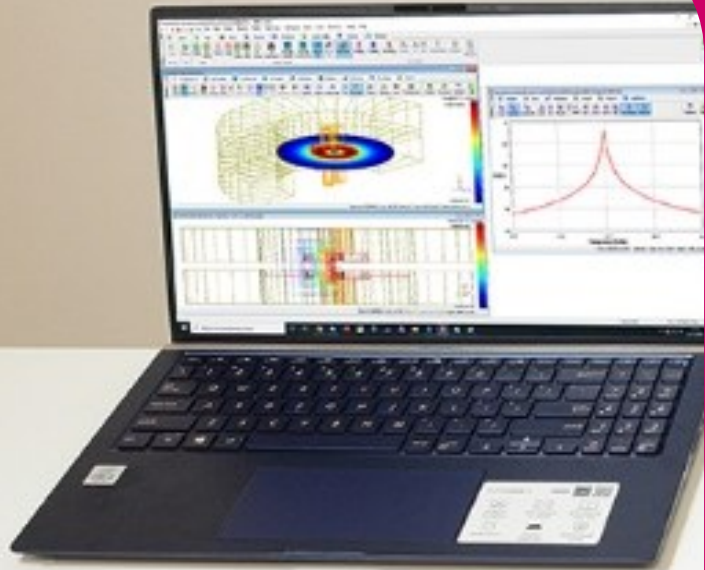


CHADA

CHADA Workflow for material measurement with dielectric resonator test-fixture

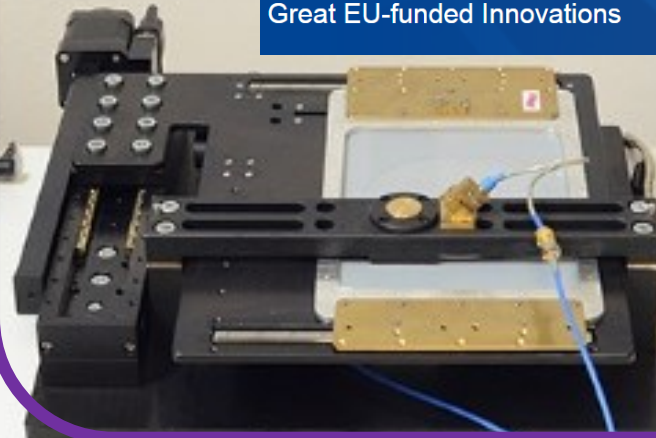


Twinned MODA + CHADA Implementation by QWED



**QuickWave™
by QWED**

<https://www.innoradar.eu/resultbykeyword/qwed>



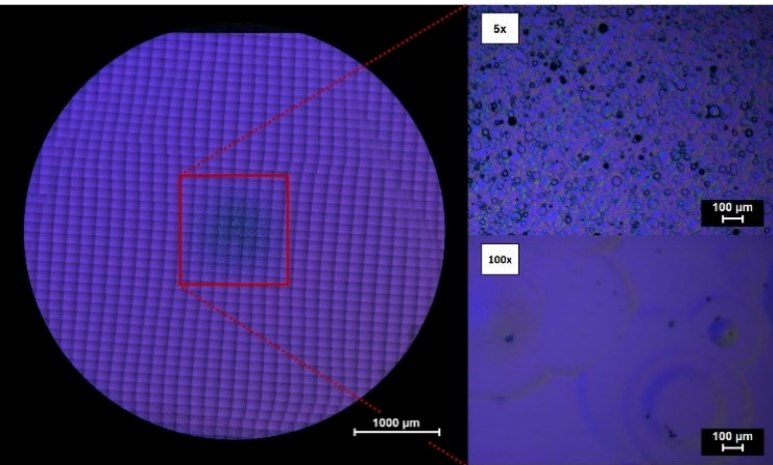
10GHz Q-Meter by QWED



Finalist of the European Innovation Radar Prize 2021

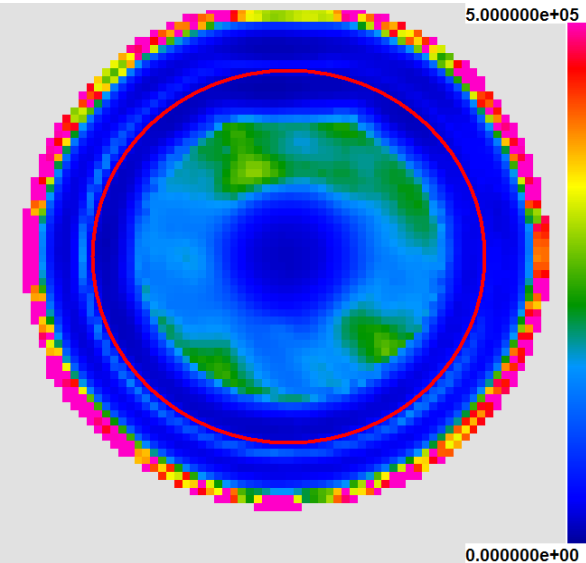


2D SPDR Imaging of HR- GaN for Light & Power Electronics Devices



Optical microscopy image at L-IMiF reveals morphology inhomogeneity in the central area:

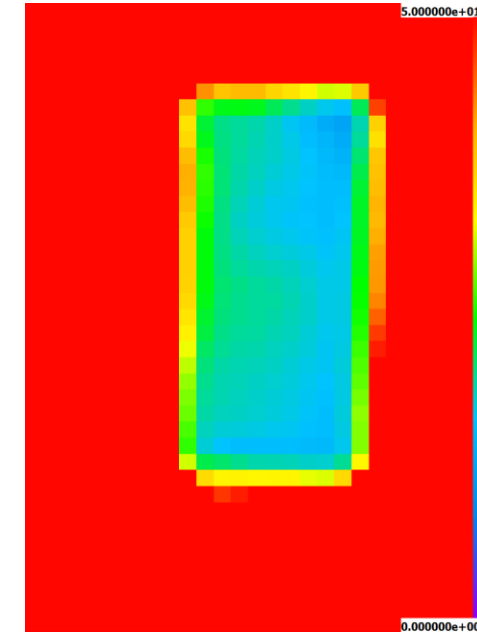
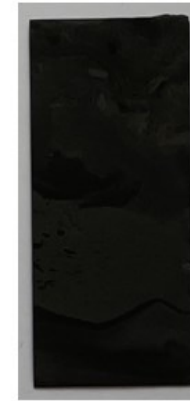
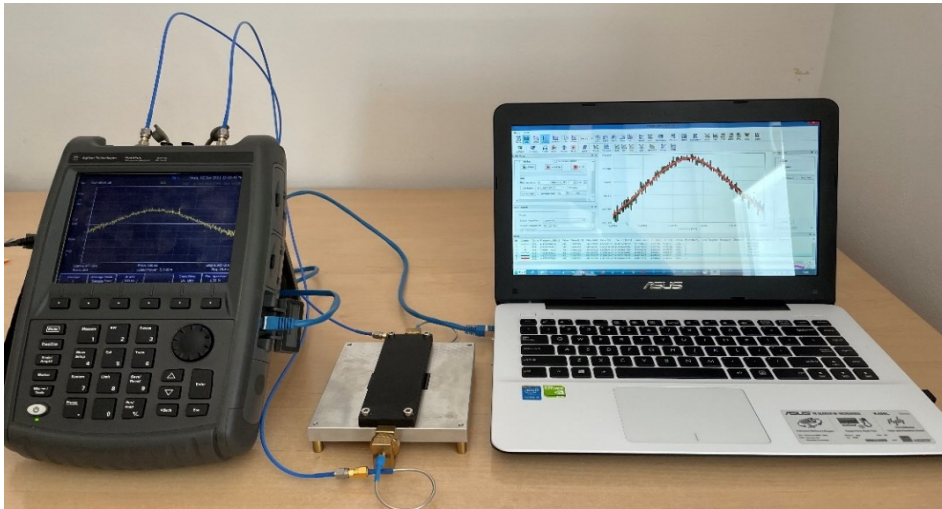
- in qualitative terms only,
- attributed to non-uniformity of the growth,
- only the central part appears useless for making devices.



SPDR image:

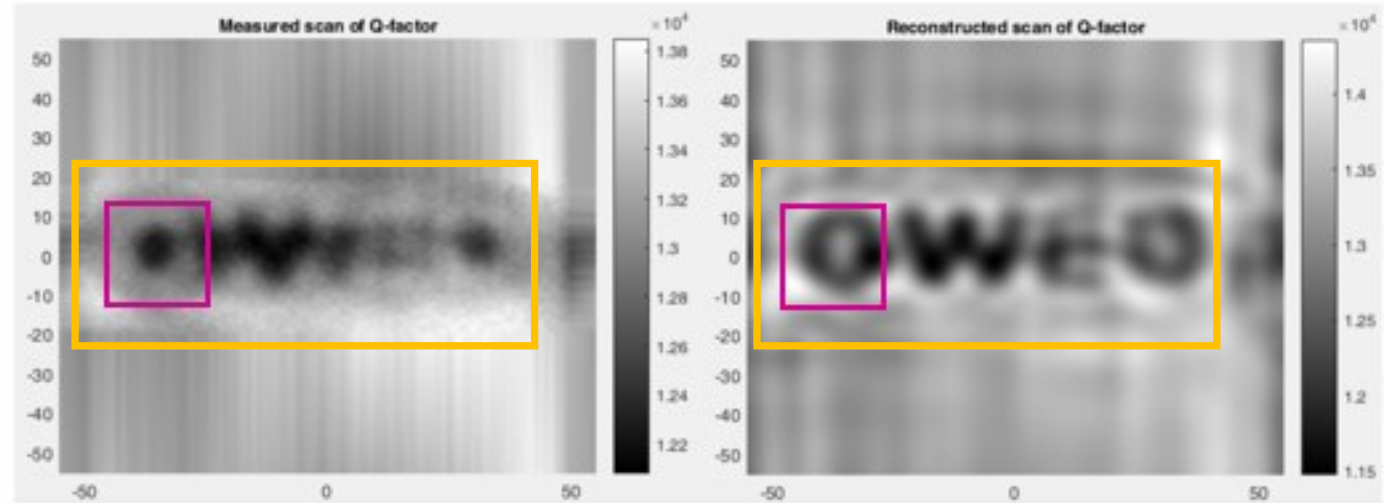
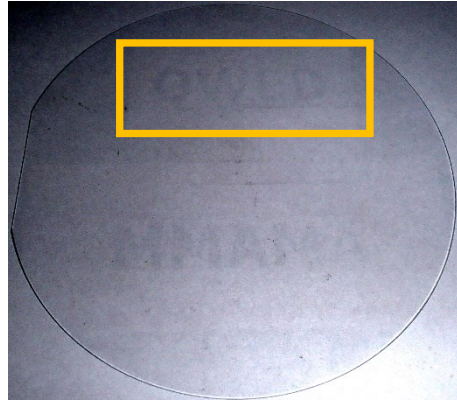
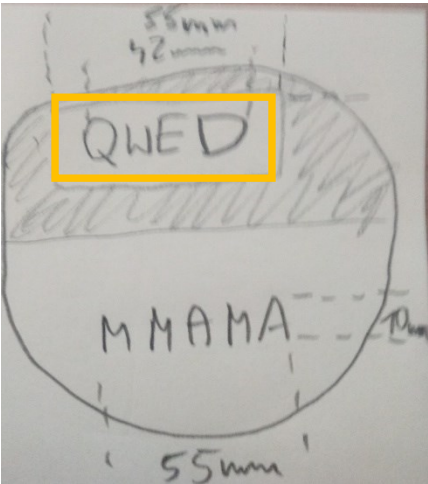
- shows this whole GaN template unusable,
- quantitative evaluation:
 - edge ring inherent to so-called edge effect,
 - ca. $2 \cdot 10^4 \Omega\text{cm}$ in the centre (dark blue),
 - ca. $5 \cdot 10^4 \Omega\text{cm}$ along the inner ring (light blue),
 - up to $1.2 - 3 \cdot 10^5 \Omega\text{cm}$ across outer SUT's area (blue-green),
 - edge effect along the circumference.

2D Imaging of Conductive Films – Application to Graphene Anodes



- ❑ Scanning area: 50 mm x 75 mm (25 mm margin around SUT)
- ❑ Uniform scanning step: 2 mm
- ❑ 1014 measurement points
- ❑ Avr thickness of the deposited graphene anode layer: 0.130 mm $\pm$ 0.02 mm
- ❑ Non-uniformities in R_s map due to sample thickness variation
- ❑ R_s extracted for average thickness value
- ❑ An absolute value of R_s can vary within uncertainty of $\pm 15\%$
- ❑ Avr R_s of 19.3 $\Omega/\text{sq.}$ in exact agreement with point-wise 5GHz SiPDR device.

Modelling-Based Resolution Enhancement of Surface Images



raw image of sample resistivity
(measured Q-Factor)

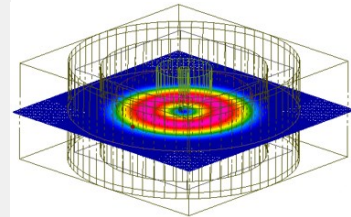
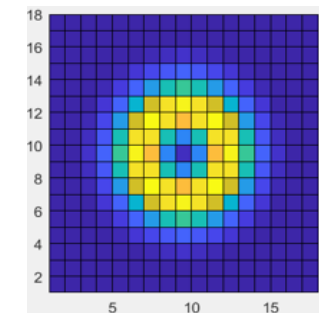
image further deconvolved
using SPDR field pattern
pre-simulated in QuickWave



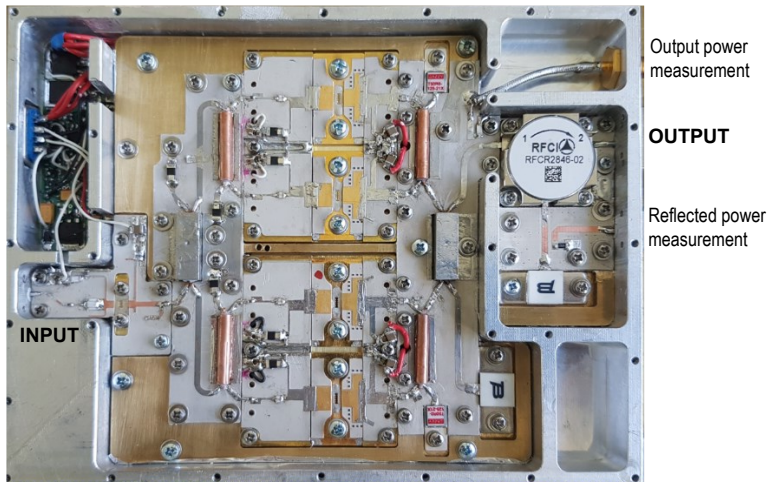
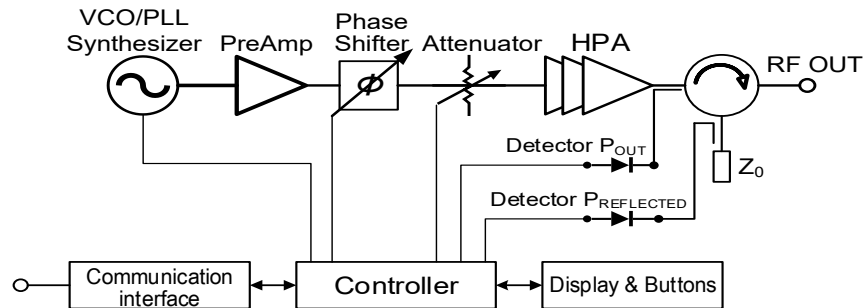
Patterned PEDOT:PSS sample
courtesy MateriaNova, Belgium



2D SPDR scanner

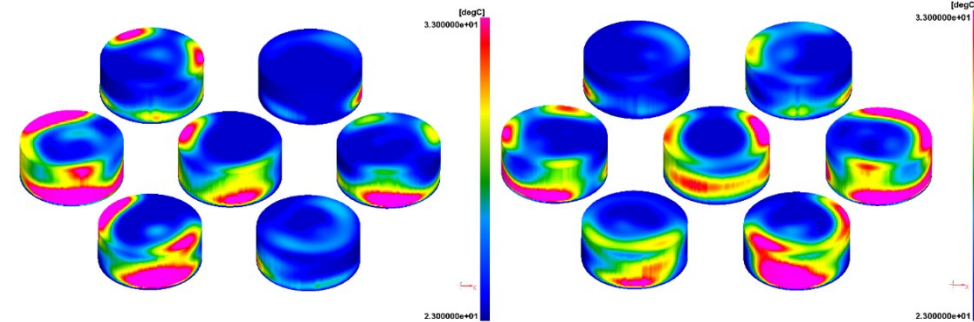


Active - Passive Methodology for Multiphysics Design

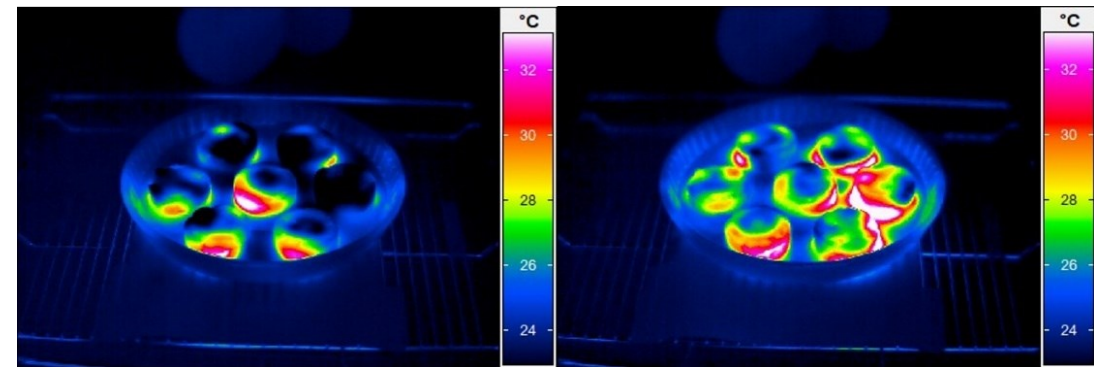


Multifunctional heating source
based on two-stage double-balanced GaN HEMT HPA
(Prof. W.Wojtasiak, Dr. D.Gryglewski Warsaw Univ.Tech.)

Temperature in mashed potato cookies, after 60 s of heating ,
for different relative phase shifts (added 110 degrees) between two sources.
(*Development of packaging and products for use in microwave ovens*, Elsevier, 2020)



QuickWave modelling by QWED



Photos courtesy BSH HAUSGERATE GmbH,
Traunreut, Germany.

B/S/H/



EU Initiatives – Joint EMMC & EMCC Reports & Input to Horizon Europe



2020 : Input for the work programme Horizon Europe in **empowering the cooperation between materials' characterisation and materials' modelling**.

This is well reflected in both **RoadMaps**.

Topic title: [Advanced materials modelling and characterisation](#)

Expected outcomes: To increase the efficiency and effectiveness of materials and product development by creating a digital continuum including materials modelling (data and physics based as well as engineering modelling), characterisation (material properties/functionalities) and safety, all supported by artificial intelligence or machine learning.

Scope: The action should investigate the development of advanced materials by rational design, with focus on the combination of theory with large-scale computational screening (e.g. Artificial Intelligence or Machine Learning). The validation by experimental methods should be included. The action should cover domains of the Green Deal Strategy (e.g. decarbonising industries or sustainable materials).



Working Groups

WG 3 Characterisation Data and Information Management.

WG 3.1 MODA & CHADA interaction with EMMC.



Report on Advanced materials modelling and characterisation: strategies for integration and interoperability

EuroNanoForum 2021 Satellite Event, 4th May 2021

Published in June 2021

DOI: [10.5281/zenodo.4912683](https://doi.org/10.5281/zenodo.4912683)

<https://zenodo.org/record/4912683#.YbH2USYxm9I>

EU Open Exchange of Ideas - EMMC International Workshops



In preparation:



<https://www.youtube.com/watch?v=jihszf4FD3o>



Javier Sanf lix



Yanaris Ortega Garcia

4th EMMC International Workshop

Vienna, 26-28 April 2023

<https://emmc.eu/emmc-2023/>

#EMMC2023

Materials & Digitalisation: the backbone of the Green Transition

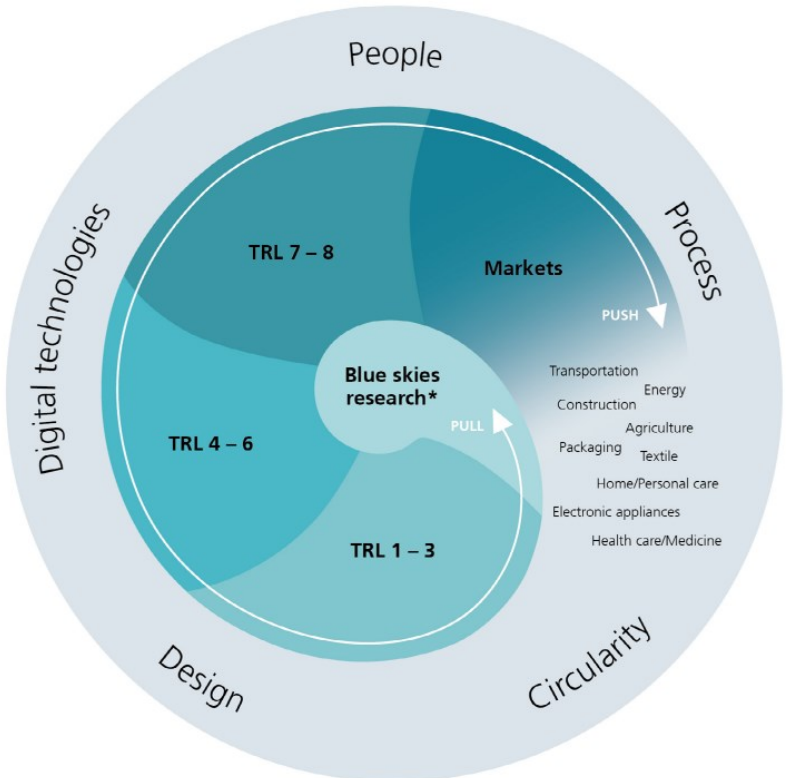
Participation & collaboration ideas welcome!



7 February 2022

<https://www.ami2030.eu/>

A strong European Materials ecosystem drives the green and digital transition as well as a sustainable inclusive European society through a systemic collaboration of upstream developers, downstream users and citizens and all stakeholders in between.



Microwave Theory & Technology ↔ Materials' Science & Technology



EU's key funding programme
for research & innovation
budget of €95.5 billion

https://ec.europa.eu/info/funding-tenders/find-funding/eu-funding-programmes/horizon-europe_en#documents



Microwave Theory & Technology ↔ Materials' Science & Technology



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https://ec.europa.eu/info/funding-tenders/find-funding/eu-funding-programmes/horizon-europe_en#documents



- a key to a project success
is the project's CONSORTIUM
- CONSORTIA building is now starting
for new Horizon Europe calls
- partners are specifically sought
in new RELEVANT applications
- Ukraine has full rights to participate
as an ASSOCIATED COUNTRY
- Marie Skłodowska-Curie Actions (MSCA)
Doctoral Networks & Postdoctoral Fellowships
are also a good way to get involved

Take-Away Messages

1. Behind every CHARACTERISATION there is always a MODEL

...but unfortunately people often prefer not to think of it

2. MODELLING increasingly replaces CUT & TRY prototyping

...but the resulting prototype must be experimentally CHARACTERISED

3. Twinned MODA+CHADA will facilitate:

- **not only the USE in modelling in industry, but also the TRUST in it,**

- **not only managing NUMBERS, but also understanding of the PHYSICS behind,**

**4. The European focus is on NOVEL MATERIALS,
with development accelerated by harmonised MODELLING+CHARACTERISATION.**

THANK YOU!

15:00-17:00 Session **WIE**: 2nd Ukrainian Microwave Week: Women in Engineering meeting

CHAIR: [Malgorzata Celuch](#) (QWED Sp. z o.o., Poland)

LOCATION: [Plenary Zoom Room](#)



Join the Women in Engineering Meeting,
UkrMW, Thursday afternoon,
for discussion on IEEE & EU initiatives

