discover accurate EM modelling

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

The National Centre for Research and Development

M-ERA.NET

NanoBat

iNEMI International Electronics Manufacturing Initiative

I4Bags

ULTCC6G_EPac

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

European Commission

Horizon 2020 Research and Innovation programme

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

HORIZON EUROPE

Marie Skłodowska-Curie Actions

M-era.Net

European Materials Modelling Council

European Materials Characterisation Council

AMI2030 ADVANCED MATERIALS INITIATIVE

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

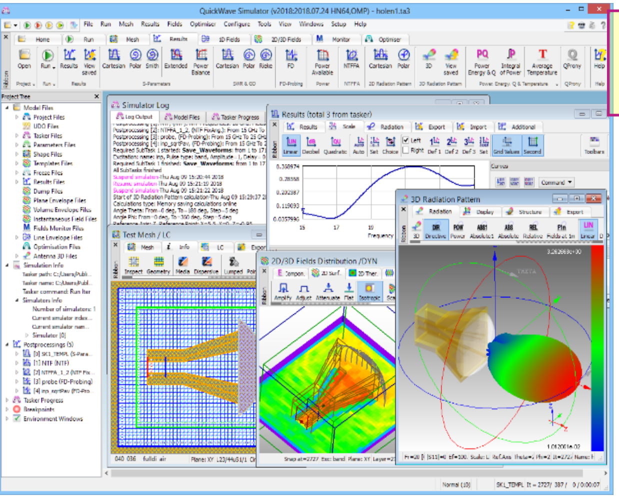
Dr. Maciej Sypniewski
Senior in CAE
- 35 years of experience in engineering software development and GHz measurements

10 employees

7 consultants

50% female

25 years in a Nutshell



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

based on 300+ publications by:

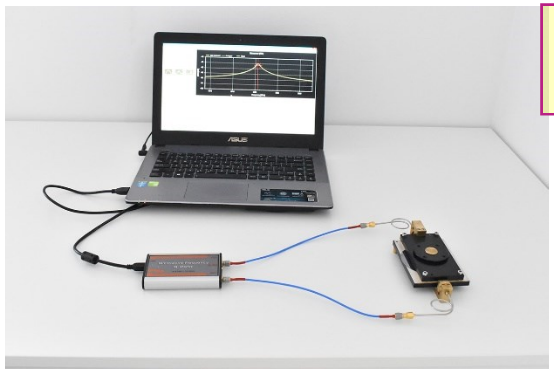
prof.W.Gwarek, IEEE Fellow, DML, Pioneer Award

dr.M.Celuch, President of QWED

Instruments for precise material measurements

based on 300+ publications

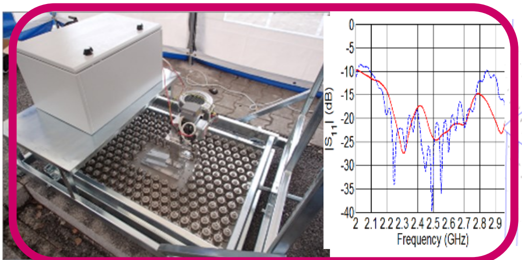
by prof.J.Krupka, IEEE Fellow

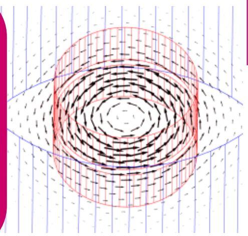


Consultancy & design services based on EM expertise & tools

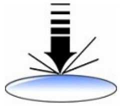
team of 10+engineers, 4 PhDs, 2 Profs

key areas: MW power appliances, customised resonators, antennas &feeds

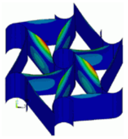




R&D projects



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



FP6 CHISMACOMB – 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

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

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.

M-ERA.NET

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

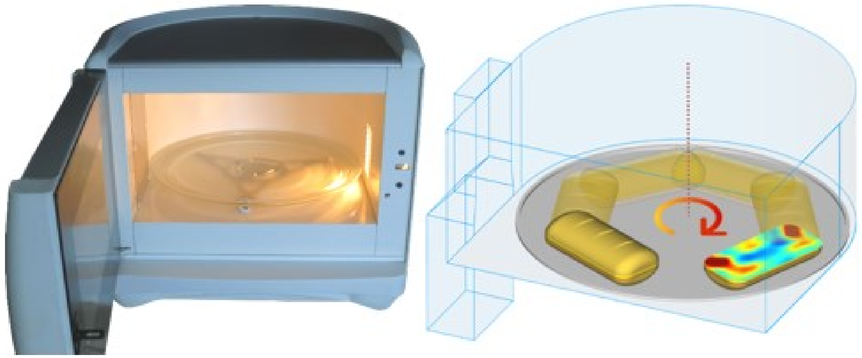
$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}$$

$$\nabla \cdot \vec{D} = \rho$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t}$$



general:

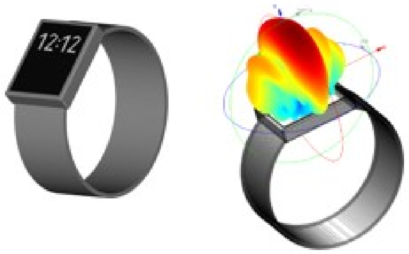
$$\vec{D}, \vec{B}, \vec{J} = F(\vec{E}, \vec{H})$$

typical:

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

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

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



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<< 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?

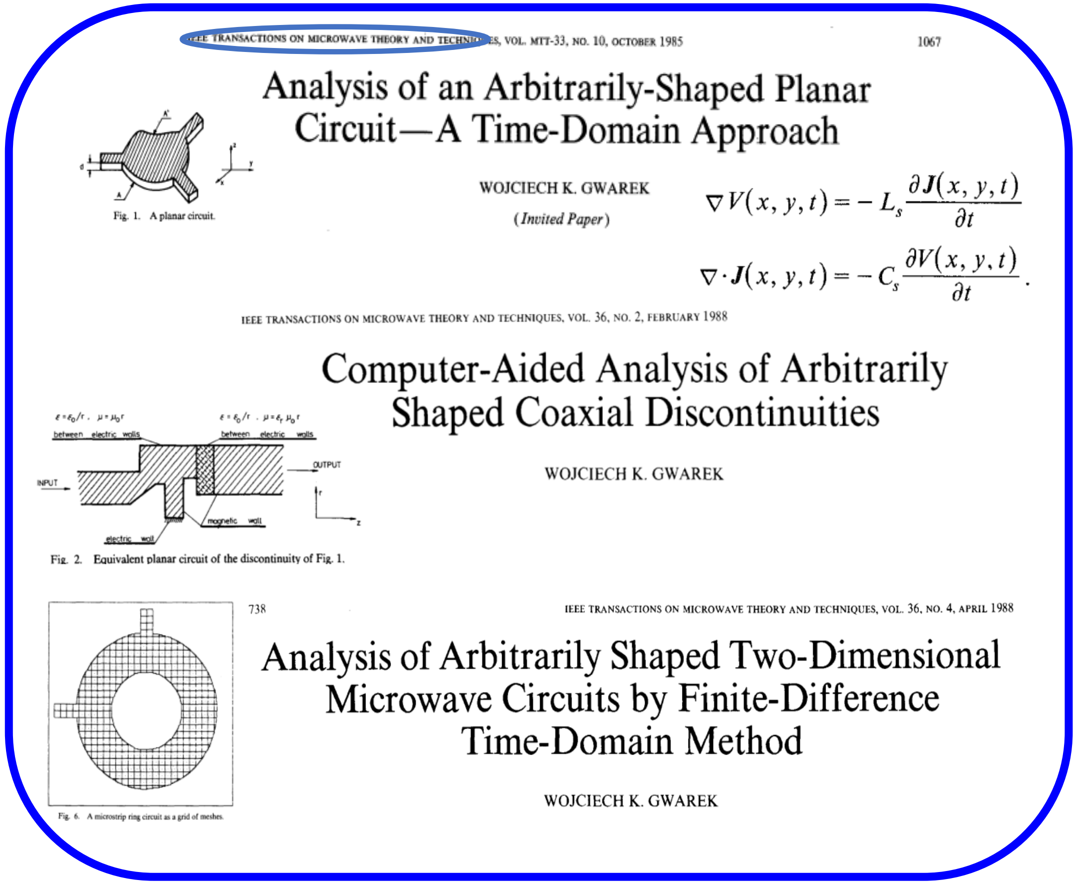
Engineers question today: can I trust EM software (to fully replace hardware prototyping)?

Origins of QWED Computer Modelling

since 1980s...

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

Fellow, Pioneeer Award, DML



IEEE TRANSACTIONS ON MICROWAVE THEORY AND TECHNIQUES, VOL. MTT-33, NO. 10, OCTOBER 1985 1067

Analysis of an Arbitrarily-Shaped Planar Circuit—A Time-Domain Approach

WOJCIECH K. GWAREK

(Invited Paper)

$$\nabla V(x,y,t) = -L_s \frac{\partial \mathbf{J}(x,y,t)}{\partial t}$$

$$\nabla \cdot \mathbf{J}(x,y,t) = -C_s \frac{\partial V(x,y,t)}{\partial t}.$$

Fig. 1. A planar circuit.

IEEE TRANSACTIONS ON MICROWAVE THEORY AND TECHNIQUES, VOL. 36, NO. 2, FEBRUARY 1988

Computer-Aided Analysis of Arbitrarily Shaped Coaxial Discontinuities

WOJCIECH K. GWAREK

Fig. 2. Equivalent planar circuit of the discontinuity of Fig. 1.

738 IEEE TRANSACTIONS ON MICROWAVE THEORY AND TECHNIQUES, VOL. 36, NO. 4, APRIL 1988

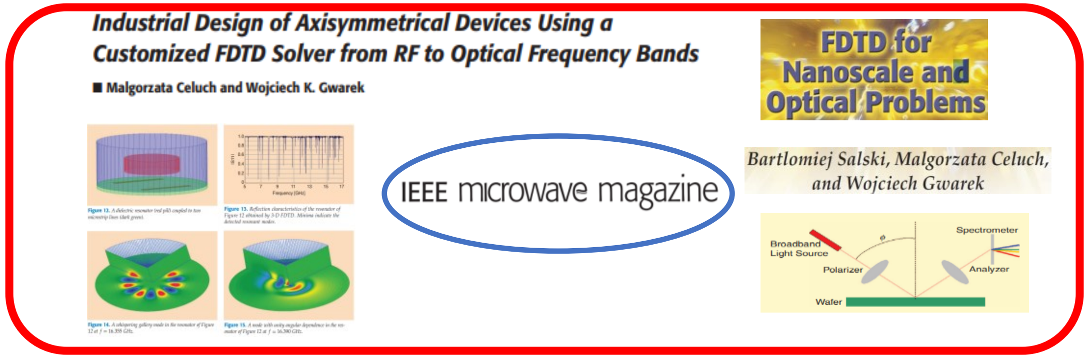
Analysis of Arbitrarily Shaped Two-Dimensional Microwave Circuits by Finite-Difference Time-Domain Method

WOJCIECH K. GWAREK

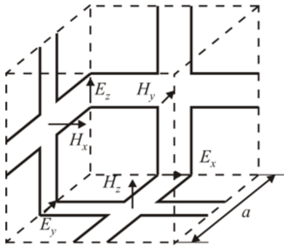
Fig. 6. A microstrip ring circuit as a grid of meshes.

... by early 2000s:

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

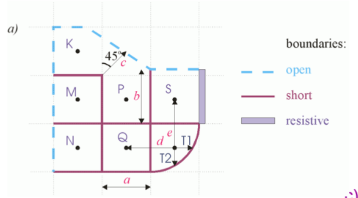


my contributions around 1990s:



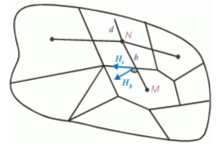
a) generalized gridding of a microwave structure

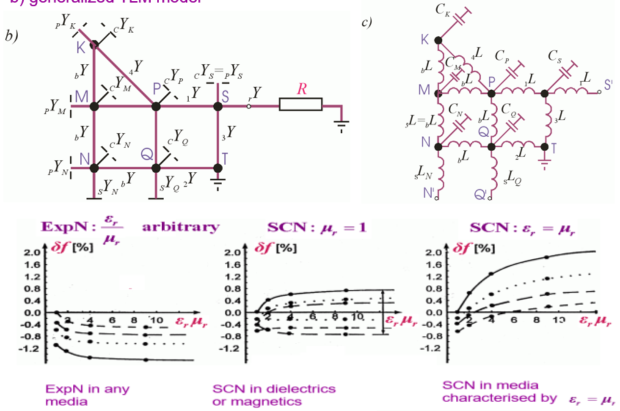
nodes: FDTD discretisation of Maxwell eqs.
connecting lines & stubs: TLM discretisation of Huygens principle

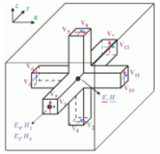


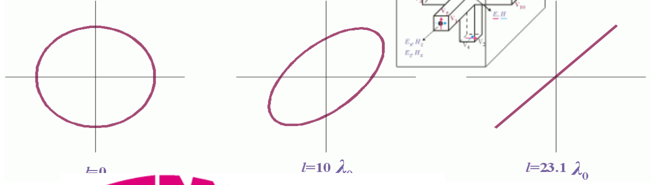
b) generalized TLM model

c) generalized FDTD model





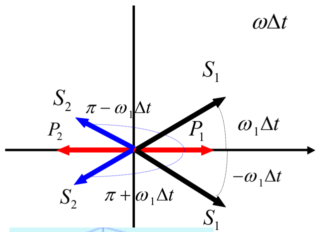


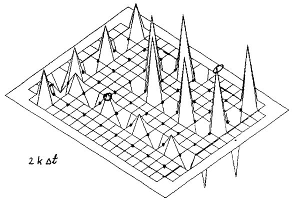


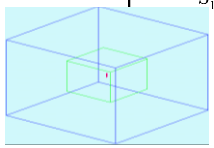
Generalised dispersion relations Theory of P- and S-eigenmodes

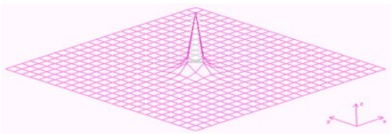
$$P(\omega\Delta t)\ S(\omega\Delta t, \beta_x a, \beta_y a, \beta_z a) = 0$$

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

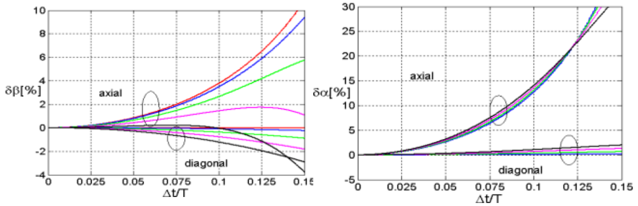




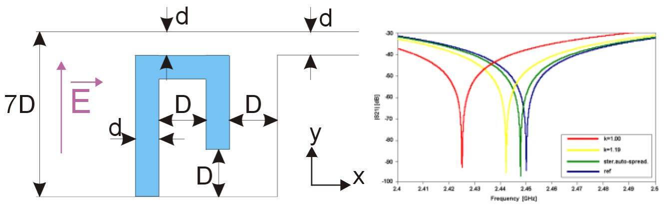




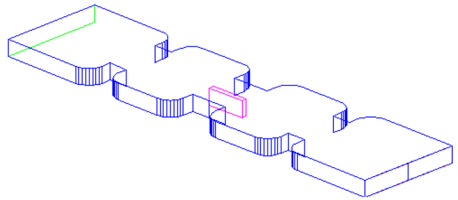
Dispersion in lossy media

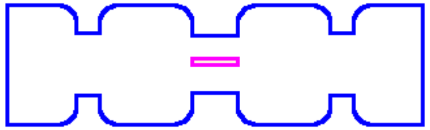


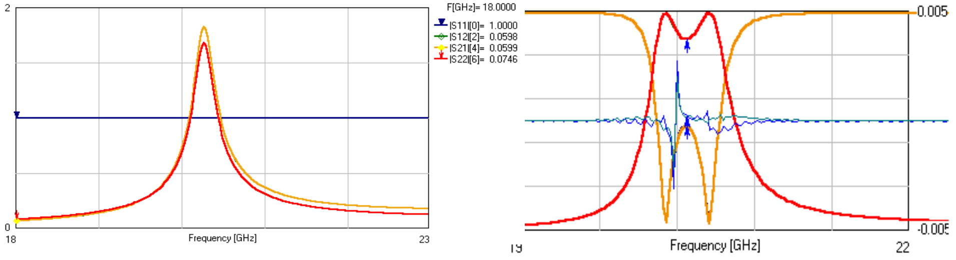
Field singularities



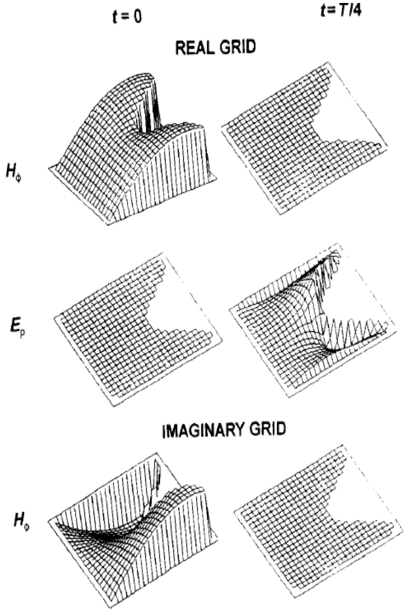
Generalised extraction of S-parameters in multi-modal transmission lines (incl. evanescent modes)



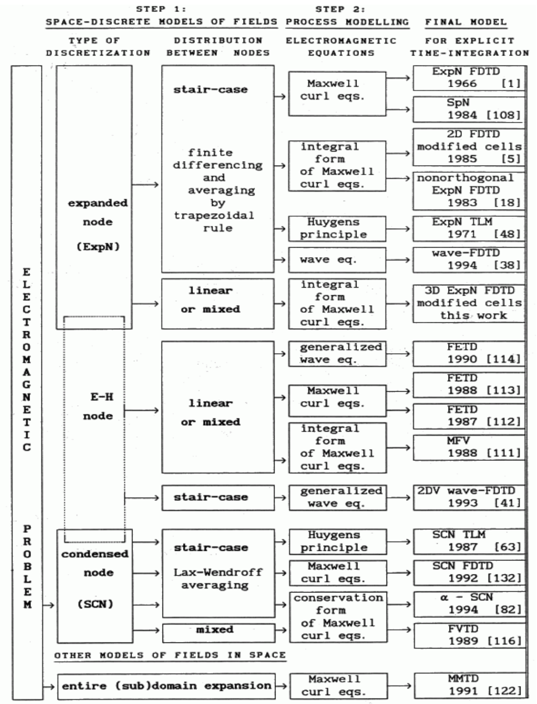




Periodic & vector 2D FDTD and TLM in real & complex form



Classification of time-domain methods

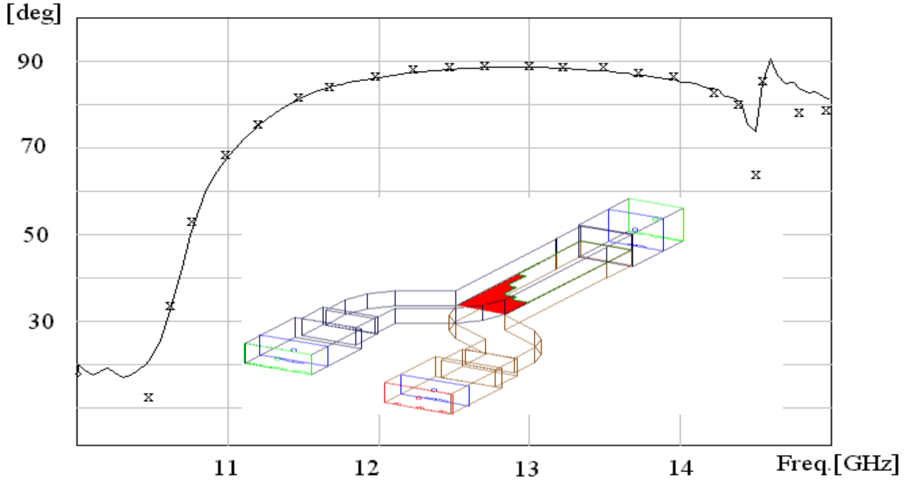


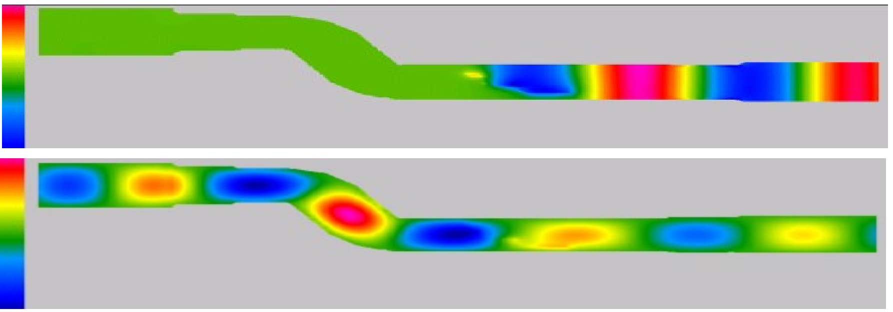
QuickWave original applications in cosmic reseach & satellite telecommunication

Septum polariser by SES

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

below: differential phase-shift



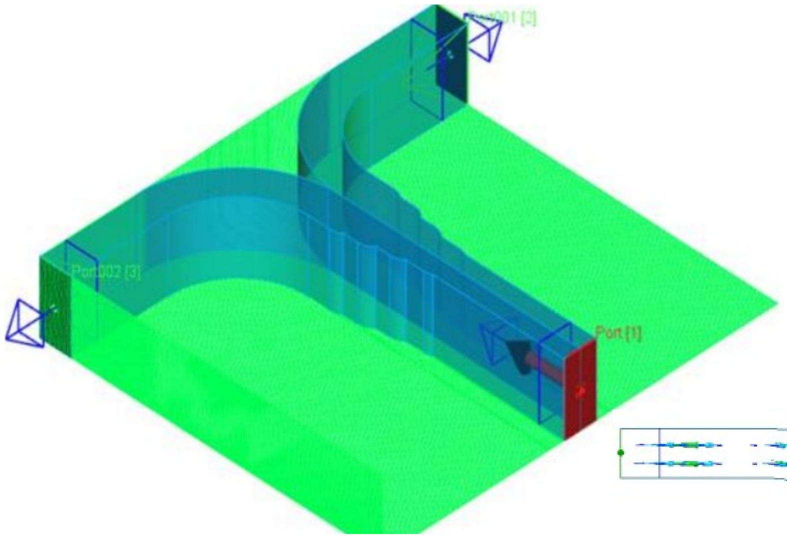


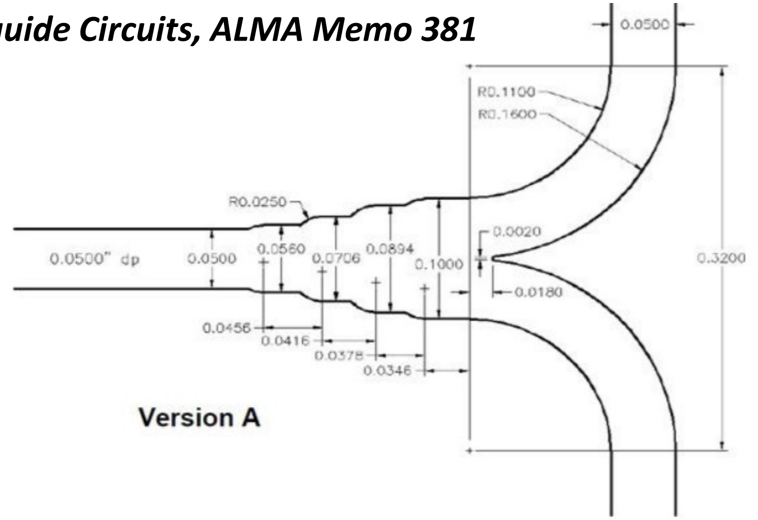
propagation of two polarisations

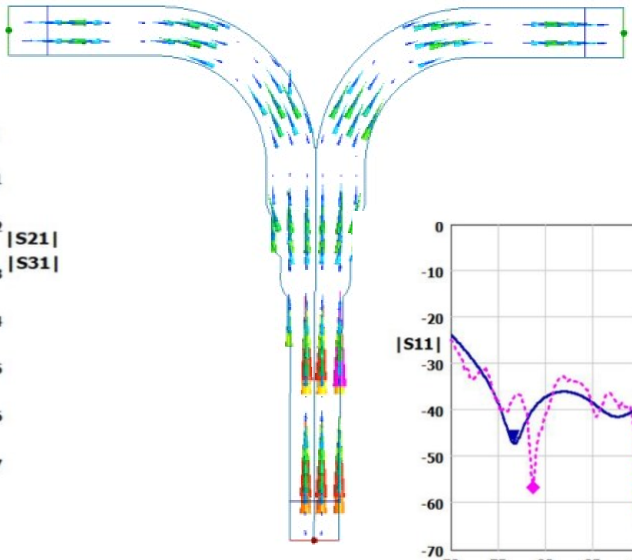
at centre frequency

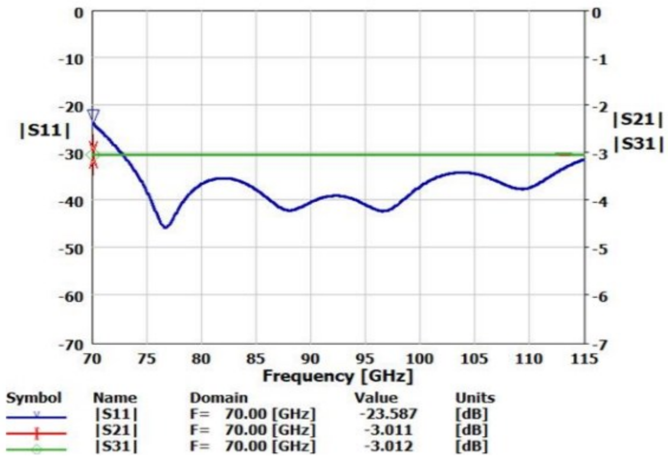
E-plane Y-junction by NRAO

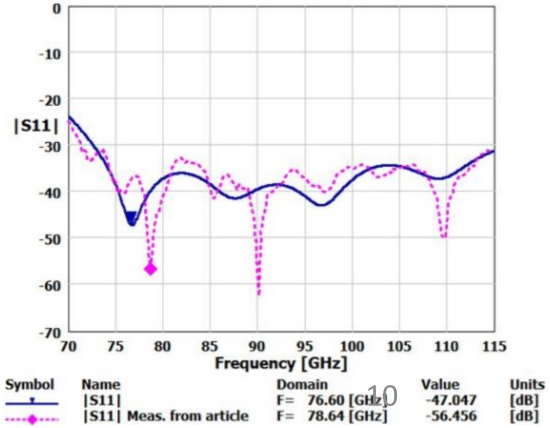
after A. R. Kerr, Elements for E-Plane Split-Block Waveguide Circuits, ALMA Memo 381





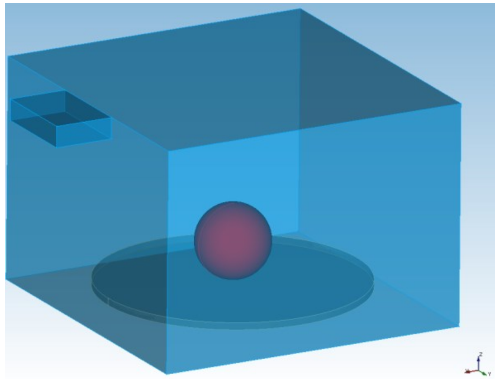


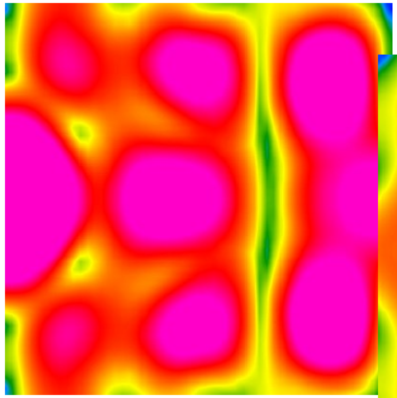




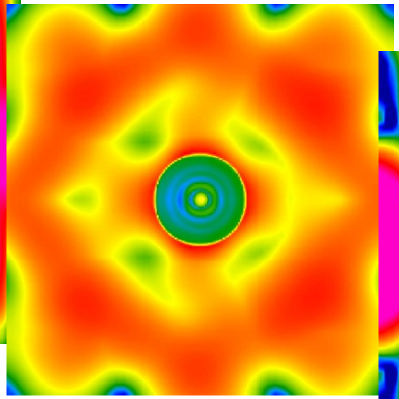
QuickWave modelling EM field interaction with tissues (for food processing & medical applicators)

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

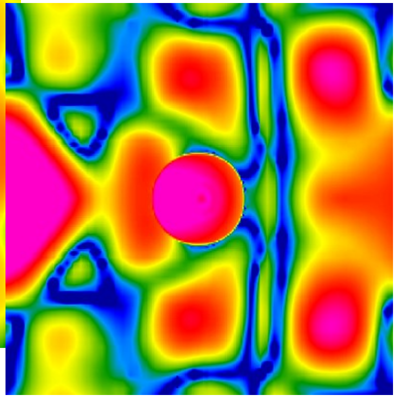




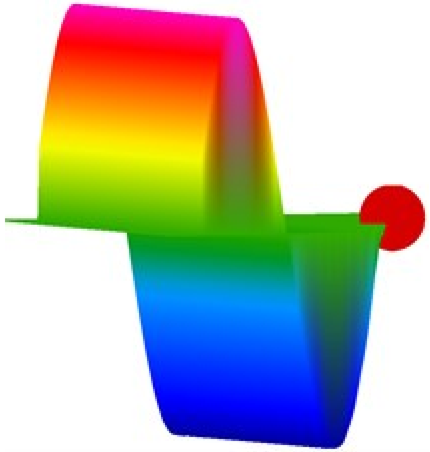
E-field in an empty cavity

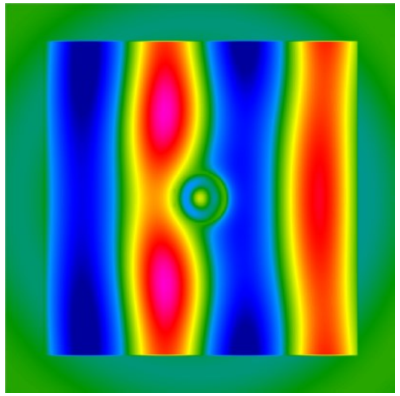


E-field in a loaded cavity

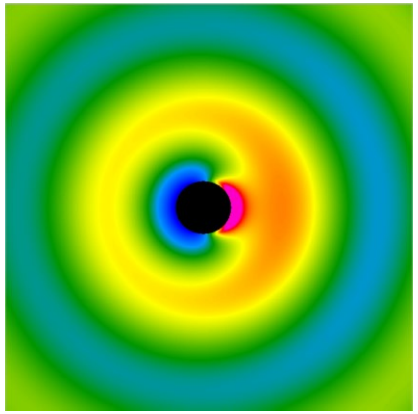


Scattered near-fied in cavity



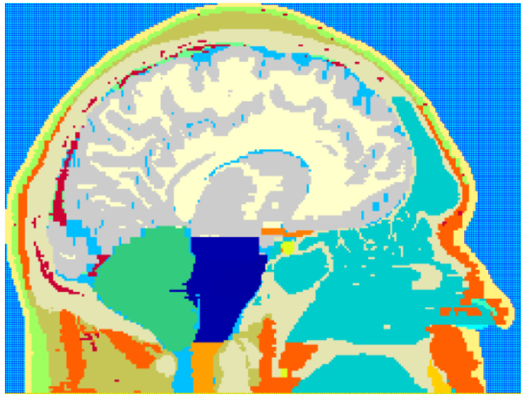


Total field
Focusing by the load
”exploding egg effect”

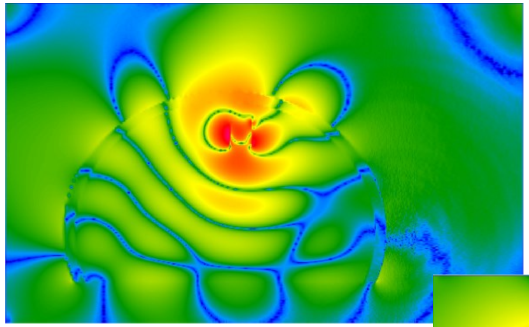


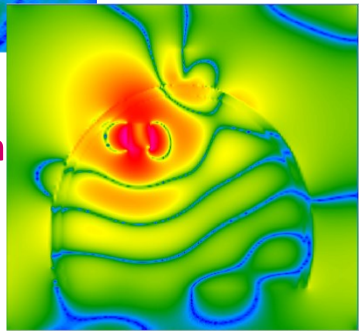
Diffracted field reveals cause of focusing: circumferential resonance

Detection of inhomogenities in tissues



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



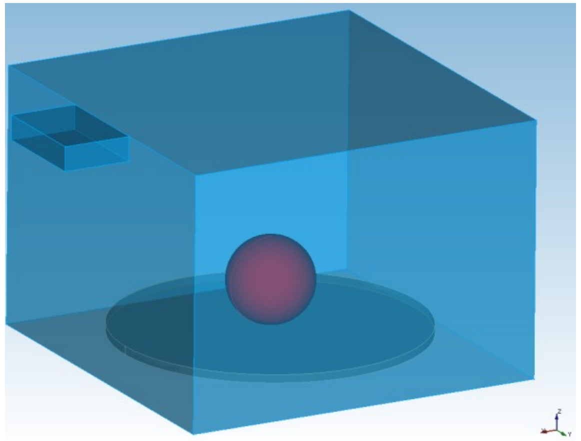


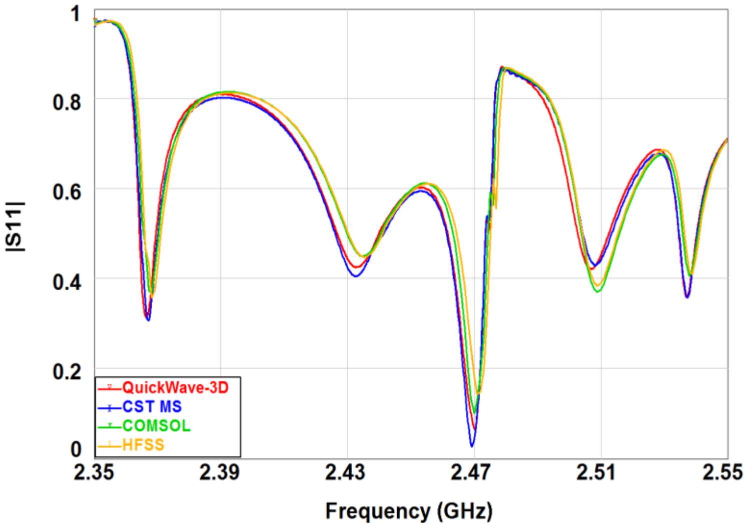
- ✓ **Tumours & haemorrhages detection**
- ✓ **Optimisation of multiantenna tomographic systems**

* https://sites.utexas.edu/austinmanaustinwomanmodels/

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

Simple microwave heating benchmarks & microwave heating phenomena studies*



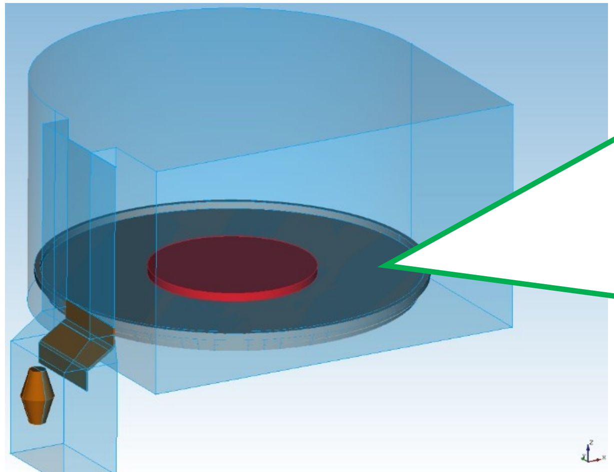


- heat transfer & load dynamics
- Load rotation & arbitrary movement during heating
- Source parameters tuning – regime for solid state sources
- Temperature dependence of material parameters

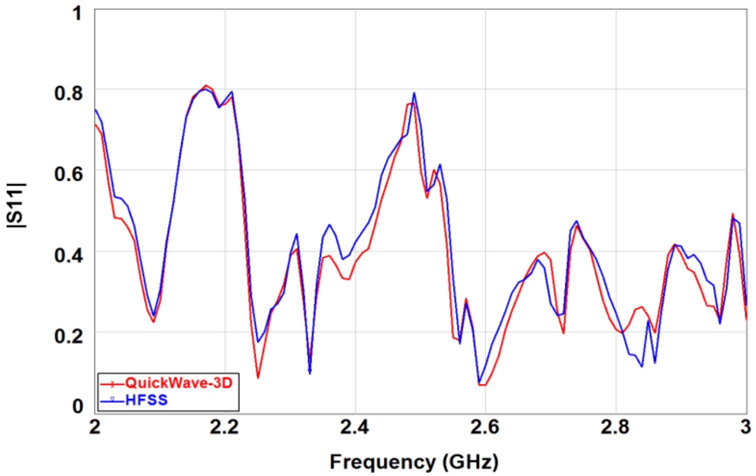
Freezing to file the state of the simulation

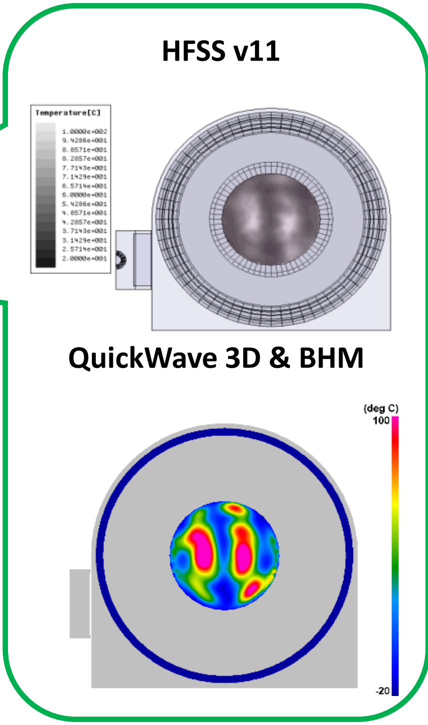
De-freezing on arbitrary computer & at convenient time

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



Courtesy of Whirlpool Inc. – Whirlpool MAX oven

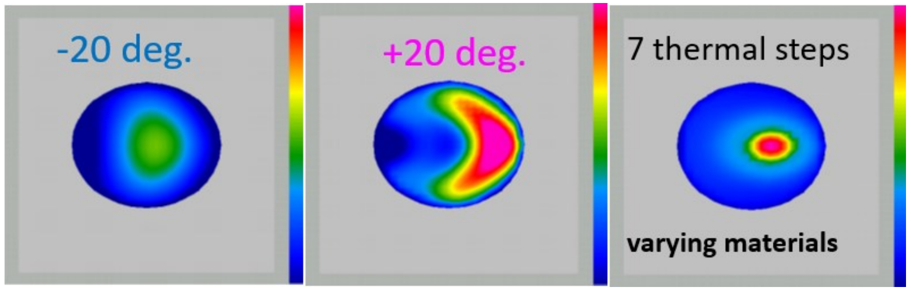


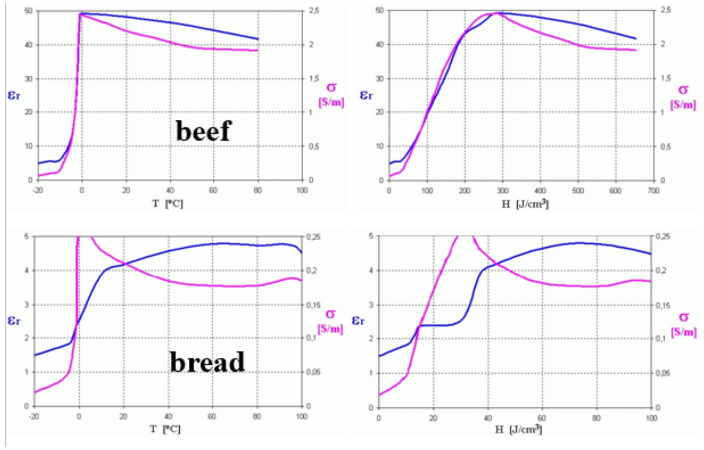


With QuickWave EM computation as fast as 1 min 18s on a low-cost video card – supporting all graphic cards with OpenCL

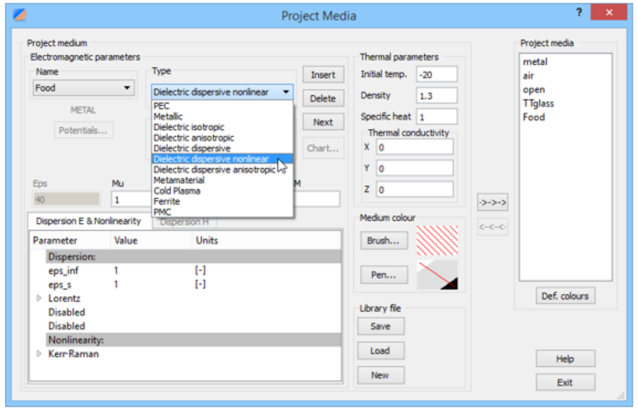
* M.Celuch, P.Kopyt & M. Olszewska-Placha in eds. M. Lorence, P. S. Pesheck, U. Erle, *Development of packaging and products for use in microwave ovens*, 2nd Ed. Elsevier 2020.

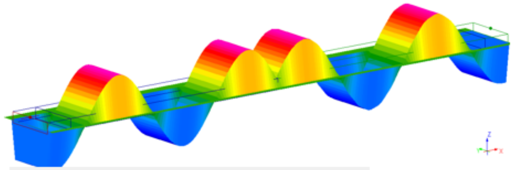
Materials' Characteristics in Microwave Engineering Design: REPRESENTATION

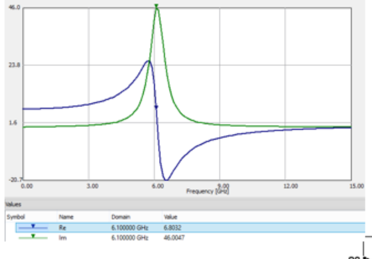





```
#Raw beef draft media file for QW-BHM module (00-09-06 POR)
#Measurements & refinements by Per O Risman, Microtrans AB, Sweden
#Modified by QWED, Poland
# DATA FROM -20 C to +80 C, dH/dV in J/cm3 reversedEnth/Temp column
!Temperature   Enthalpy      EPa         SIGa     SpecHeat Density  Ka
# Data deg C   J/cm3                     S/m
-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
```







Arbitrary Lorentz model parameters from QuickWave™

text-files for a coupled EM-thermal process

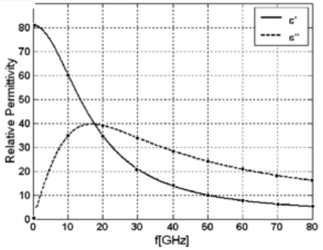
$$Drude: \quad \varepsilon_r(\omega) = \varepsilon_\infty + \frac{(2\pi f_p)^2}{(j\omega 2\pi \nu_c - \omega^2)}$$

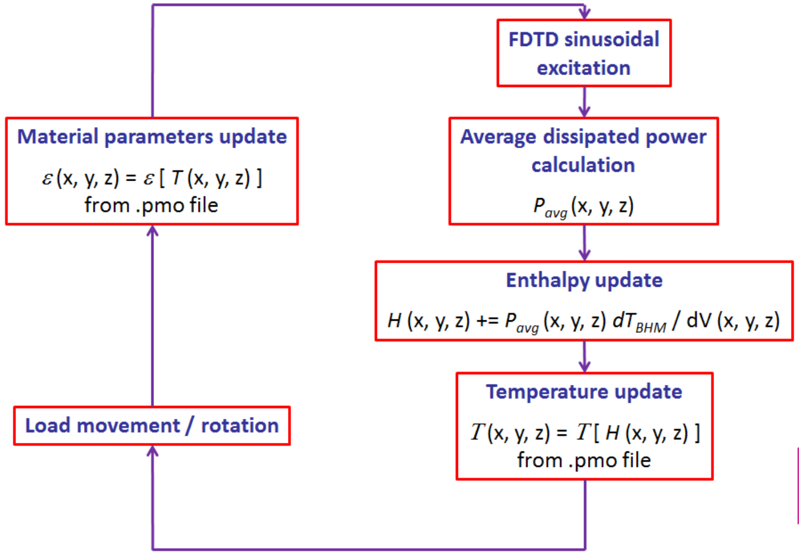
$$Debye: \quad \varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{(1 + j\omega\tau)}$$

$$Lorentz: \quad \varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty (2\pi f_p)^2}{((2\pi f_p)^2 + j\omega 2\pi \nu_c - \omega^2)}$$

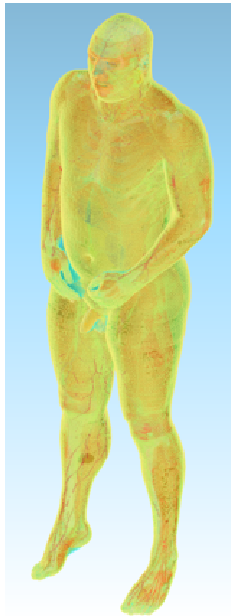
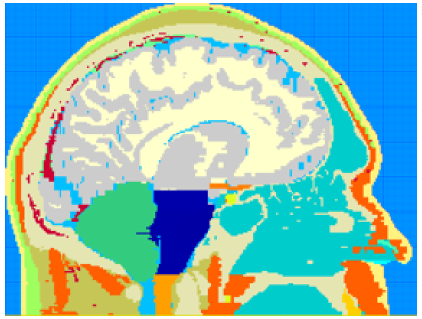
material parameters from equations

Water parameters





Materials' Characteristics in Microwave Engineering Design: SOURCE of DATA


*

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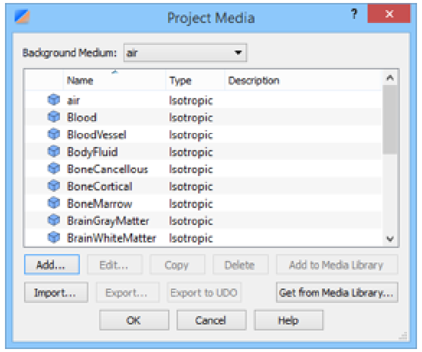
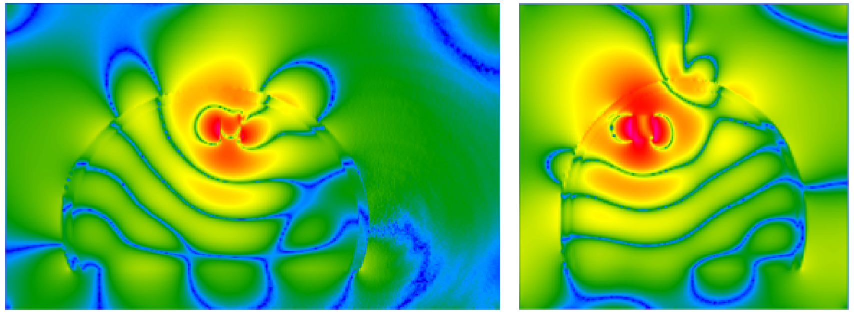


**

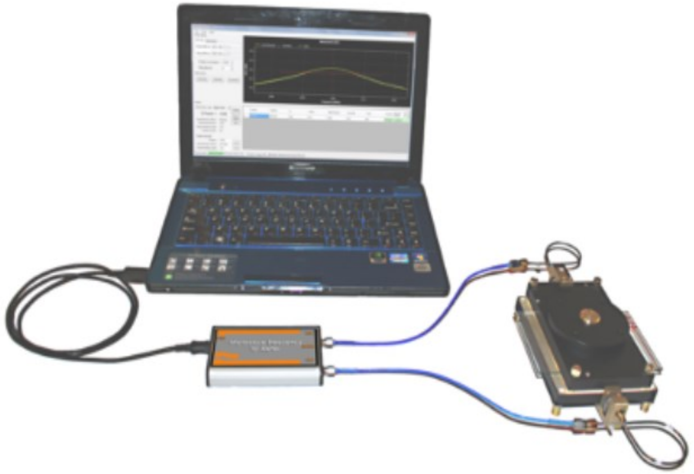


Detection of inhomogeneities in human tissues, e.g. tumours, haemorrahages

Design and development of diagnostic devices

Macroscopic parameters of tissues taken from a public database

Own (proprietary) measurements

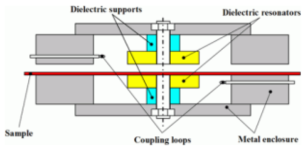


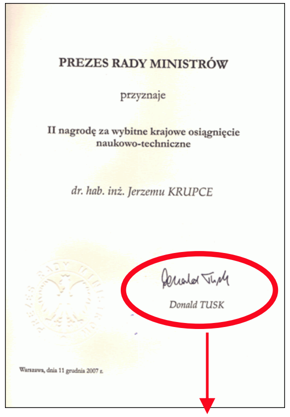
* AustinMan model (https://sites.utexas.edu/austinmanaustinwomanmodels/) converted to **QuickWave EM** software for Mälardalen University, Sweden

**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)




PREZES RADY MINISTRÓW

przyznaje

II nagrodę za wybitne krajowe osiągnięcie naukowo-techniczne

dr. hab. inż. Jerzemu KRUPCE

Donald TUSK

by Donald Tusk
Prime Minister of Poland 2007-2014
President of the European Council 2014-2019


DIPLOMA

Eureka!

THE BELGIAN AND INTERNATIONAL TRADE FAIR FOR TECHNOLOGICAL INNOVATION

Jerzy KRUPKA

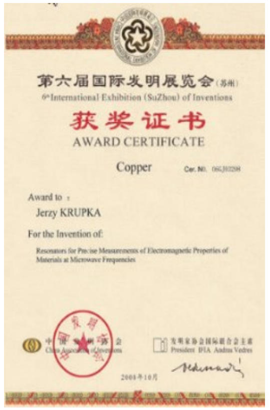
for the innovation

Résonateurs pour des mesures précises des propriétés électromagnétiques de matériaux à bande de fréquence micro-ondes.

Médaille d'or

THE PRESIDENT OF THE INTERNATIONAL JURY

THE PRESIDENT


第六届国际发明展览会(苏州)

6th International Exhibition (SuZhou) of Inventions

获奖证书

AWARD CERTIFICATE

Copper

Award to :

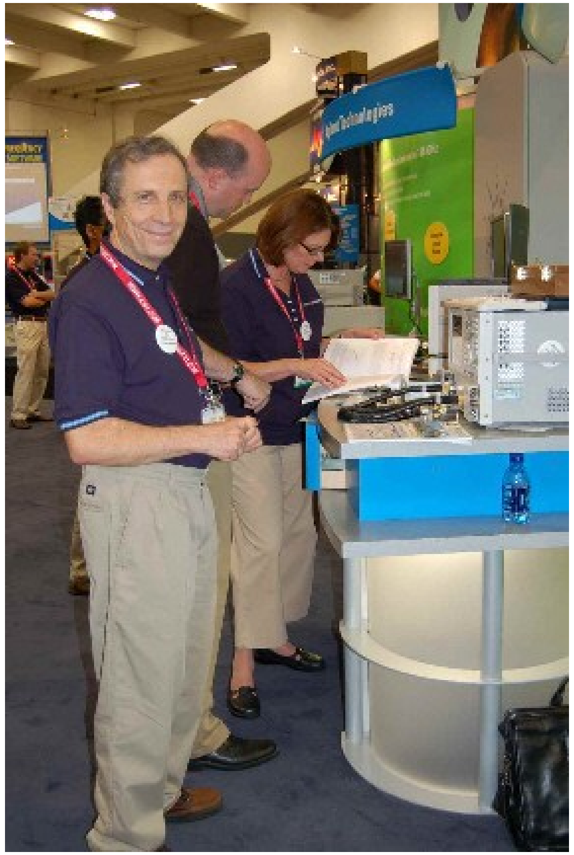
Jerzy KRUPKA

For the Invention of:

Resonators for Precise Measurements of Electromagnetic Properties of Materials at Microwave Frequencies

President IFIA Andras Vedres

… by early 2000s:
QWED commercialises the SPDRs
endorsement by Agilent / Keysight
publication of standard IEC 61189-2-721:2015

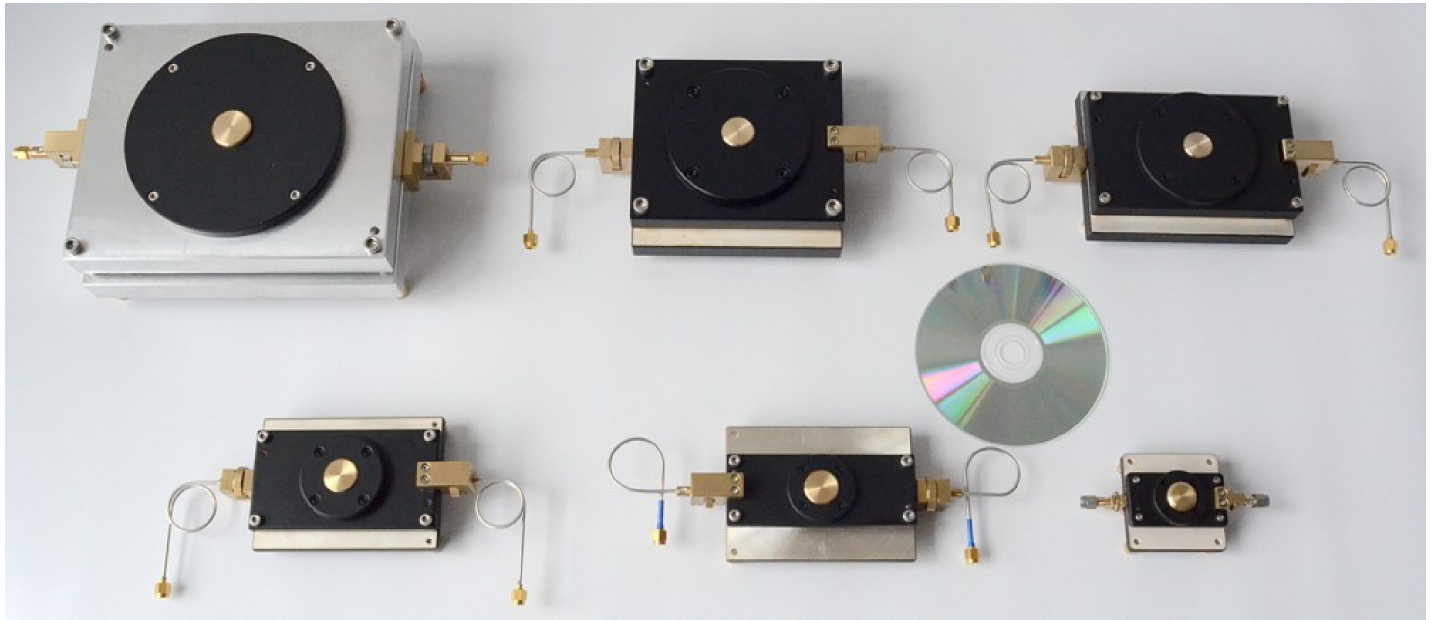


Agilent Both
IEEE IMS 2006, San Francisco, CA

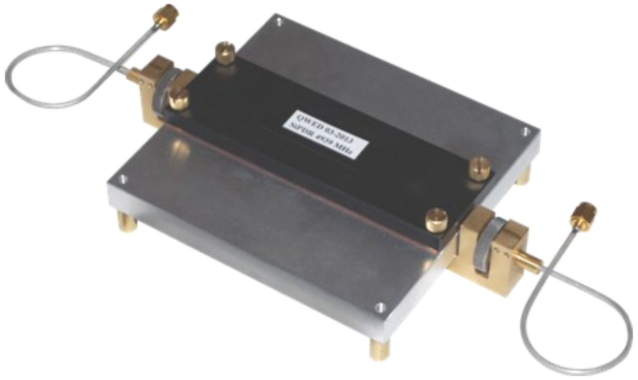
MMA-2010, Warsaw PL
co-organised by QWED & Warsaw Univ.Tech.

Popular Dielectric Resonators by QWED

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

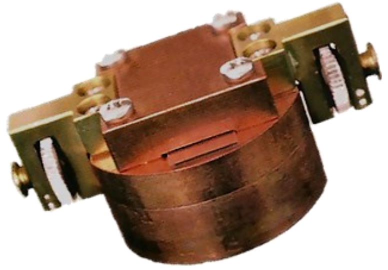


5 GHz SiPDR for resistive sheets

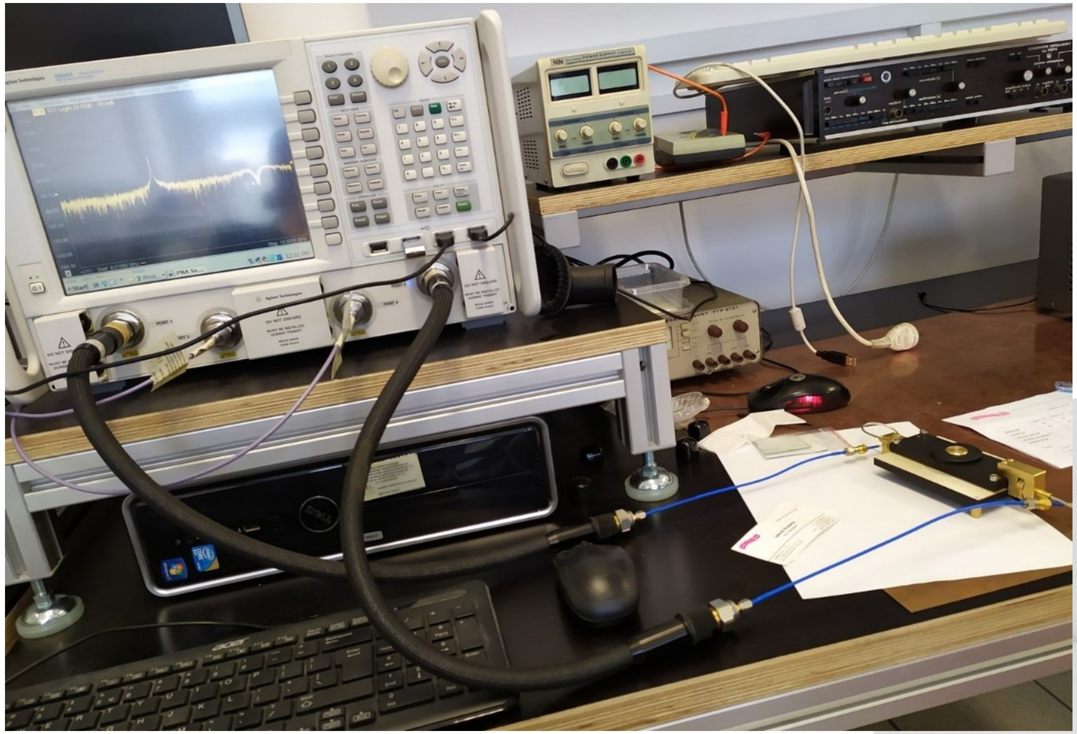


TE01δ cavities, typically 1 – 10 GHz
for bulk low-loss dielectrics

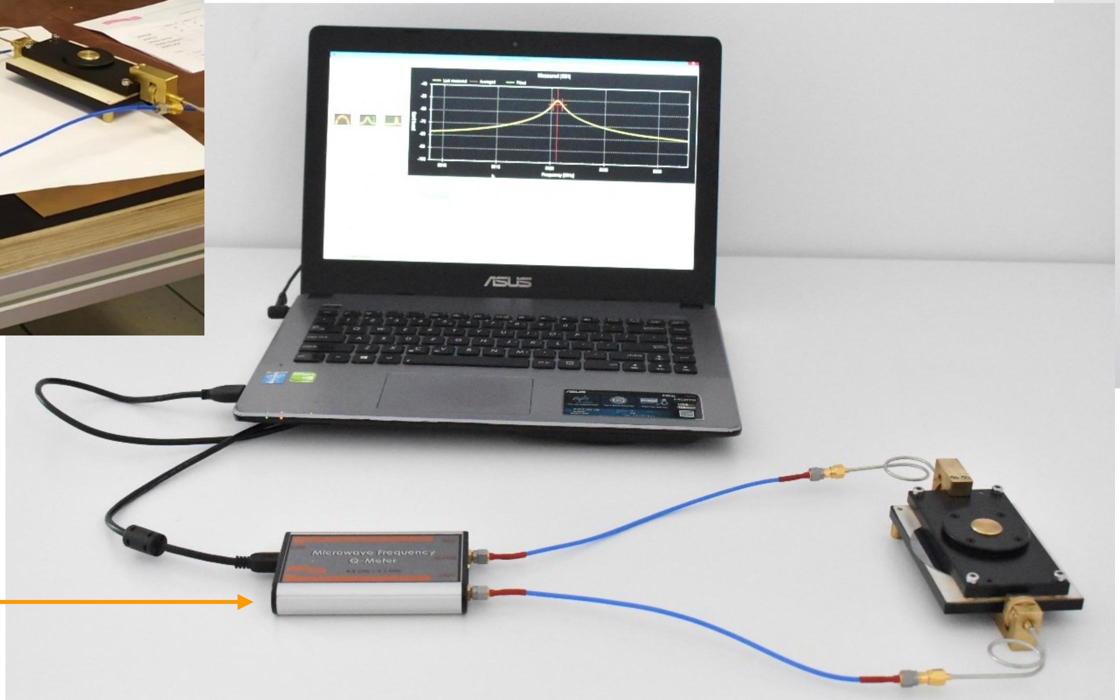
modified SiPDR for graphene



Resonators Operating in Different Setups

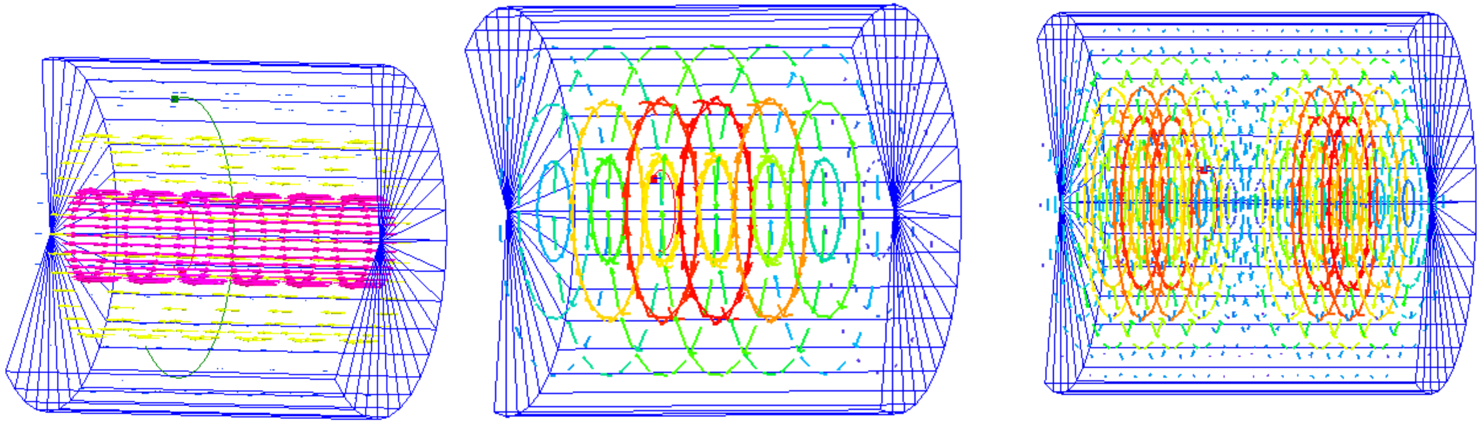


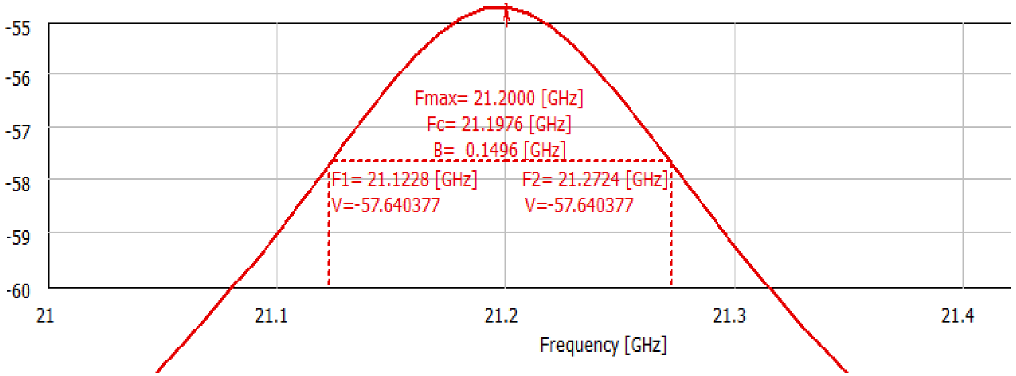
also for home-office!



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

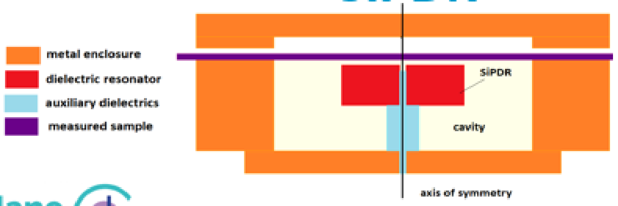
Where Modelling and Measurements Meet: Enhanced Design & Calibration of Resonators



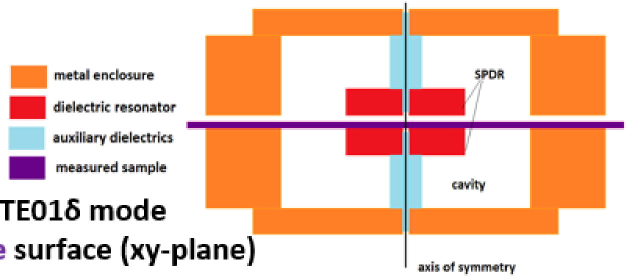


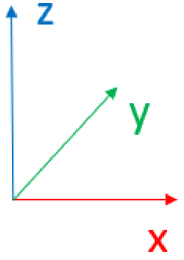
Tutorial examples on
NanoBat Open Platform
https://qwed.eu/nanobat.html

SiPDR

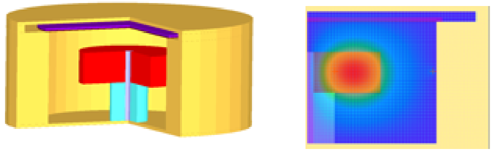


SPDR



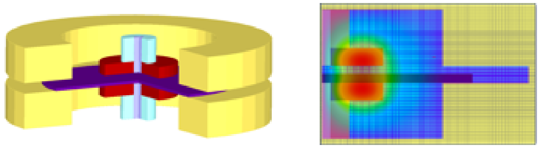


two configurations used with TE01δ mode
E-field tangential (parallel) to sample surface (xy-plane)



E-field distribution in the half cross-section

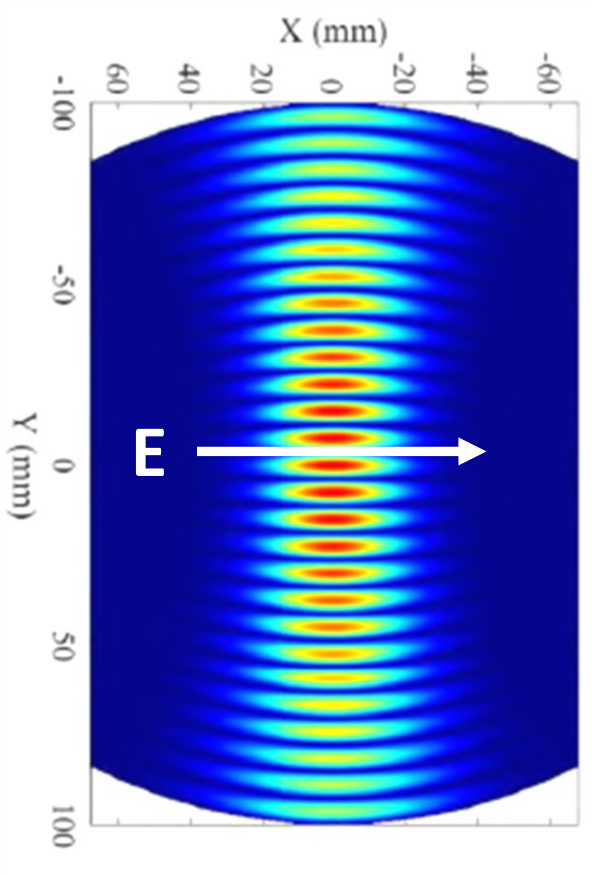
sample between the **single post dielectric** and the **ground plane**

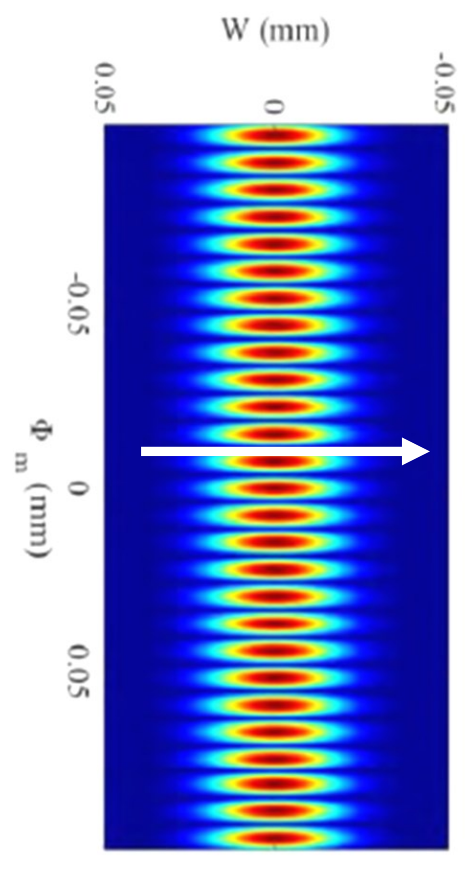


E-field distribution in the half cross-sectio

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

New: Fabry-Perot Open Resonator 20 – 110 GHz



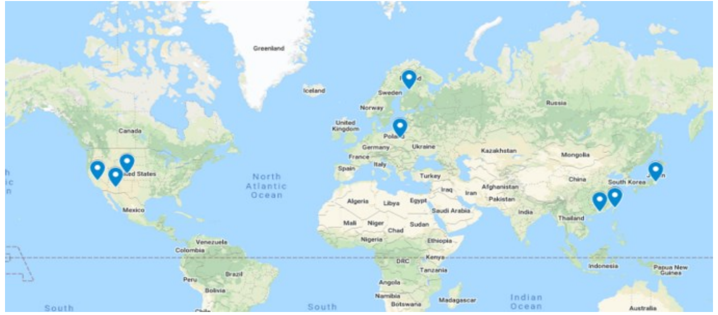


continuing the successful collaboration with Warsaw Univ. Tech. (Profs. J.Krupka, B.Salski, P.Kopyt)

Validation in iNEMI Round Robin - STRATEGY

Our project: iNEMI

- 3M
- AGC-Nelco
- Ajinomoto USA
- AT&S
- Centro Ricerche FIAT-FCA
- Dell
- Dupont
- EMD Electronics (Co-Chair)
- Flex
- Georgia Tech
- Showa Denko Materials
- IBIDEN Co Ltd
- IBM
- Intel
- Isola
- ITRI (Co-Chair)
- Keysight (Co-Chair)
- MacDermid-Alpha
- Mosaic Microsystems
- NIST
- Nokia
- Panasonic
- QWED
- Shengyi Technology Company
- Sheldahl
- Unimicron Technology Corp
- Zestron



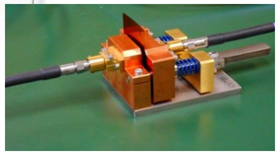
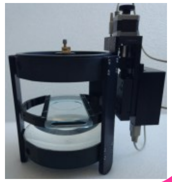
Sample Material Requirements
- Stable, Low loss
- Low moisture absorption / temperature dependency
- Isotropic
- Good mechanical & handling properties

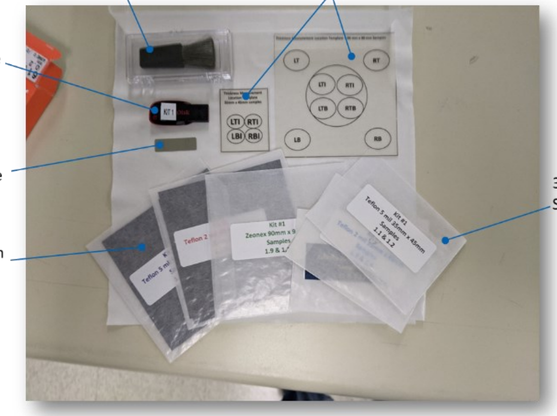
1st Project Stage
- Precision Teflon
- Cyclo Olefin Polymer

2nd Project Stage
- Rexolite
- Fused Silica

Industrial
- Automotive

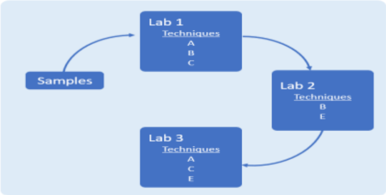
Techniques Included
- Split Post Dielectric Resonator
- Split Cavity Resonator
- Fabry-Perot
- Balanced Circular Disk Resonator

→ Frequency Span : 10GHz – 100GHz with overlaps

10 Laboratory Round Robin



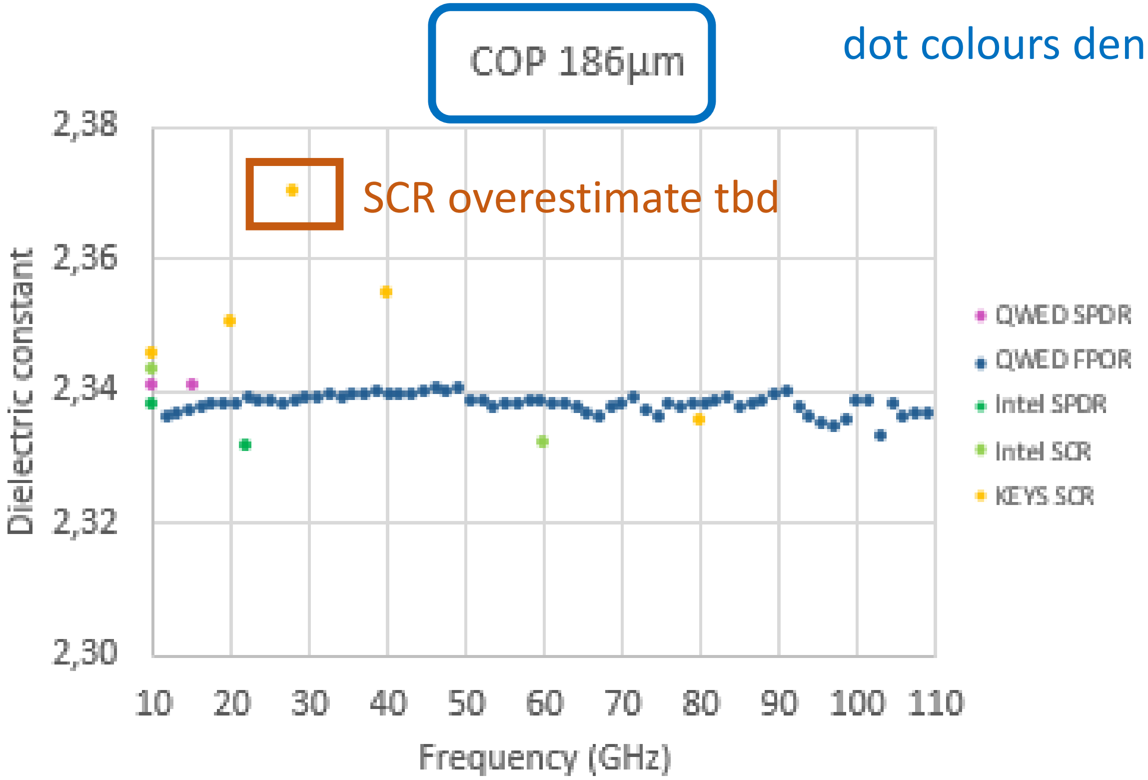
10 Sample Kits Created
- Sample sizes 35 mm x 45 mm, 90 mm x 90 mm
- circulated between 10 labs

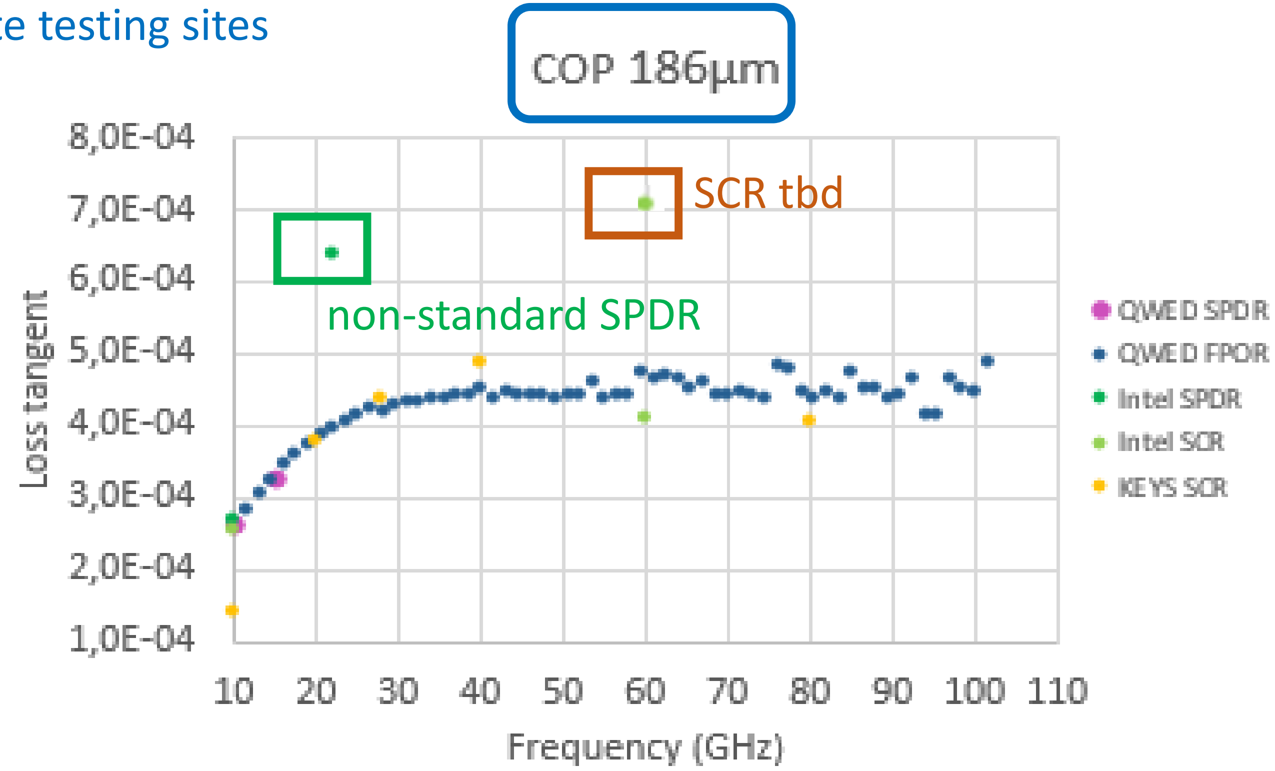
Validation in iNEMI Round Robin – EXAMPLE RESULTS

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.

dot colours denote testing sites





Dk spread < 1% (within ± 0.5% from average)
(< 2% incl. outliers)

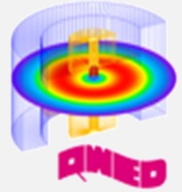
> 40GHz 2x increase in Df compared to 10GHz

Exploring Synergies between Computer Modelling and Material Measurements

Commercial since 1997
QuickWave Simulation Software
~1000 licences implemented

THE EUROPEAN ICT PRIZE WINNER

Modelling (EM, MW, multiphysics,...)
- waves in free space is "easy" Maxwellian
- wave interaction with matter is "complicated"...



Applicator design & model for parameter extraction

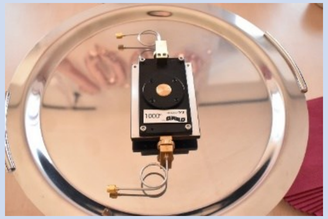
INNOVATION

Material measurements

Accurate material parameters (constitutive relations)

Commercial resonator test-fixtures since 2001

1000th unit sold in 2020



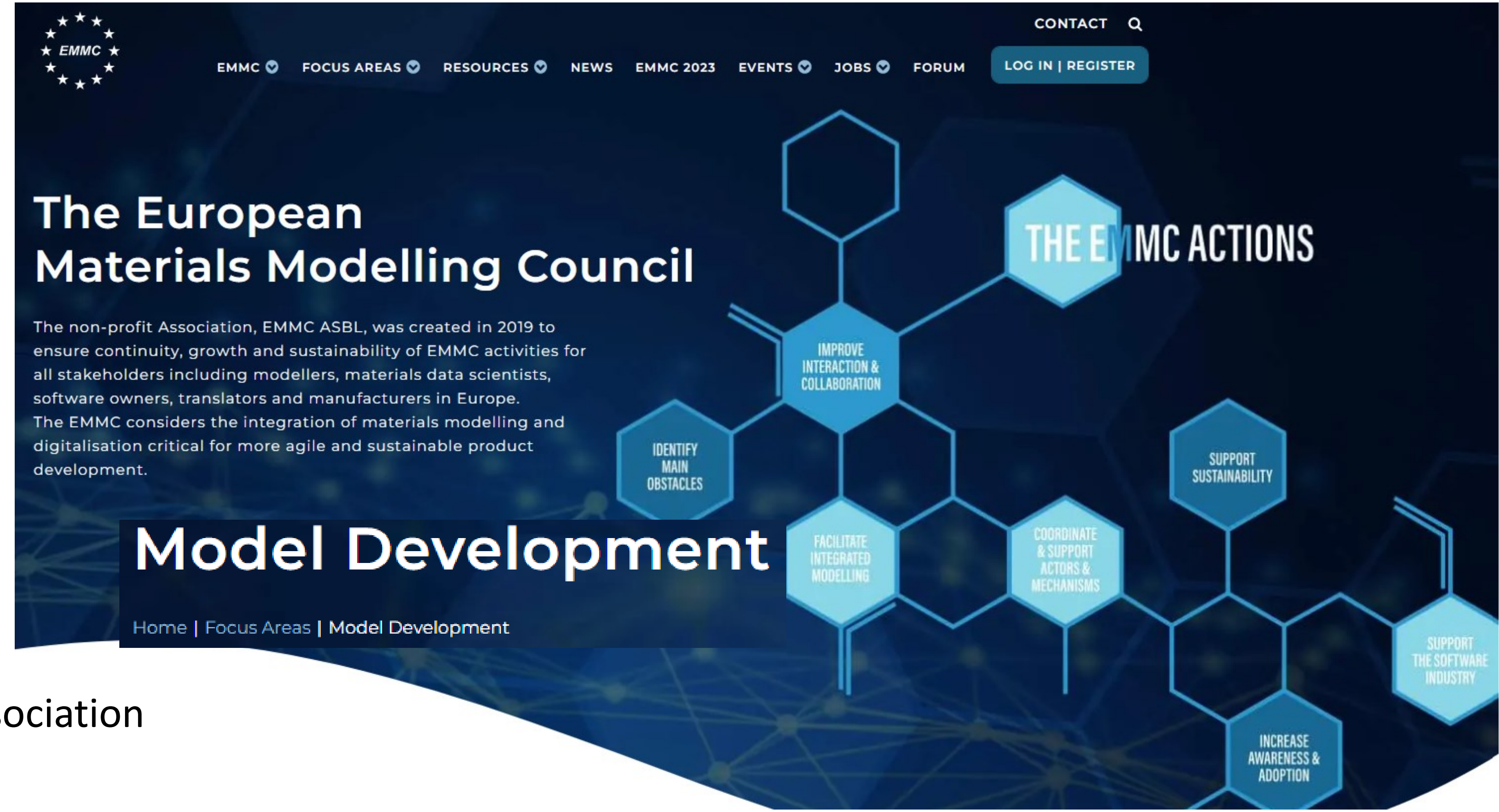
Open Platform Examples & Tools

QW-Modeller for QuickWave
Free general purpose 3D CAD modeller for QuickWave.

Open Platform Examples:
SMM tip presented at Numerical Electromagnetic

European Standard:
IEC 61189-2-721:2015
CEN-CENELEC Workshop 2021

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.

EMCC Focus Areas

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

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: Malrgorzata 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

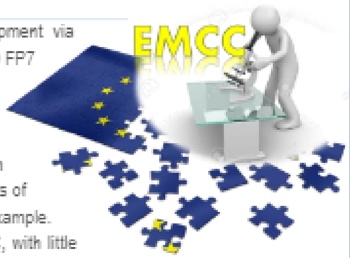
2016
European Materials Characterisation Council

initiative, not a legal body

European Commission

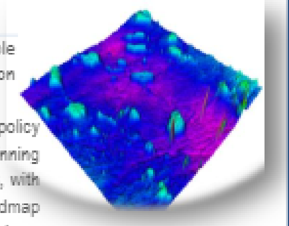
European Materials Characterisation Council (EMCC)

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.)

EMMC

NanoSafety Cluster

EPP

European Cluster on Catalysis

LinkedIn

follow ECC on the social networks

EUMAT

Photovoltaics & nanotechnology

Materials Modelling – Characterisation Problems Addressed by EU Initiatives

★ EMMC ★

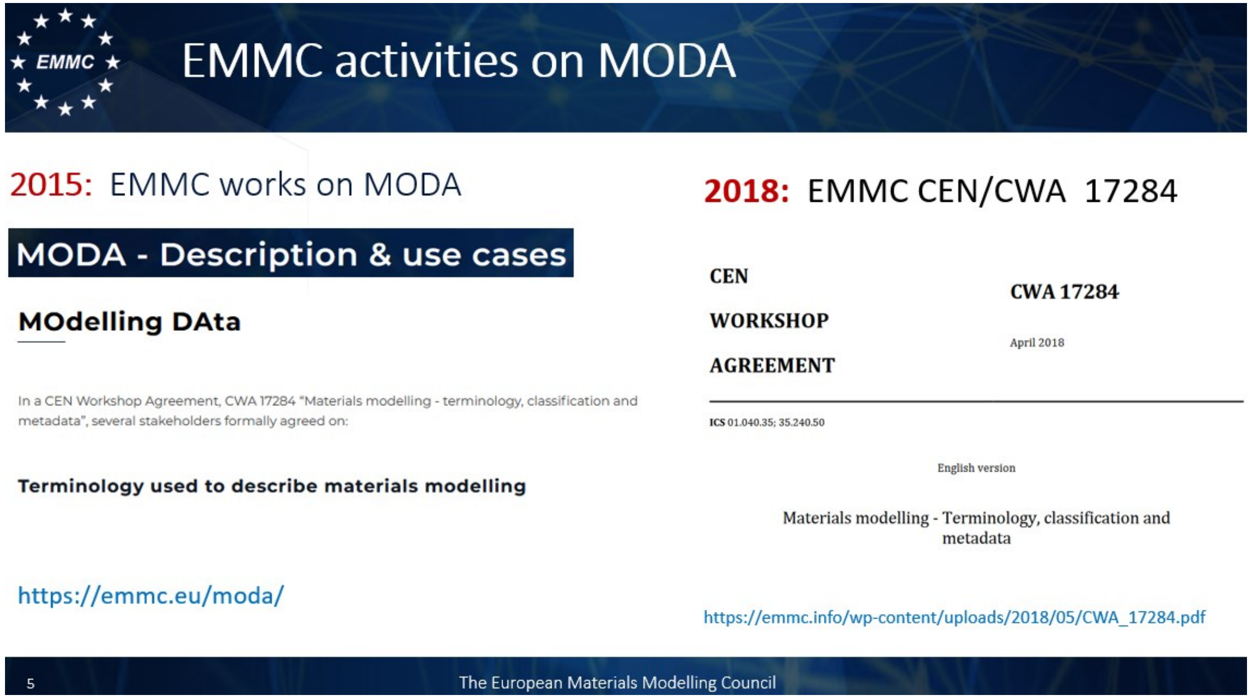
Typical materials model descriptions ...

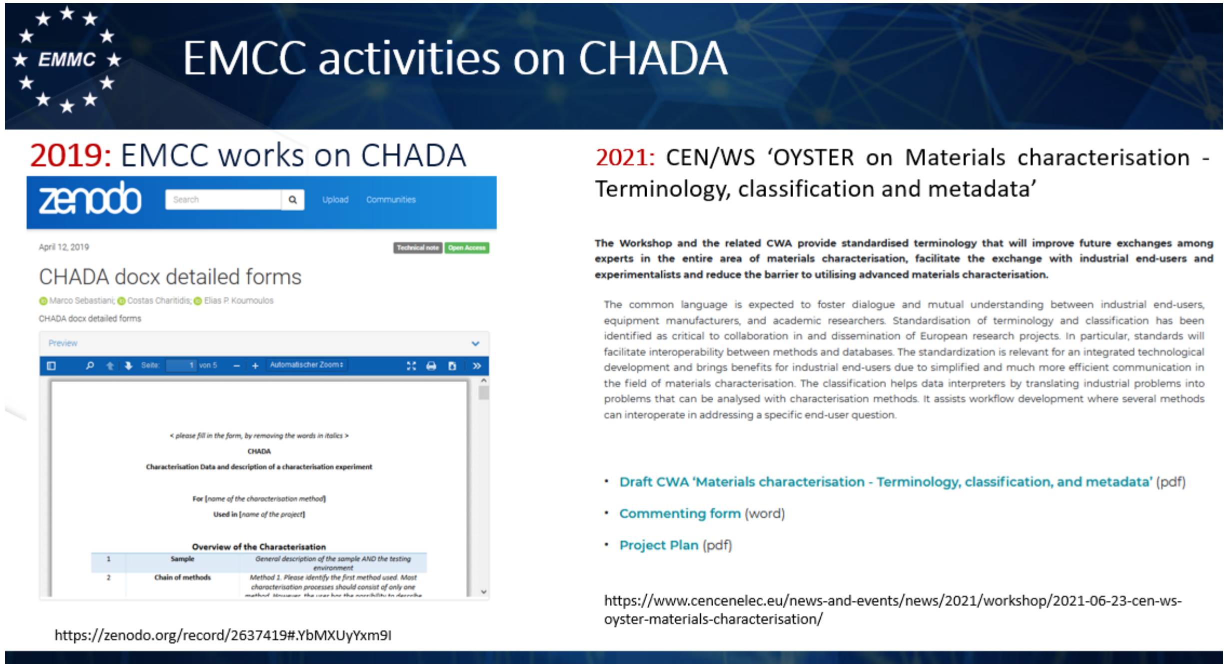
- By **phenomena (application)**:
  - "I have a mikro-kinetics model."
- By **scale** of the phenomena:
  - "I have a mesoscale model."
- By name of the **software (code)**
  - "I use the Uppsala model"
- By **solver**:
  - "I have a FE model"

The European Materials Modelling Council

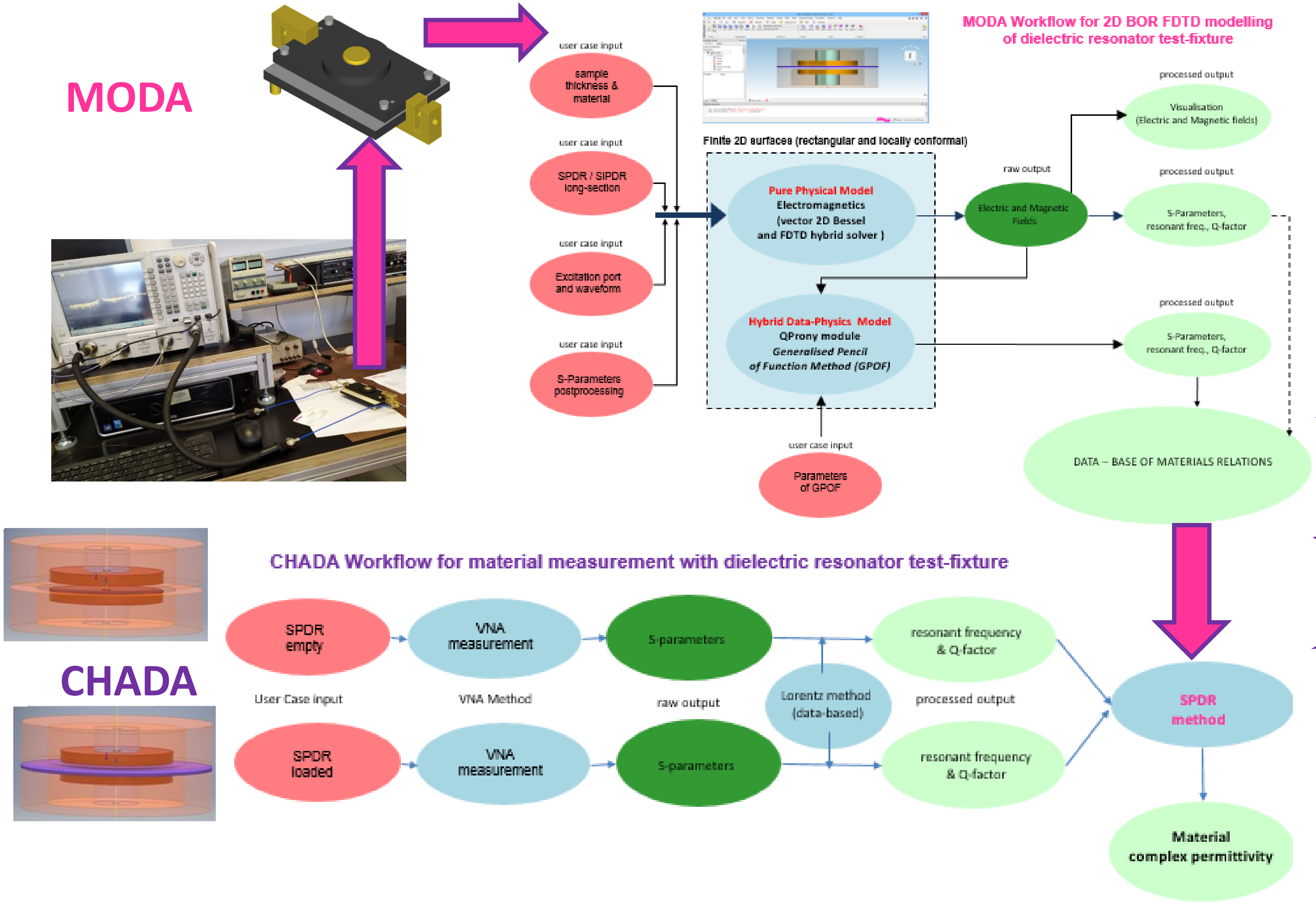
Materials Modelling – Characterisation Solutions Proposed by EU Initiatives

- 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





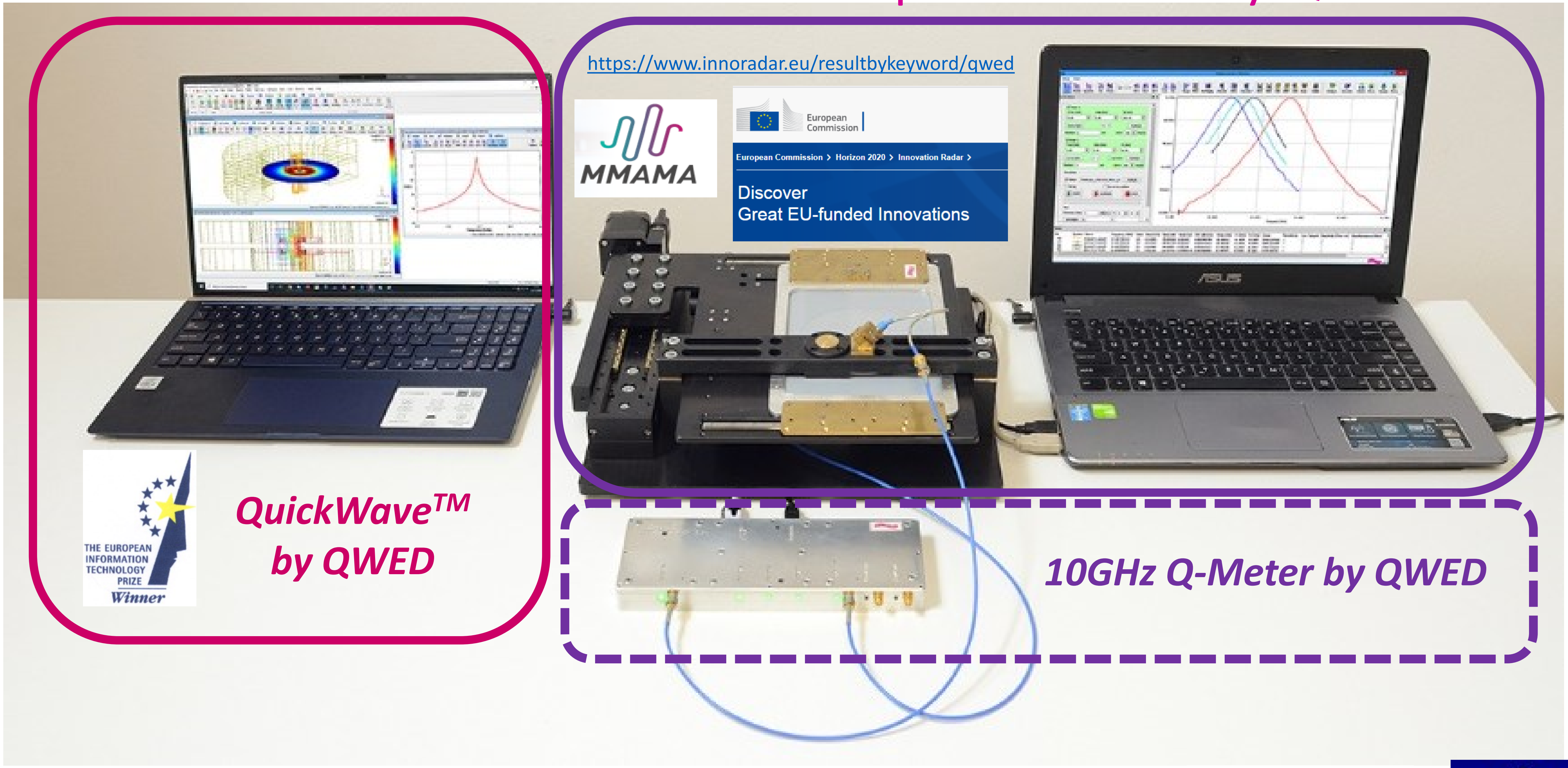
Twinned MODA + CHADA Example by QWED



...more physics behind...

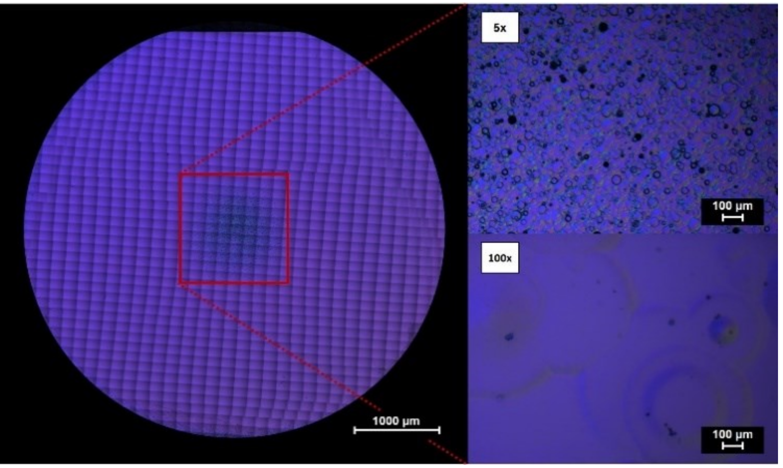
input from MODA is ESSENTIAL to complete CHADA!

Twinned MODA + CHADA Implementation by QWED



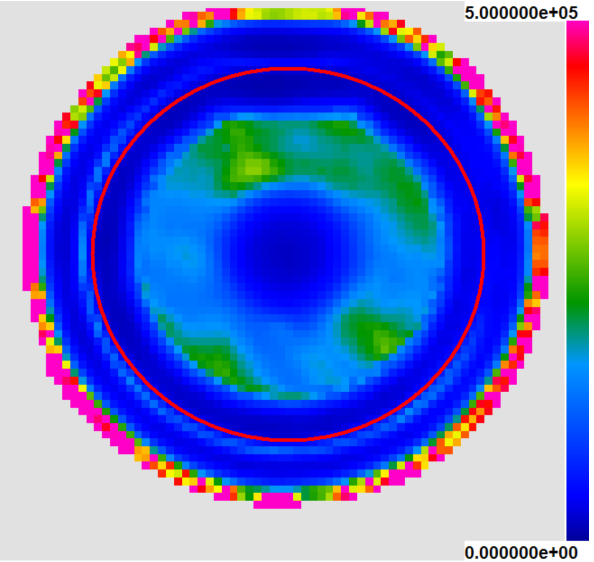
Finalist of the European Innovation Radar Prize 2021

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 unuseful for making devices.

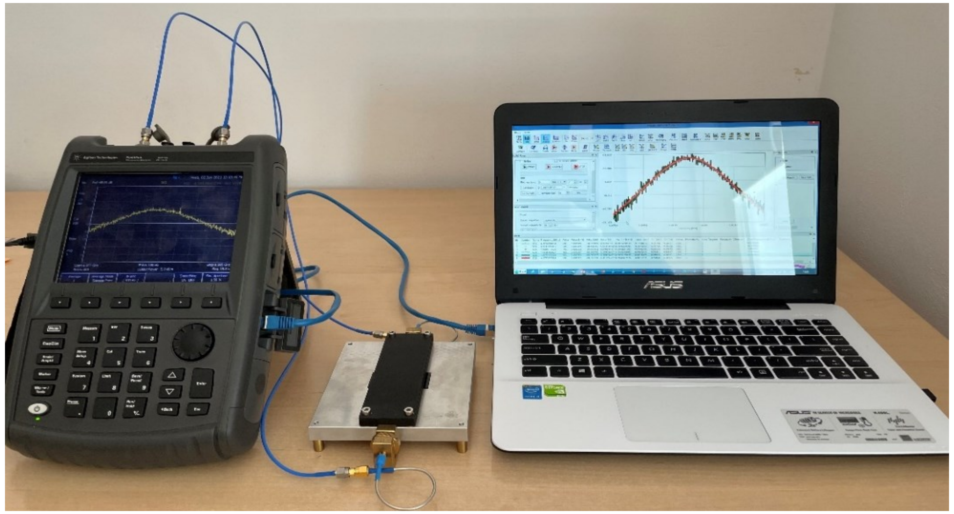


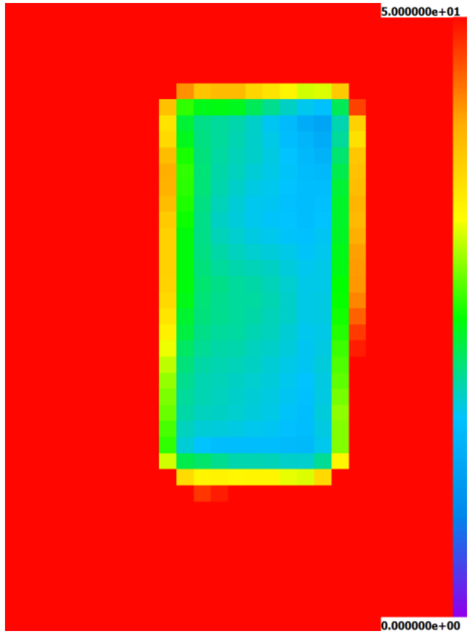
SPDR image:

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

M-ERA.NET
The National Centre for Research and Development
Łukasiewicz IMiF

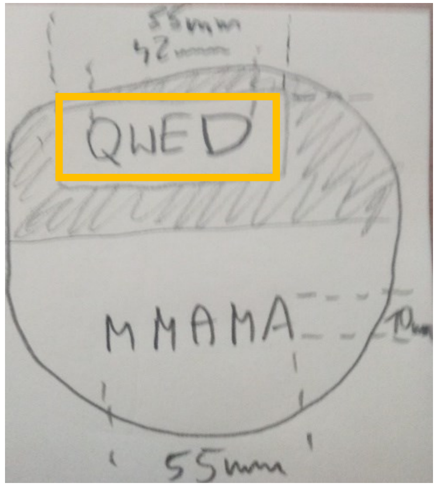
2D Imaging of Conductive Films – Application to Graphene Anodes

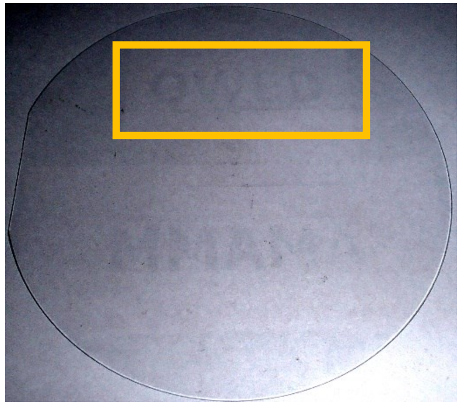


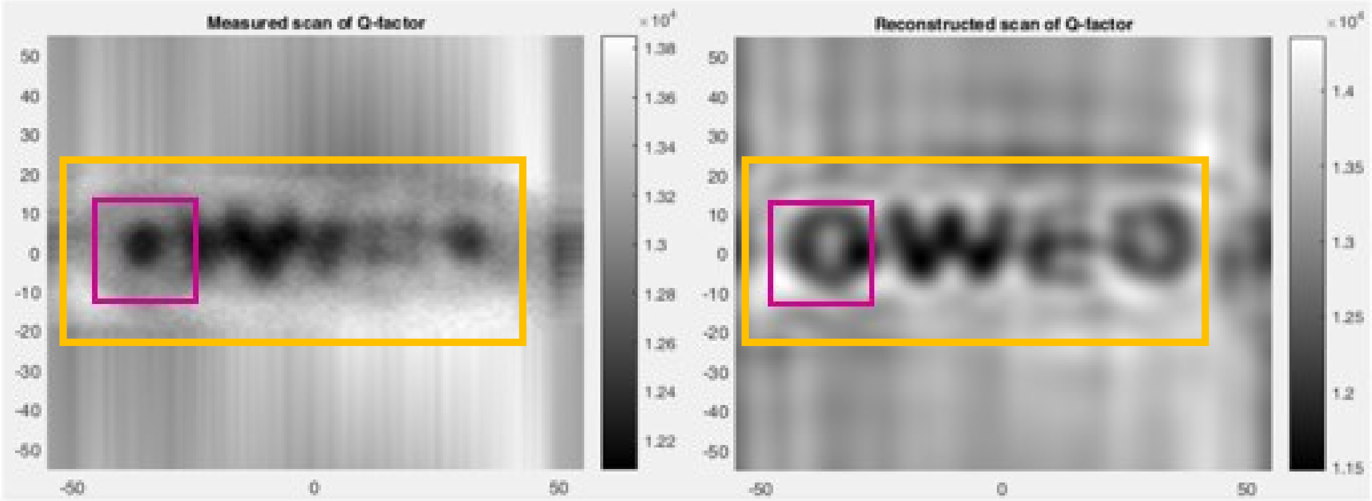


- Scanning area: 50 mm x 75 mm (25 mm margin around SUT)
- Uniform scanning step: 2 mm
- 1014 measurement points
- Avr thickness of the deposited graphene anode layer: 0.130 mm ± 0.02 mm
- Non-uniformities in R_s map due to sample thickness variation
- R_s extracted for average thickness value
- An absolute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

Modelling-Based Resolution Enhancement of Surface Images





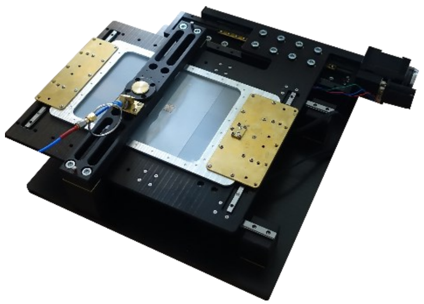


raw image of sample resistivity (measured Q-Factor)

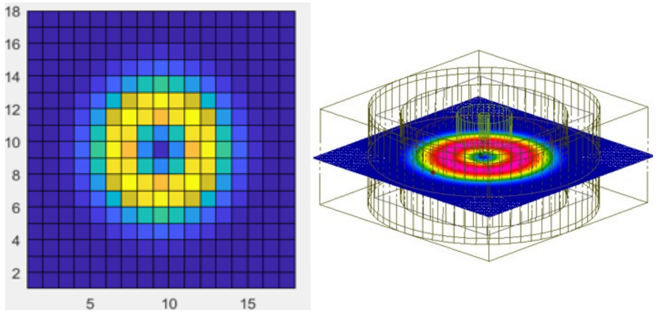
image further deconvolved using SPDR field pattern pre-simulated in QuickWave

MMAMA MATERIA NOVA M-ERA.NET

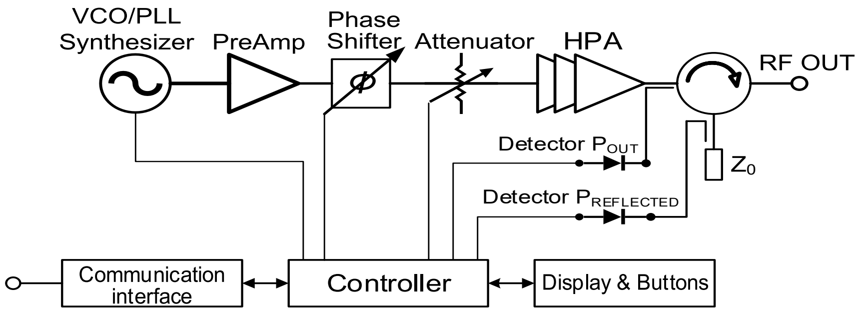
Patterned PEDOT:PSS sample courtesy MateriaNova, Belgium

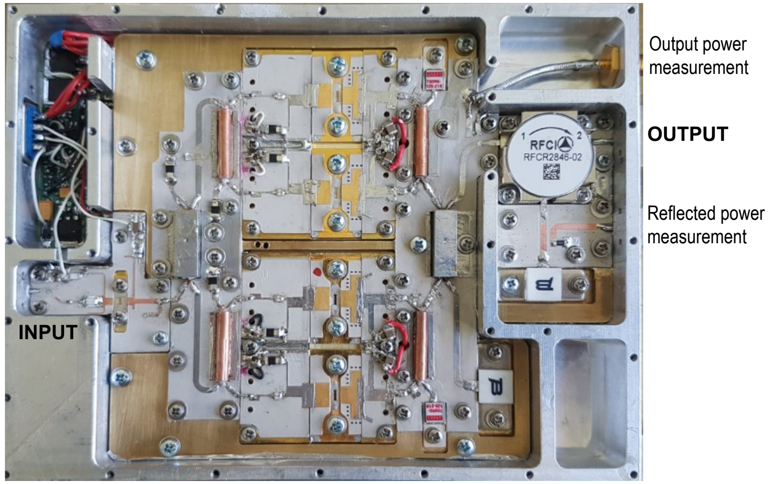


2D SPDR scanner



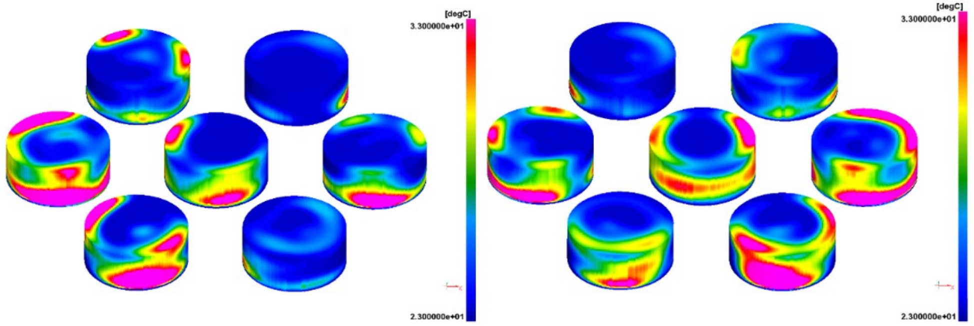
Active - Passive Methodology for Multiphysics Design



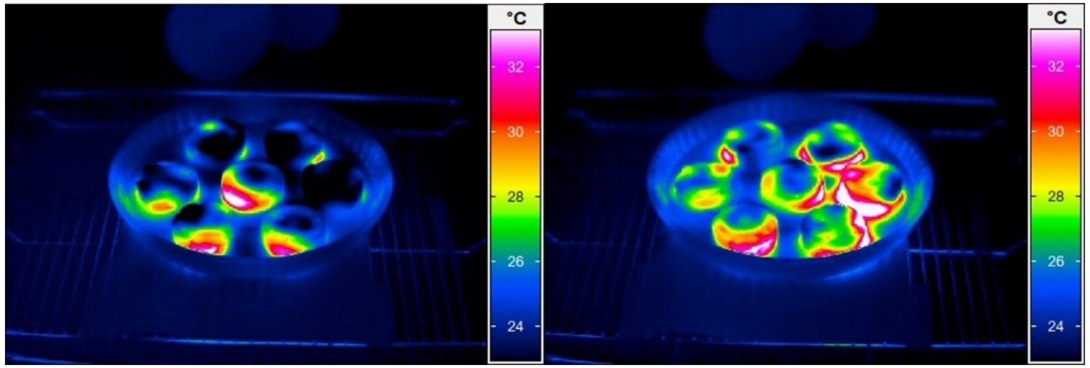


Multifunctional heating source
based on two-stage double-balanced GaN HEMT HPA
(Prof. W.Wojtasiak, Dr. D.Gryglewski Warsaw Univ.Tech.)

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

Horizon Europe: contributions EMMC & EMCC

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.

EuroNanoForum 2021

European Materials Modelling Council

European Materials Characterisation Council

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://zenodo.org/record/4912683#.YbH2USYxm9I

EU Open Exchange of Ideas - EMMC International Worshops

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

In preparation:

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!

New EU Initiative – Ami2030

https://www.ami2030.eu/

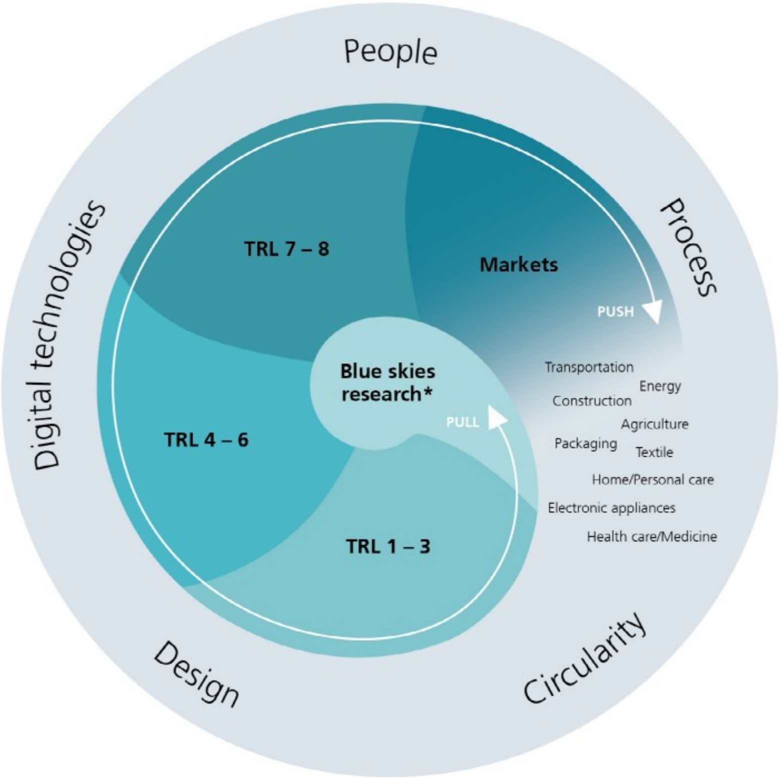
AMI2030 ADVANCED MATERIALS INITIATIVE

MATERIALS 2030 MANIFESTO

Systemic Approach of Advanced Materials for Prosperity – A 2030 Perspective

7 February 2022

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.



life.augmented

UNIVERSITY OF OXFORD

Fraunhofer

cea

INL INTERNATIONAL IBERIAN NANOTECHNOLOGY LABORATORY

umicore

BEDA The Bureau of European Design Associations

QWED

Microwave Theory & Technology ↔ Materials' Science & Technology

EuMA European Microwave Association

EurAAP

MTT-S IEEE MICROWAVE THEORY & TECHNOLOGY SOCIETY

IEEE Antennas and Propagation Society

European Commission

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

EMMC

AMI2030 ADVANCED MATERIALS INITIATIVE

Microwave Theory & Technology ↔ Materials' Science & Technology

European Commission

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

- 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 Slodowska-Curie Actions (MSCA)
  Doctoral Networks & Postdoctoral Fellowships
  are also a good way to get involved

Acknowledgements

The work of my research team at QWED is currently co-funded by:

Nano Bat

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The National Centre for Research and Development

the *Polish National Centre for Research and Development* under contracts *M-ERA.NET2/2020/1/2021* and *M-ERA.NET3/2021/83/I4BAGS/2022*.

M-ERA.NET

M-ERA.NET 3 has received funding from *the European Union's Horizon 2020* research and innovation programme under grant agreements *No 958174*.

ULTCC6G_EPac

I4Bags

We kindly acknowledge the collaborations with our partners in the above European projects.

iNEMI International Electronics Manufacturing Initiative

We acknowledge the iNEMI "5G" partnerships for round-robin experiments and discussions.

Special thanks to all our industrial clients and partners for driving our developments and their kind permission to publish selected industrially-representative results.

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 facilite:

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

- not only mamaging 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

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