discover accurate EM modelling

From Computational Electromagnetics to Modelling-Based Characterisation of Materials for Electronic and Energy Technologies

Malgorzata Celuch
Co-Founder, President, Senior Scientist
QWED Sp. z o.o., Poland

4th EMMC International Workshop 2023

Vienna
26-28 April 2023

Nano Bat

M-ERA.NET

The National Centre for Research and Development

ULTCC6G_EPac

I4Bags

Talk Outline

1. QWED in a Nutshell

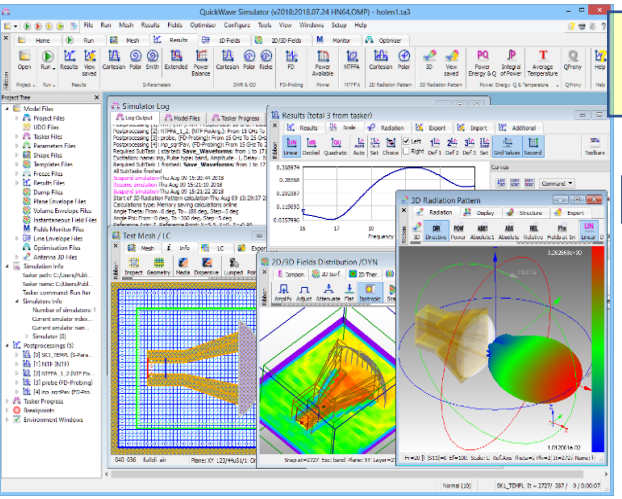
2. Origin of QWED's Electromagnetic Modelling (back in 1980s!)

3. Origin of Material Measurements at QWED (almost as far back in time...)

4. Twinned MODA + CHADA (2019)

5. Acknowledgements & Outlook

25 years in a Nutshell

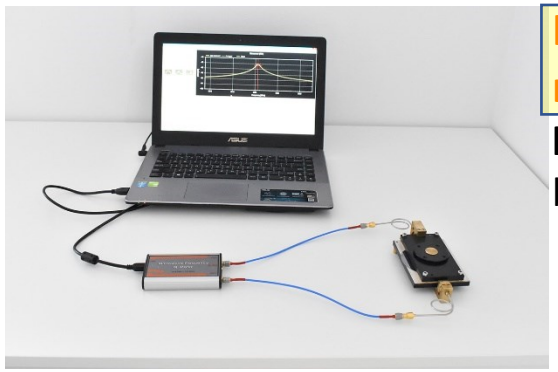


Electromagnetic simulation & design software, 3D & BOR 2D tools

based on 300+ publications by:

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

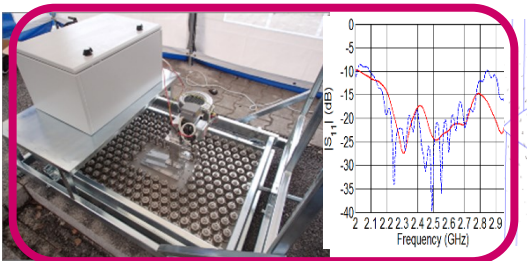
dr.M.Celuch, President of QWED

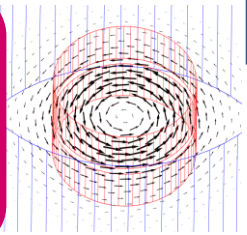


Instruments for precise material measurements

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.

ULTCC6G_EPac – development & application of novel ceramics for 5G & beyond

I4BAGS – modelling & characterisation of ion-implanted battery & graphene-enabled devices

What Is Computational Electromagnetics?

Electromagnetic Modelling, Electromagnetic Simulations, Computational Electromagnetics (CEM)…

*solving Maxwell **Physical Equations***

general (integral):

$$\oint_l \vec{E}\,\overrightarrow{\mathrm{dl}} = -\frac{\mathrm{d}}{\mathrm{d}t}\iint_S \vec{B}\cdot\vec{\mathbf{n}}\,\mathrm{ds}$$

$$\oint_l \vec{H}\,\overrightarrow{\mathrm{dl}} = \iint_S \left(\vec{J} + \frac{\partial \vec{D}}{\partial t}\right)\cdot\vec{\mathbf{n}}\,\mathrm{ds}$$

$$\oiint_s \vec{D}\cdot\vec{\mathbf{n}}\,\mathrm{ds} = \iiint_V \rho\,\mathrm{dv}$$

$$\oiint_S \vec{B}\cdot\vec{\mathbf{n}}\,\mathrm{ds} = 0$$

$$\oiint_s \vec{J}\cdot\vec{\mathbf{n}}\,\mathrm{ds} = -\iiint_V \frac{\partial \rho}{\partial t}\,\mathrm{dv}$$

popular (differential):

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

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

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

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

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

*subject to **Material Relations***

general:

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

typical:

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

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

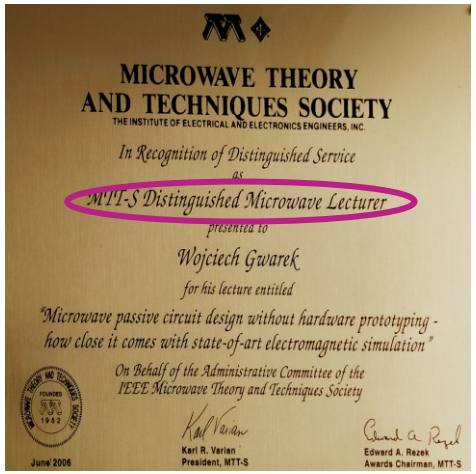
$$\vec{J} = \underline{\underline{\sigma}}\cdot\vec{E}$$

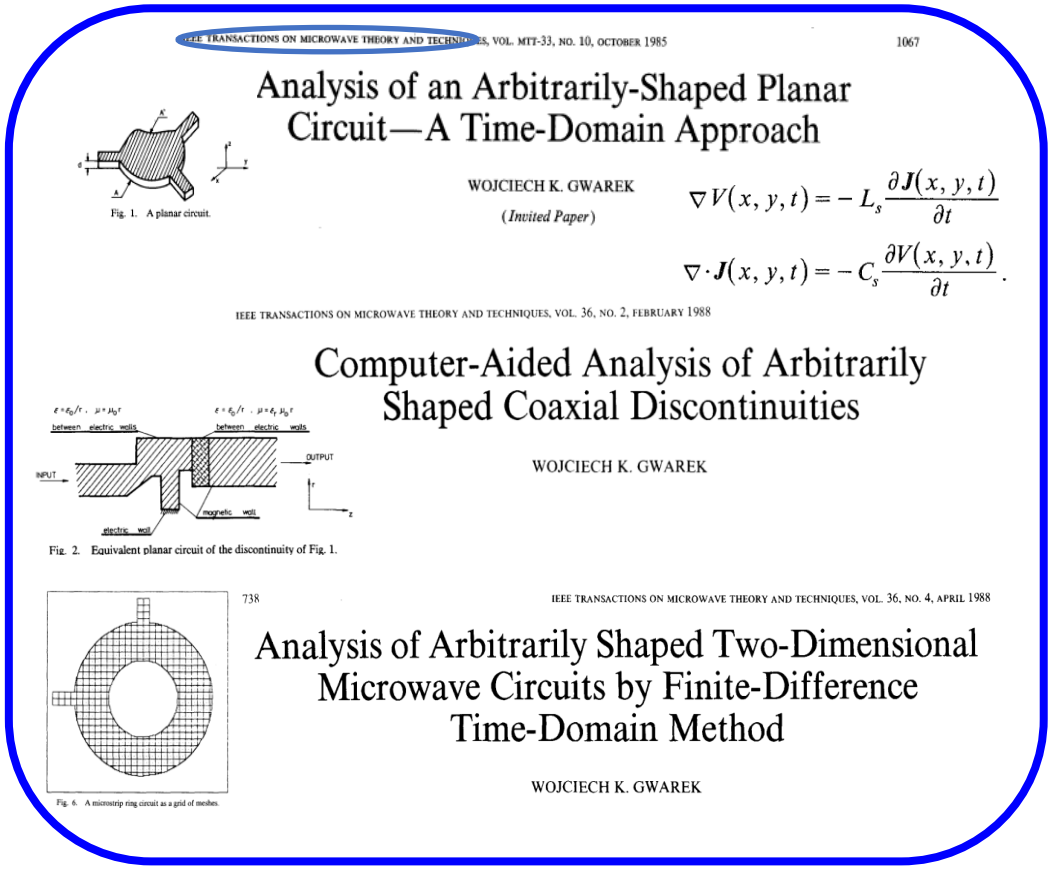
QWED's expertise:
fast & accurate solutions
in complex geometries,
wide frequency range

expertise needed

Origins of QWED's Electromagnetic Modelling

IEEE- awarded research of Prof. Wojciech Gwarek

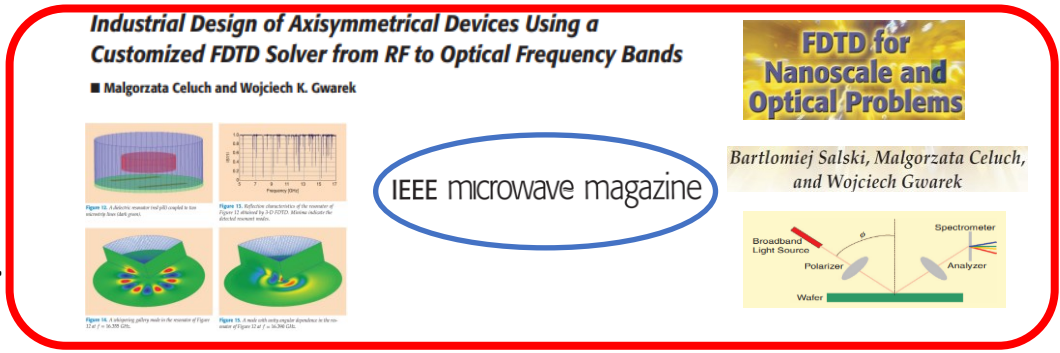




New conformal FDTD method:

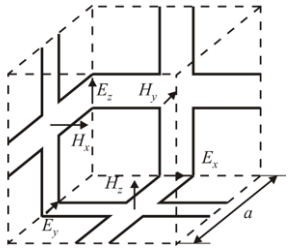
+ Conformal Space Discretisation
  (similar to FEM - arbitrary shapes).

+ Time-Domain Solution
  (faster than FEM - wide frequency band, diagonal mass matrices).

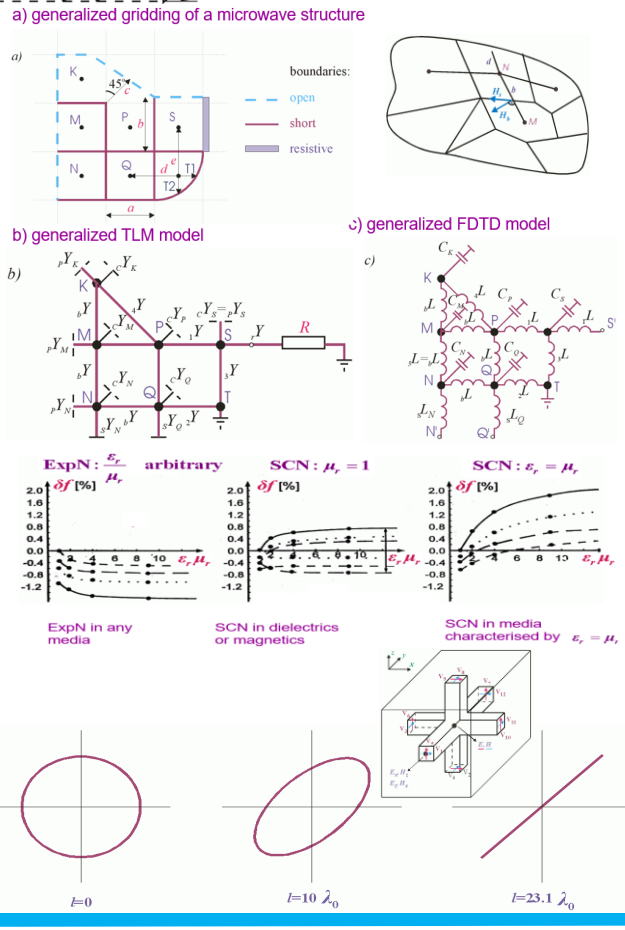


My Contributions 1990s

FDTD versus TLM Theorem of Formal Equivalence



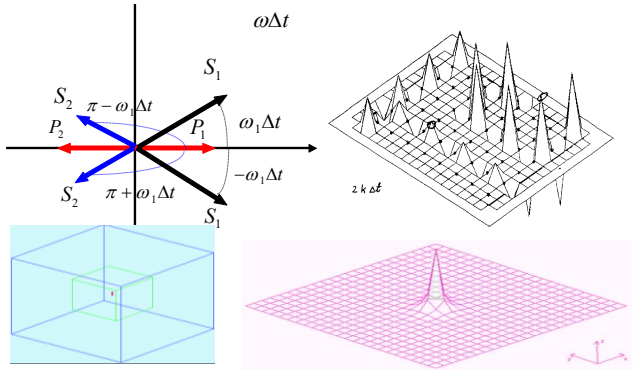
nodes: FDTD discretisation of Maxwell eqs.
connecting lines & stubs: TLM discretisation of Huygens principle



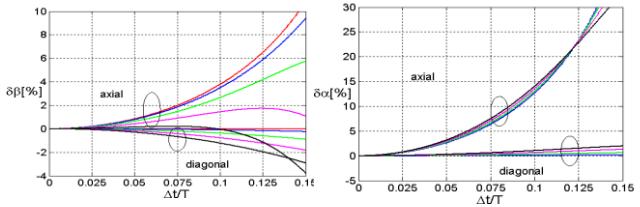
Generalised dispersion relations Theory of P- and S-eigenmodes

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

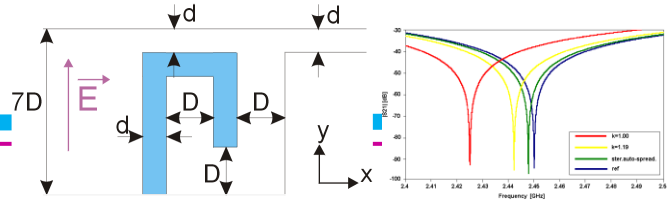
$$\omega_{ph}^2[-\omega_{ph}^2\mu\varepsilon + \beta_{xph}^2 + \beta_{yph}^2 + \beta_{zph}^2]^2 = 0$$



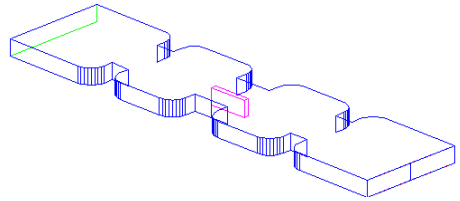
Dispersion in lossy media

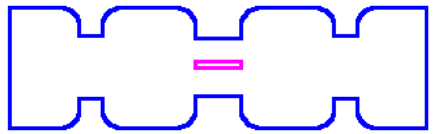


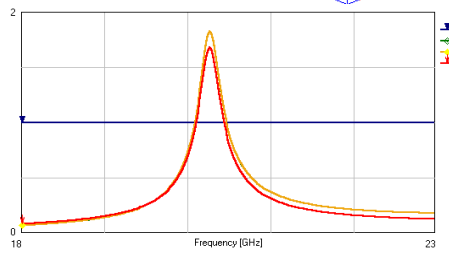
Field singularities

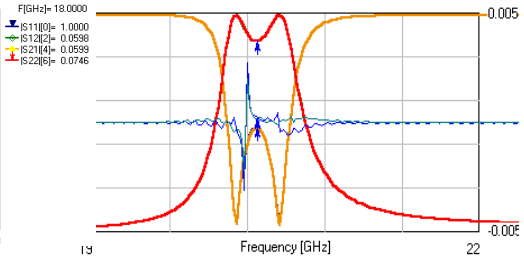


Generalised extraction of S-parameters in multi-modal transmission lines (incl. evanescent modes)

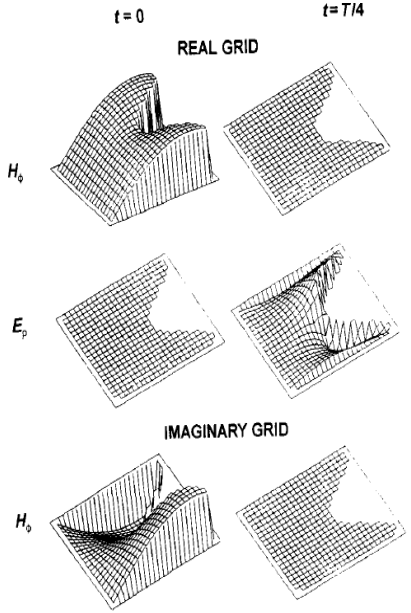




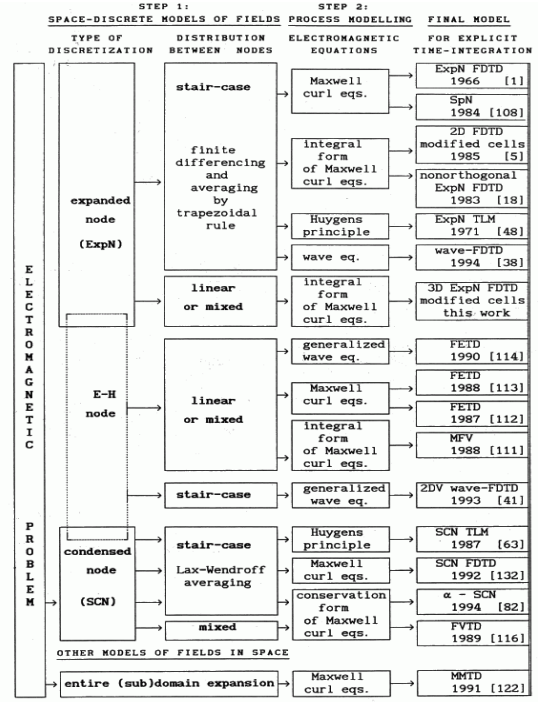




Periodic & vector 2D FDTD and TLM in real & complex form



Classification of time-domain methods

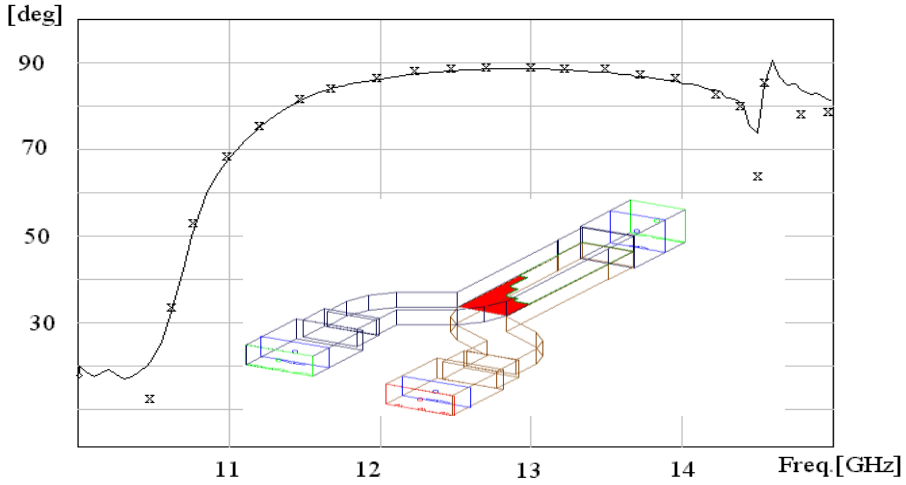


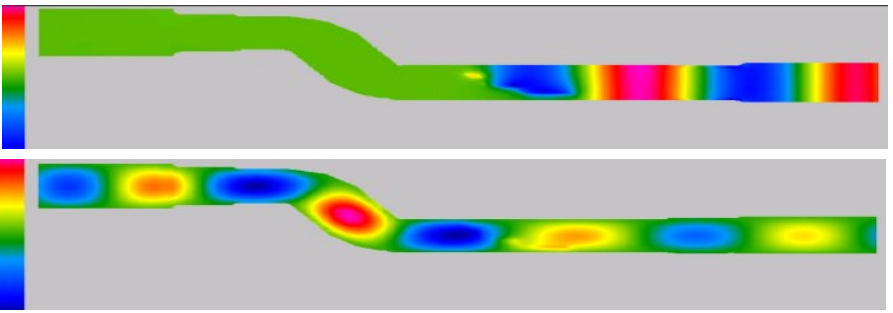
QuickWave™ original applications in cosmic reseach

Septum polariser by SES

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

below: differential phase-shift



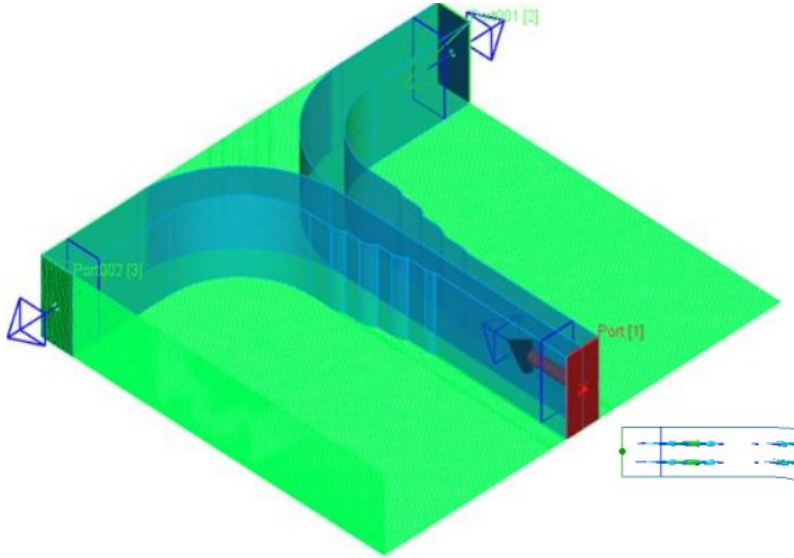


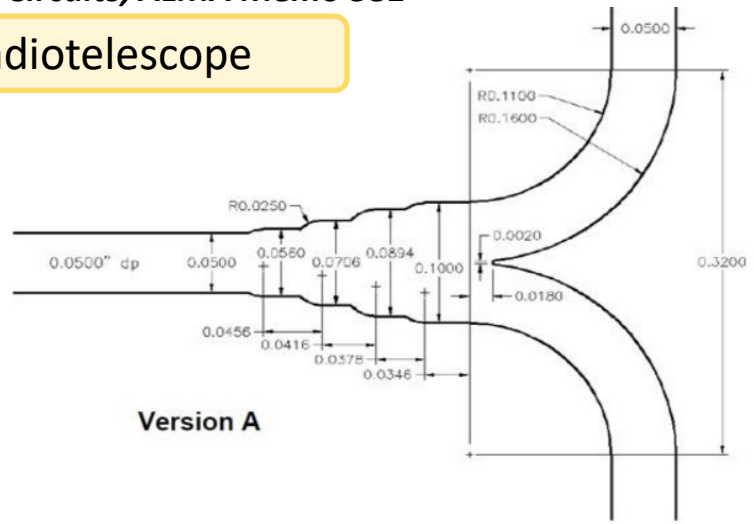
propagation of two polarisations at centre frequency

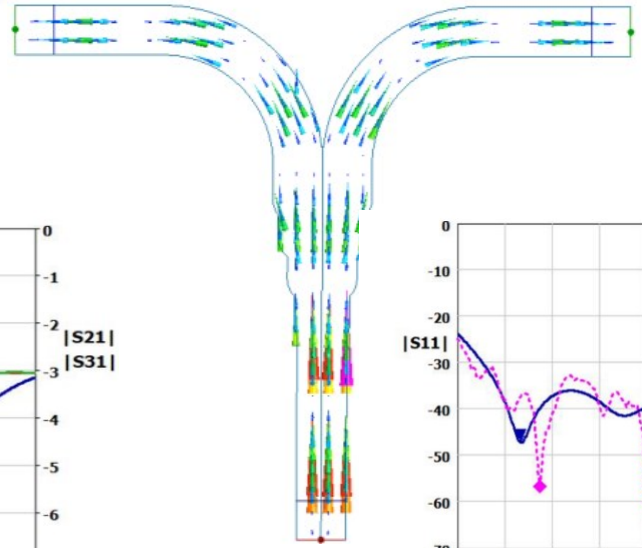
E-plane Y-junction by National Radio Astronomy Observatory, Charlottesvile, VA

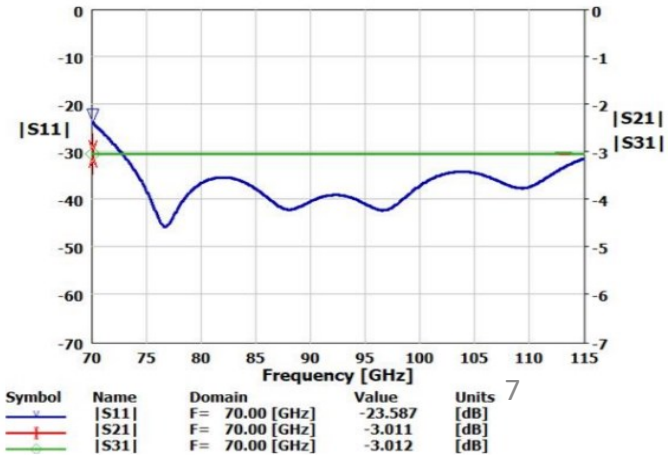
after A. R. Kerr, Elements for E-Plane Split-Block Waveguide Circuits, ALMA Memo 381

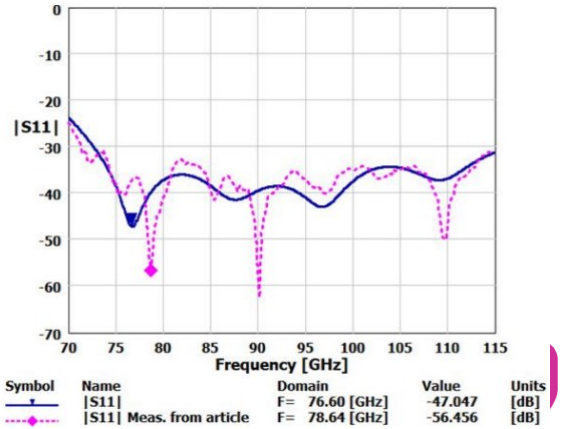
ALMA = Atacama Large Millimiter Array radiotelescope







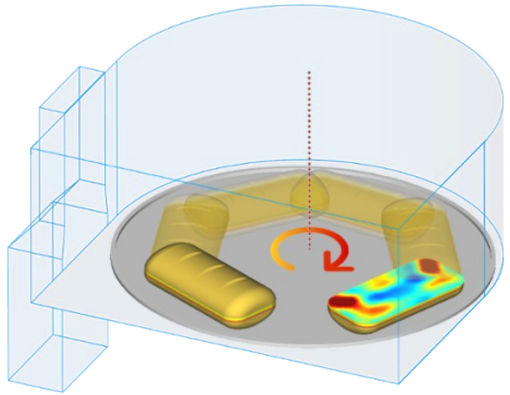




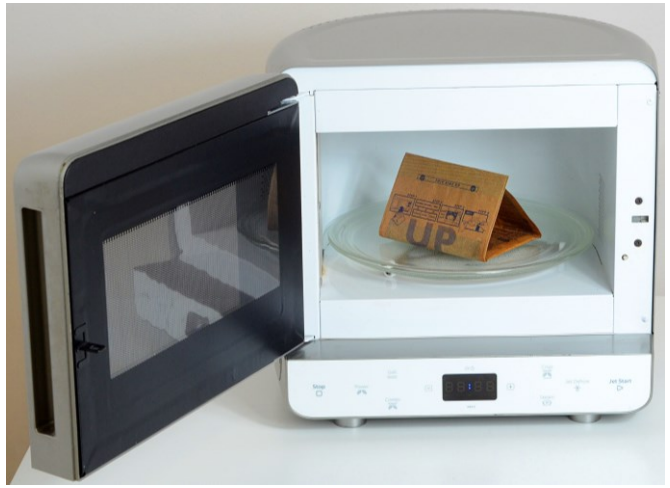
Modelling of Microwave Processing of Materials - for Research, Industry, Home

EMB-1998, Linkoping, Sweden:

complex geometries of ovens & feeds, enthalpy-dependent material parameters, load rotation, microwave popcorn



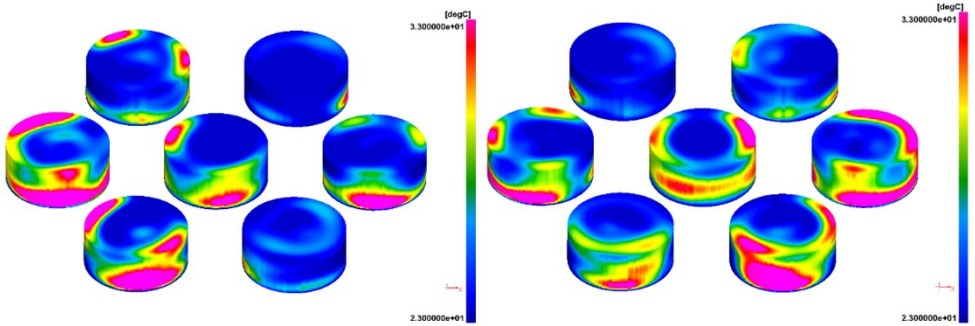
Whirlpool – MAX domestic oven



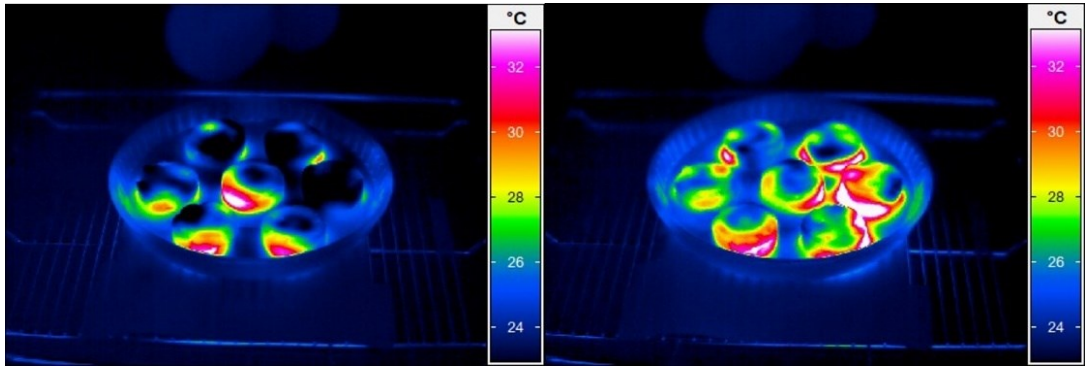
Elsevier, 2020

"Development of packaging and products for use in microwave ovens"

Temperature in mashed potato cookies,
for different relative phase shifts between two solid-state sources



QuickWave modelling by QWED

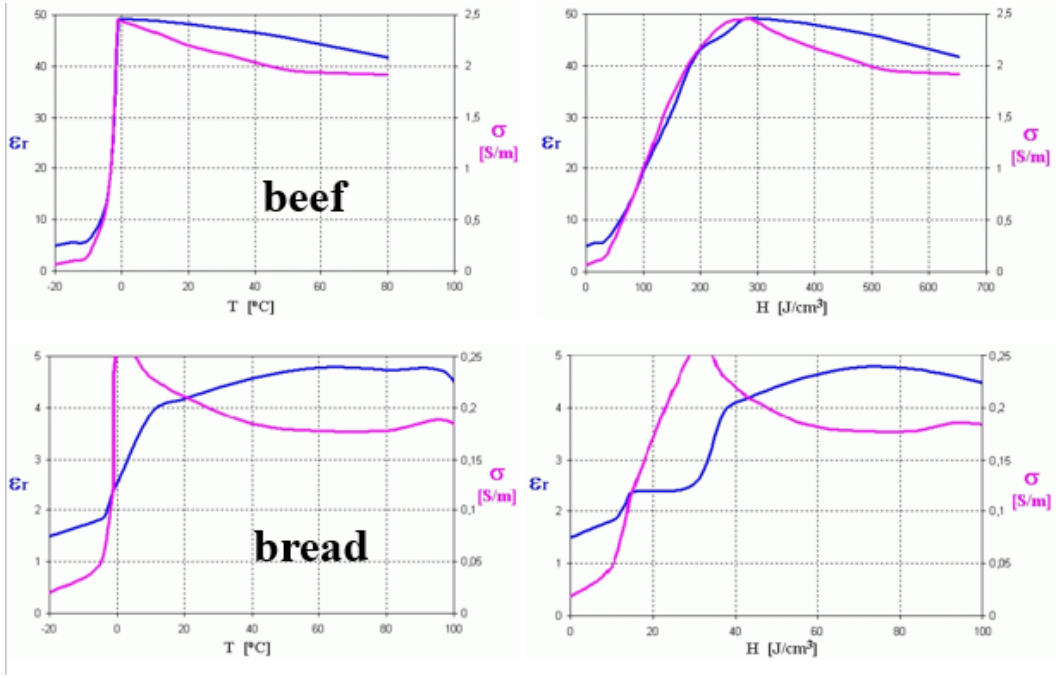


Photos courtesy BSH HAUSGERATE GmbH,
Traunreut, Germany.

B/S/H/

Multiphysics Modelling for Microwave Heating Applications

QW-BHM 2000



FDTD analysis with sinusoidal excitation at ***f=f0***

Calculation of 3D pattern of ***dissipated power*** $P_{avg}(x,y,z)$

Enthalpy update in 3D domain

$$H^{n+1}(x,y,z) = H^{n}(x,y,z) + \frac{P^{n}_{avg}(x,y,z)\Delta\tau^{n}}{\Delta V(x,y,z)}$$

Temperature update in 3D domain

$T(x,y,z) = T[H(x,y,z)]$

from *.pmo file

Load movement/rotation

Translation of the object and thermal quantities along user-defined trajectory

Calculation of heat transfer

Enthalpy and ***temperature*** update in 3D domain

Material and ***thermal parameters*** update in 3D domain

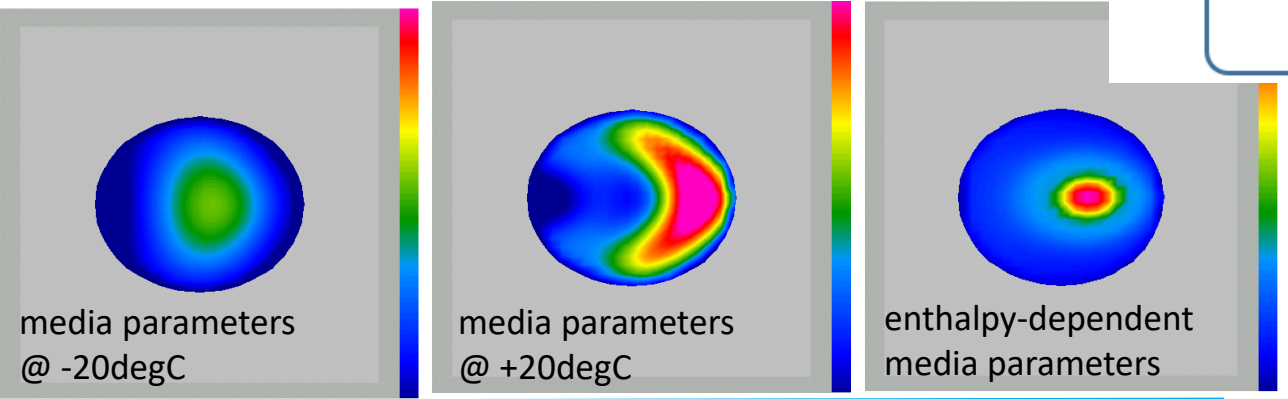
$\varepsilon(x,y,z) = \varepsilon[T(x,y,z)]$

$\sigma(x,y,z) = \sigma[T(x,y,z)]$

from *.pmo file

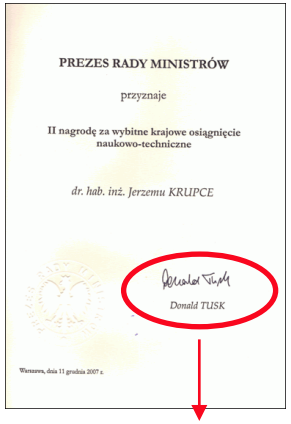
Source tuning to ***f=f1***

Changing operating frequency: automatically to the deepest resonance or manually upon user's criterion



Material Measurements: from WUT to QWED

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

Warszawa, dnia 11 grudnia 2007 r.

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

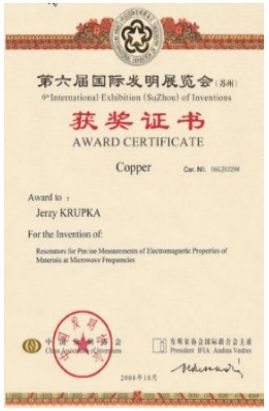

DIPLOMA

Eureka!

THE BELGIAN AND INTERNATIONAL TRADE FAIR FOR TECHNOLOGICAL INNOVATION

Jerzy KRUPKA

Médaille d'or


第六届国际发明展览会

6th International Exhibition (SuZhou) of Inventions

获奖证书

AWARD CERTIFICATE

Copper

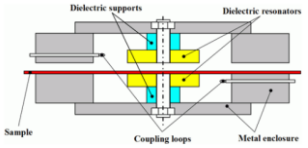
Award to

Jerzy KRUPKA

For the Invention of:

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

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



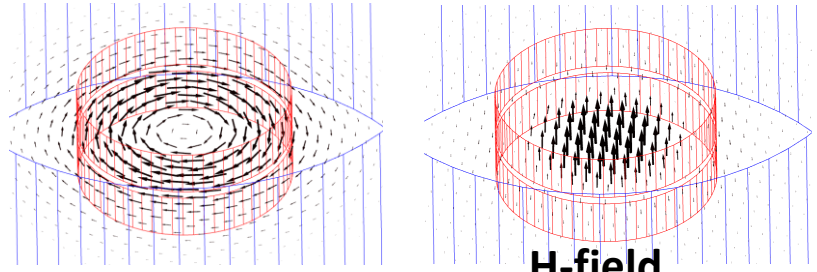
1000th unit sold in 2020.

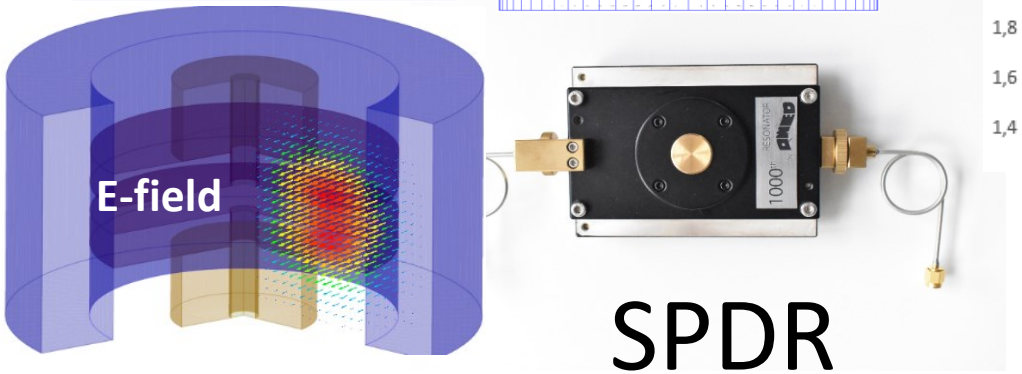
Today ~120 units/year.


Agilent Both
IEEE IMS 2006, San Francisco, CA

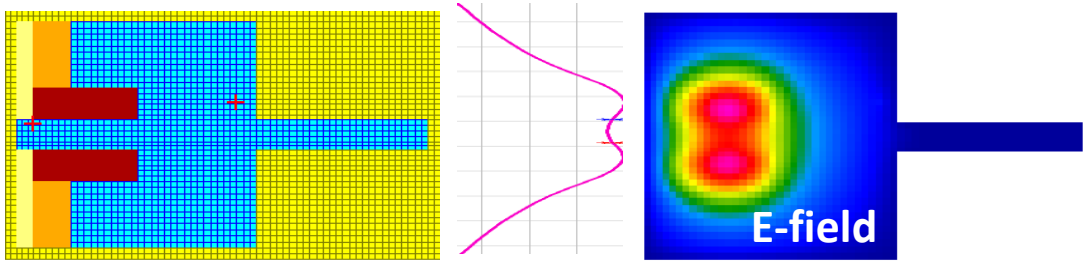
MMA-2010, Warsaw PL
co-organised by QWED & WUT

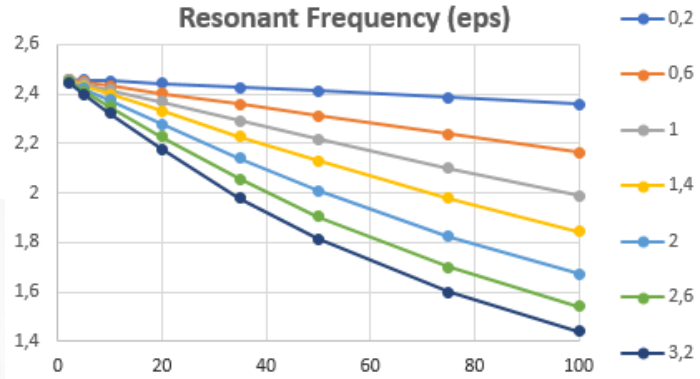
Materials' Characterisation Enhanced by Accurate Computational Modelling





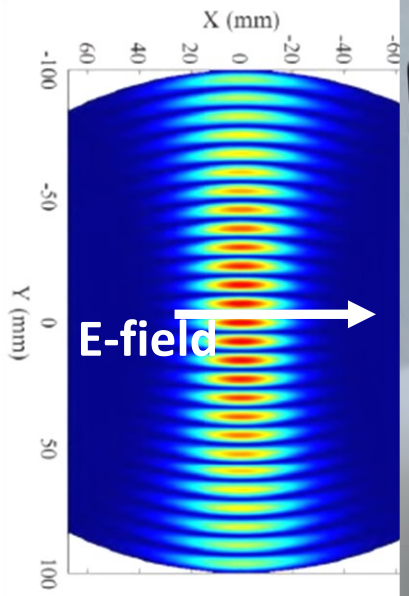
SPDR





Simulated Data Base
for Calibration
& Measurement Support

FPOR

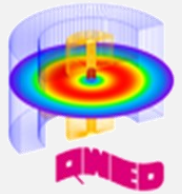


Field distributions obtained from full-wave EM simulations (QuickWave™ software by QWED).

Current Work: Bridging Computer Modelling with Material Measurements

Commercial since 1997
QuickWave Simulation Software
~1000 licences implemented

THE EUROPEAN ICT PRIZE WINNER



Applicator design
& model for
parameter extraction

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

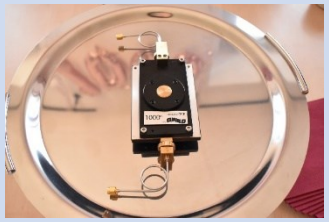
INNOVATION

Material measurements

Accurate material
parameters
(constitutive
relations)

Commercial resonator test-fixtures since 2001

1000th unit sold in 2020



Open Platform Examples & Tools

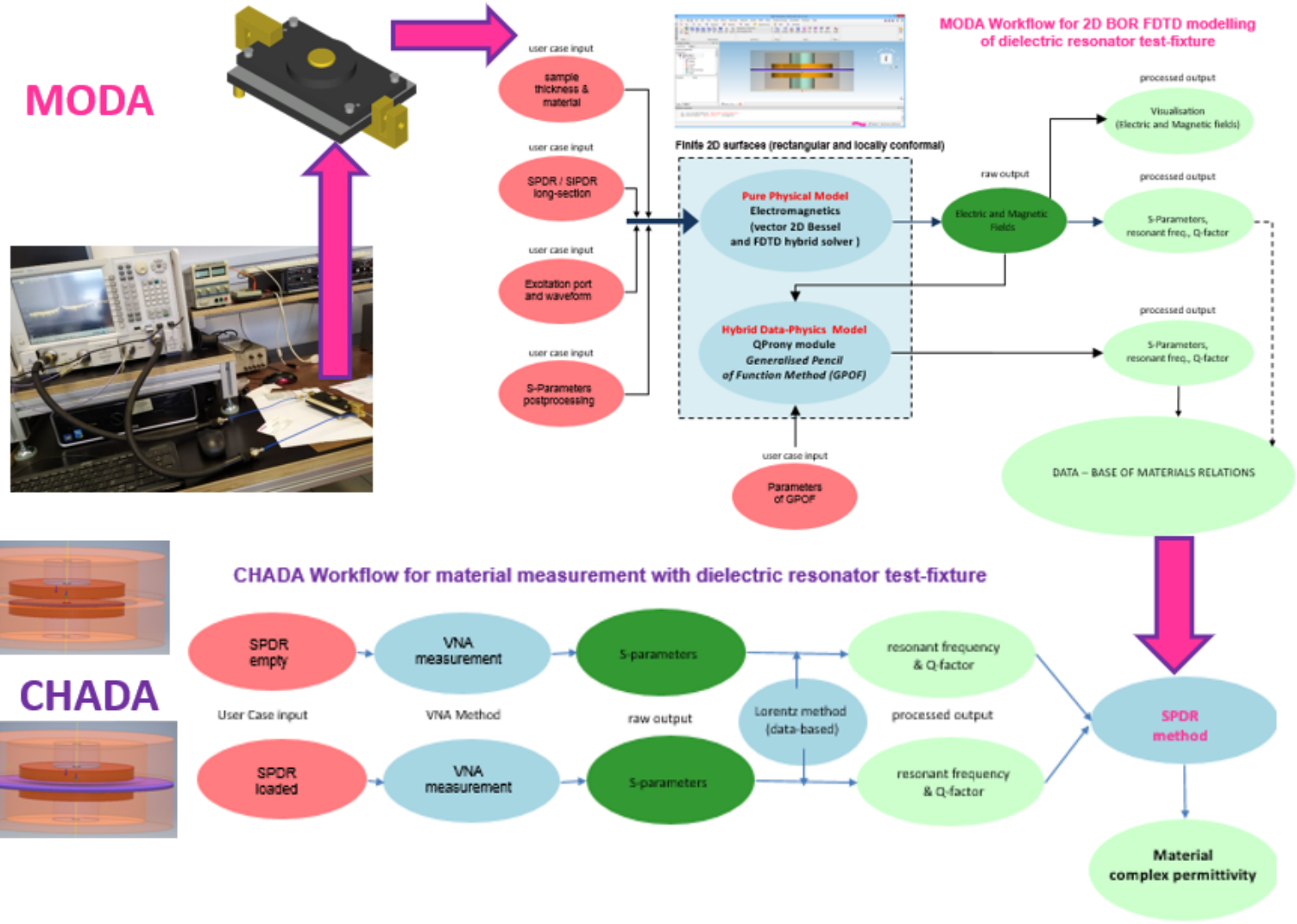
QW-Modeller for QuickWave
Free general purpose 3D CAD modeller for QuickWave.

Open Platform Examples:

SMM tip presented at Numerical Electromagnetic

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

Twinned MODA + CHADA Representation of QWED's Research



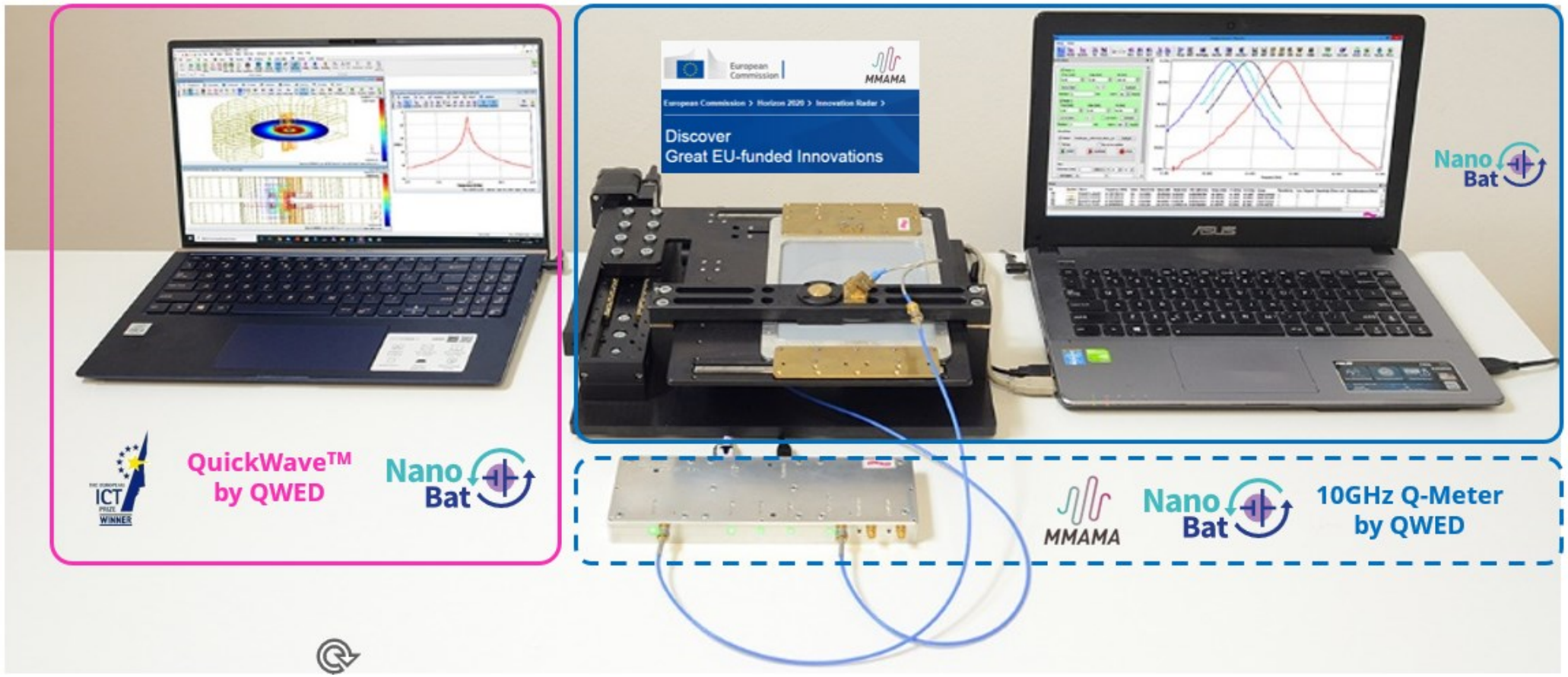
Behind each measure
is a model of the physical
processes assumed to be taking place
in the material.

The measurement
serves to identify those model parameters.

Hence, a reliable simulation
of the measured scenario
is needed to
validate the constructed model
under various conditions.

Implementation of Twinned MODA + CHADA:

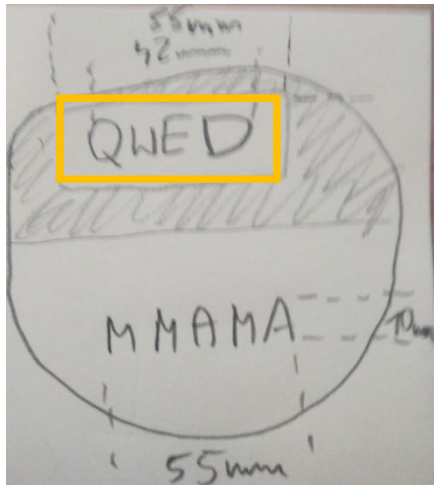
Modelling-based System for GHz Imaging of Material Surfaces

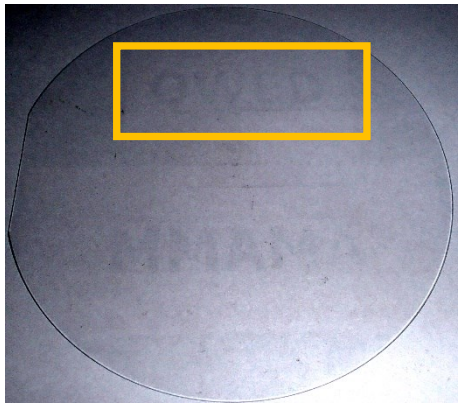


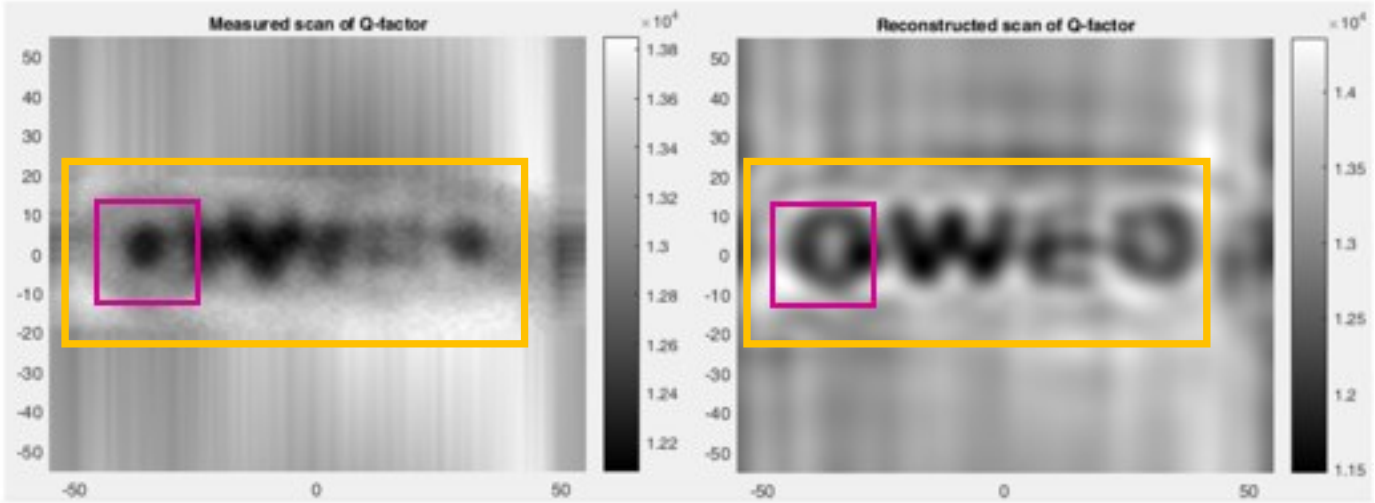
Finalist of the European Innovation Radar Prize 2021

2D Imaging of Organic Semiconductors for Solar Cells

Modelling-Based Resolution Enhancement of Surface Images







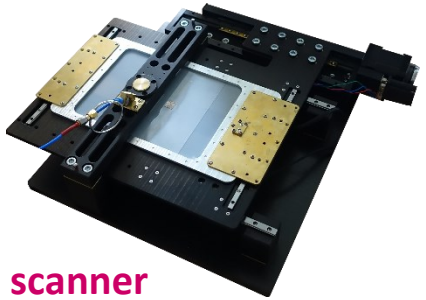
Patterned PEDOT:PSS sample
courtesy MateriaNova, Belgium

raw image of sample resistivity
(measured Q-Factor)

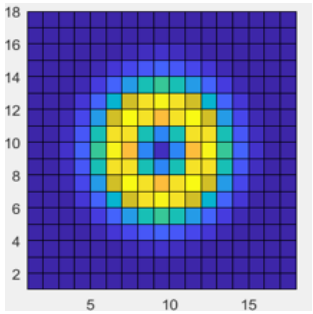
image further deconvolved
using SPDR field pattern
pre-simulated in QuickWave

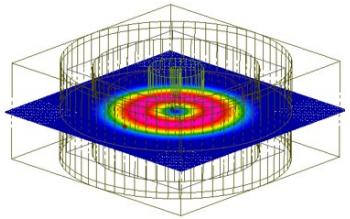
MMAMA

MATERIA NOVA



2D SPDR scanner

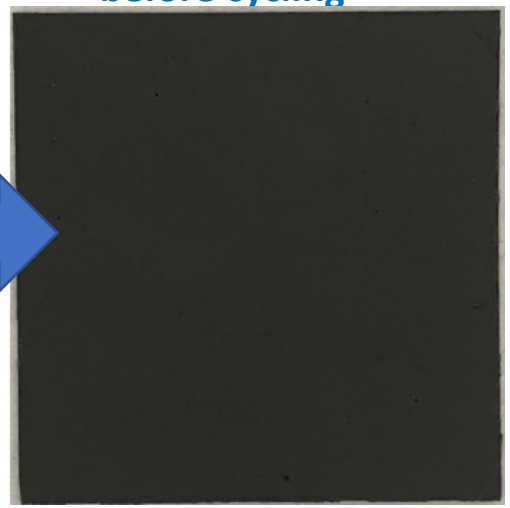




2D Imaging of Conductive Films – Graphene Anodes Before & After Cycling

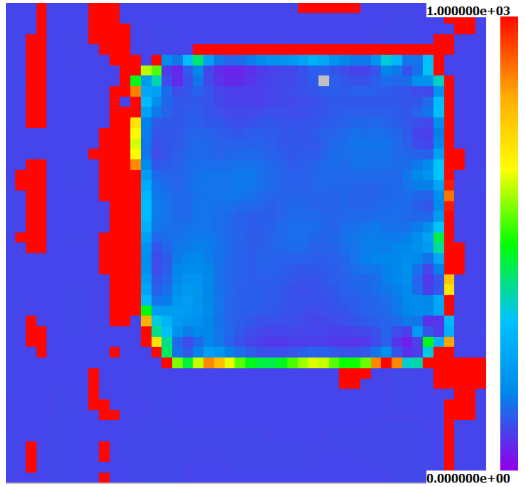
Copper electrode

Graphene –based battery anode before cycling



Scanning range: 80 x 80 mm,
scanning step: 2mm
Measurement points: 1681
Scanning time: ca. 2h

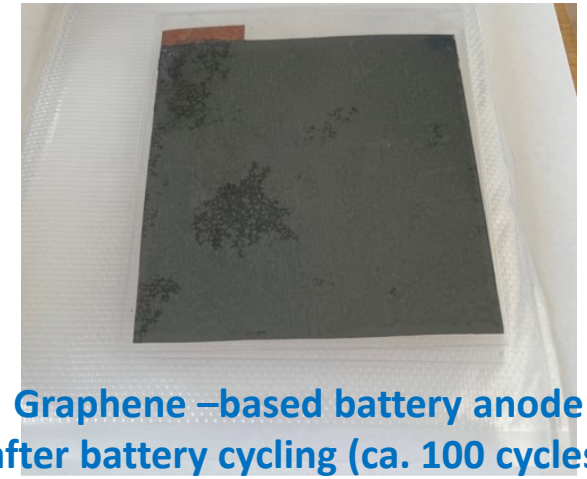
2D map of Rs [Ω/sq.]



values of Rs [Ω/sq.]

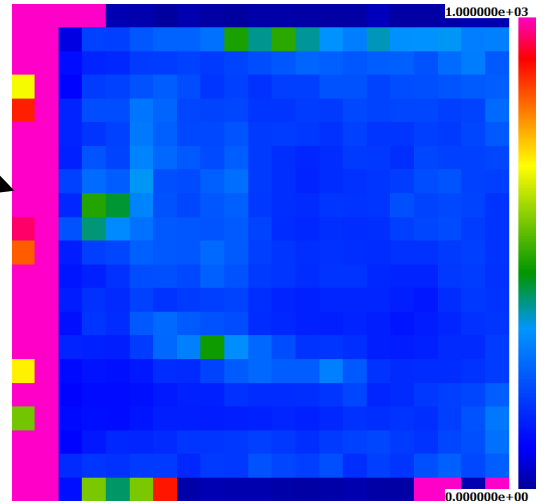
85 – 160 [Ω/sq.]

**courtesy PLEIONE Energy, Greece*



Graphene –based battery anode after battery cycling (ca. 100 cycles)

Sample edge (protecting foil)



110 – 340 [Ω/sq.]

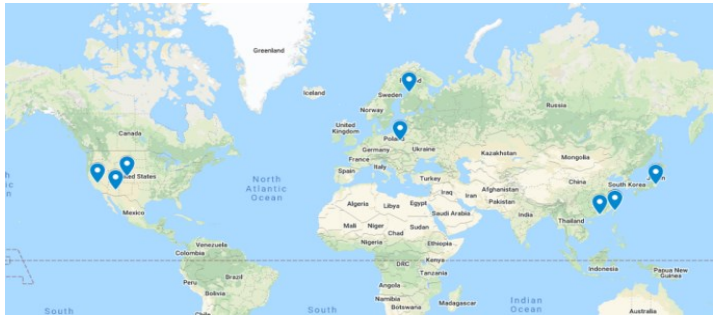
increase indicates SEI formation

Recent Industrial Benchmarking: iNEMI 5G Round Robin Overview

iNEMI International Electronics Manufacturing Initiative

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



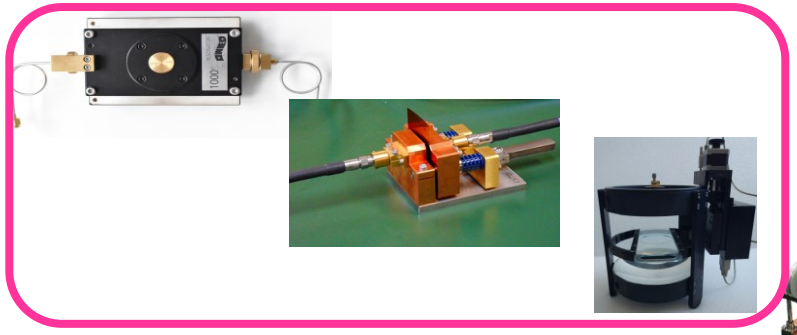
Sample Material Requirements
- Stable, Low loss
- Low moisture absorption / temperature dependency
- Isotropic
- Good mechanical & handling properties

1st Project Stage
- Precision Teflon
- Cyclo Olefin Polymer

2nd Project Stage
- Rexolite
- Fused Silica

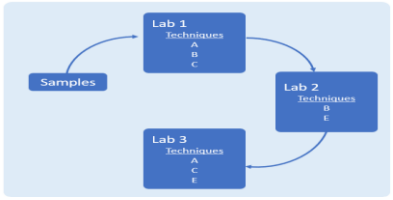
Industrial
- Automotive

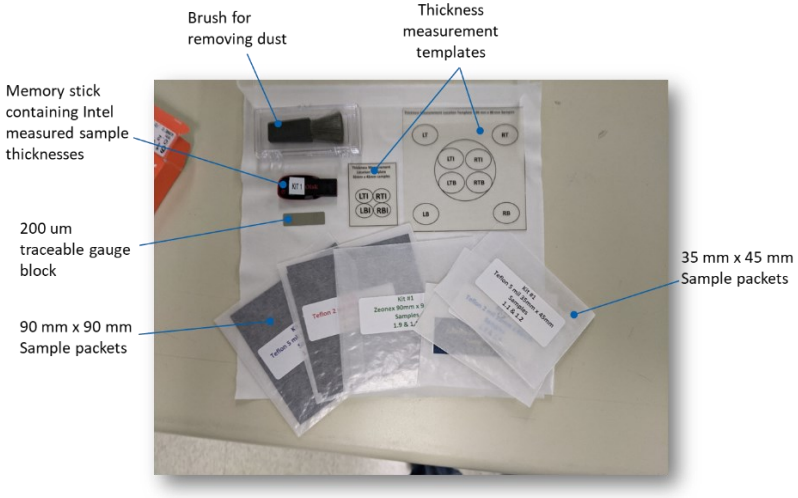
Techniques Included
- Split Post Dielectric Resonator
- Split Cavity Resonator
- Fabry-Perot
- Balanced Circular Disk Resonator



→ Frequency Span : 10GHz – 100GHz with overlaps

10 Laboratory Round Robin





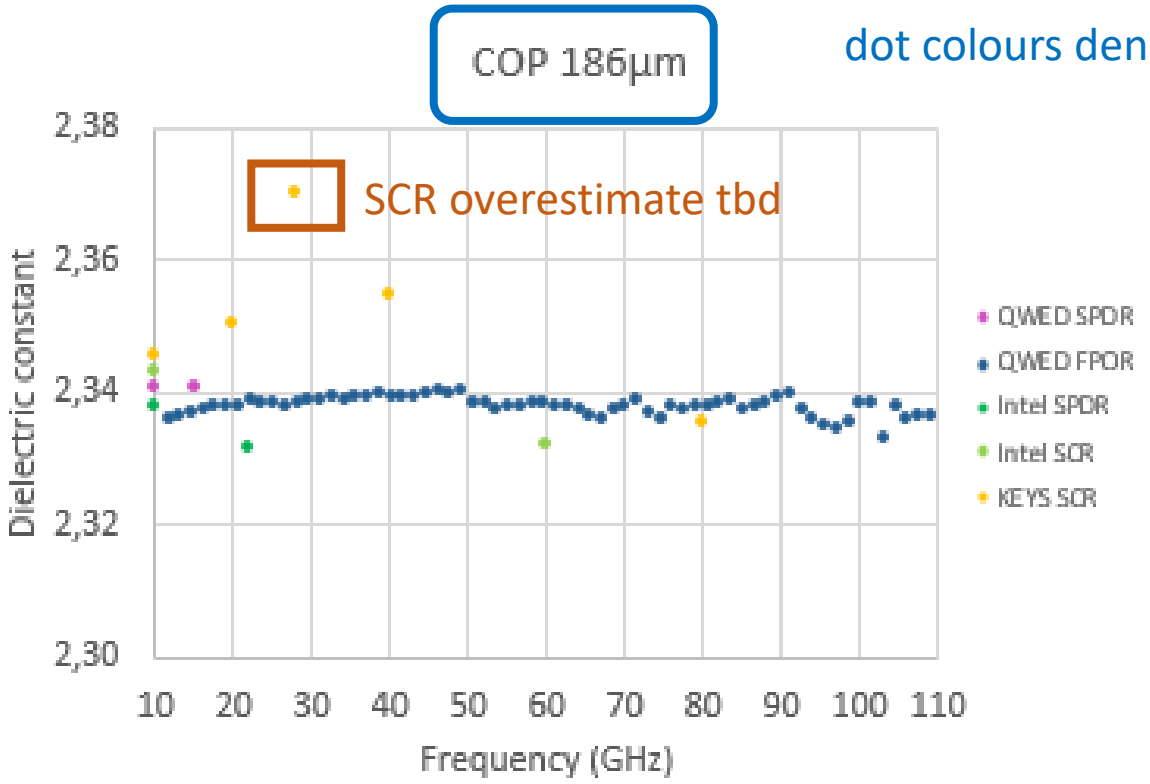
10 Sample Kits Created
- Sample sizes 35 mm x 45 mm, 90 mm x 90 mm
- circulated between 10 labs

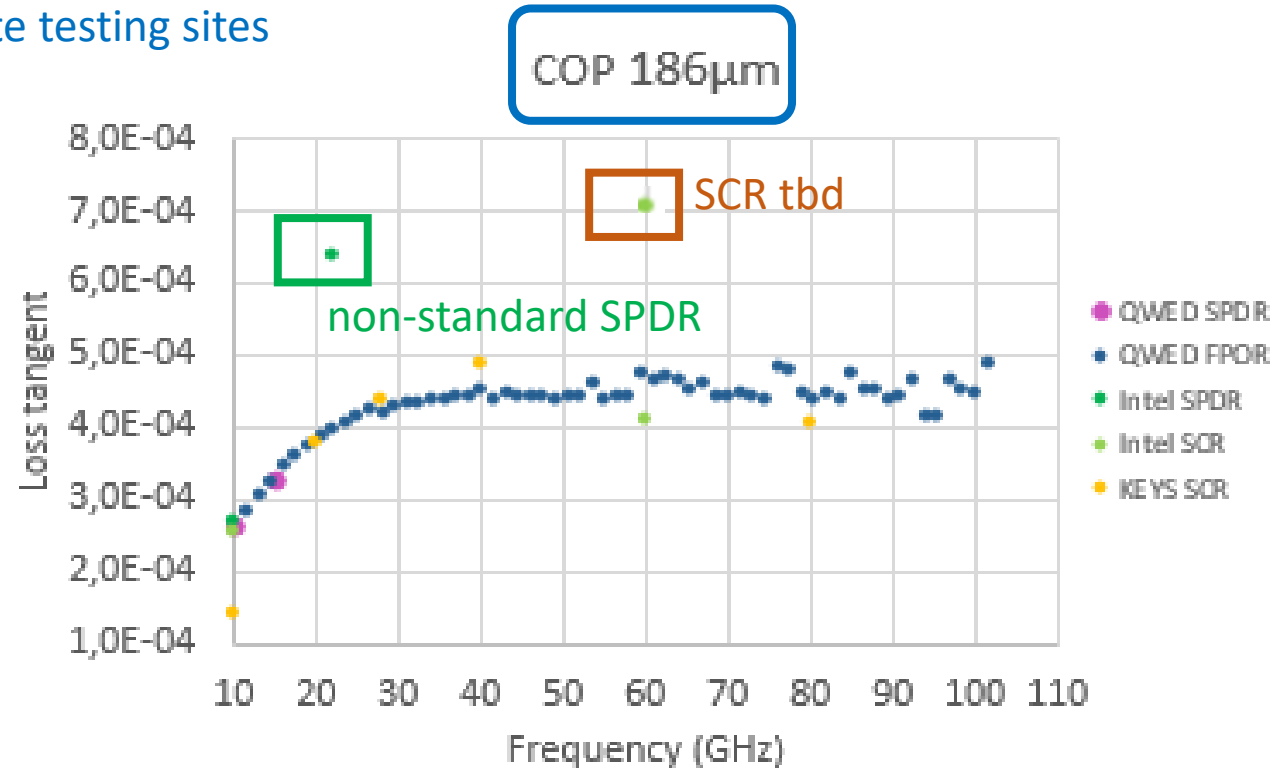
iNEMI 5G Round Robin: Example Results

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

QWED's Modelling & Characterisation Competences & Products Today

Continuum Physics-Based Modelling

Electromagnetics, Heat Flow, Load Movement,
Fluid Flow, Thermal Radiation…

QuickWave™ software gave origin to QWED.

First licence sales in 1997
(to NASA-related labs and a leading microwave oven producer).

By today: ~ 1000 licences implemented worldwide.

Fast & accurate solutions with arbitary Boundary Conditions.

Wide frequency band covered (including 5G/6G technologies).

Compares favourably to competitiors' software.

Needs more material data.

Material Characteristion

Electrical & Dielectric & Magnetic

Industrial testing of materials.

Validation of material models & designs.

Superior accuracy (especialy for practically relevant low-loss materials).

Fast, easy-to-use, non-destructive.

Affordable & popular.

120-200 instruments sold per year.

Contributions to Open Modelling Platforms

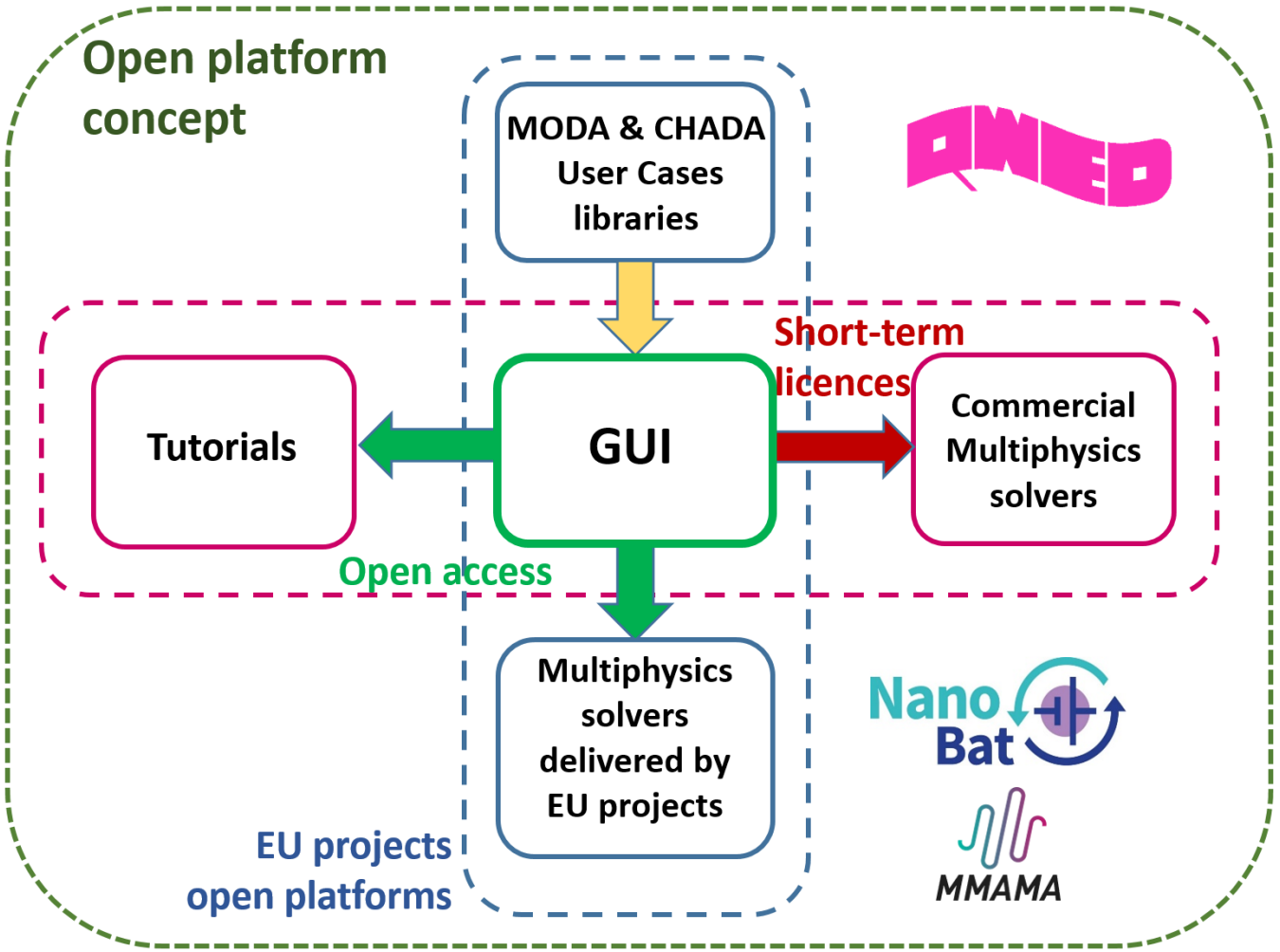
Leading Team

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



Contributions to TG 1.1 of EMMC FA 1 welcome!

M-ERA.NET I4Bags

Nano Bat

QWED

Contributions to European Initiatives and Policy Making

2008 Paris, France

Consolidating Research and Innovation for European SMEs Conference
Paris, France
September 15-16, 2008

Dr. M. Celuch was an invited speaker in the high level Conference jointly organised by the European Commission and OSEO ***"Consolidating Research and Innovation for European SMEs: How to do more and better"***, which took place at the French Ministry for Economy, Industry and Employment, place on September 15-16, on the occasion of the French Presidency of the European Union. Video recordings of the Conference are available at http://www.ue-recherche-et-pme.oseo.fr/. Dr. Celuch participated in Debate: *How to adapt support for SMEs within an enhanced networking approach*.

The European Commission also organised, in parallel with and in complement to the main conference, a ***dedicated EC press programme*** for journalists present at the Conference. QWED was proud to be ***one of fifteen European research success stories*** selected for presentation.

EMMC

Materials characterisation challenges to support the industry transition in the digital era

MODA and CHADA; challenges and opportunities for integration and exploitation to industrial stakeholders beyond EU projects.

N. Adamovic[1], G. Goldbeck[2], M. Celuch[3]
1] TU-Wien, Vienna, Austria. H2020 OntoCommons, OntoTrans
2] Goldbeck Consulting Ltd, Cambridge, UK. H2020: OYSTER, NanoMECommons
3] QWED. Poland. H2020 NanoBat

nanoMECommons Co-Creation Workshop
13 December 2021

zenodo Search Upload Communities

June 8, 2021 Report Open Access

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

Adamovic, Nadja; Boskovic, Bojan; Celuch, Małgorzata; Charitidis, Costas; Friis, Jesper; Goldbeck, Gerhard; Hashibon, Adham; Hurtós, Esther; Sebastiani, Marco; Simperler, Alexandra

Materials are Key Enablers for Green & Digital Transition

IndTech 2022

QWED

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ULTCC6G_EPac

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

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.

Thank you for your attention!

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

May 2022: QWED team celebrating our 25 years

- and looking forward to new collaborations and new challenges for the next 25 years

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