Thessaloniki, Greece
8 July 2021

ISFOE Session (hybrid): ***Open Innovation, Standardisation and Business Development***

Linked CHADA and MODA for GHz characterisation and modelling of energy materials in the H2020 NanoBat project

Malgorzata Celuch and Marzena Olszewska-Placha

QWED Sp. z o.o.
Warsaw, Poland

www.qwed.eu

IEEE Poland Section
Women in Engineering AG

www.ieee.pl/wie

European Materials
Modelling Council

www.emmc.eu

CEN-OYSTER
Workshop

www.cen.eu/news/workshops
/Pages/WS-2020-010.aspx

H2020 NanoBat project

www.nanobat.eu

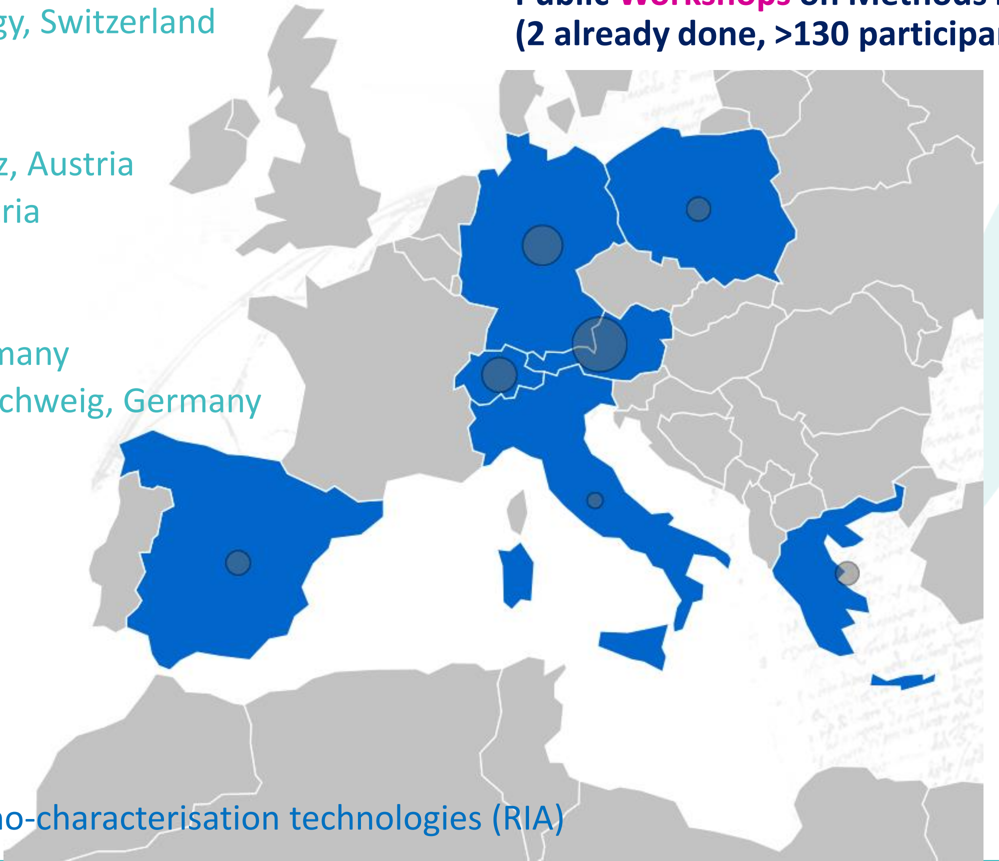
NanoBat has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 861962.

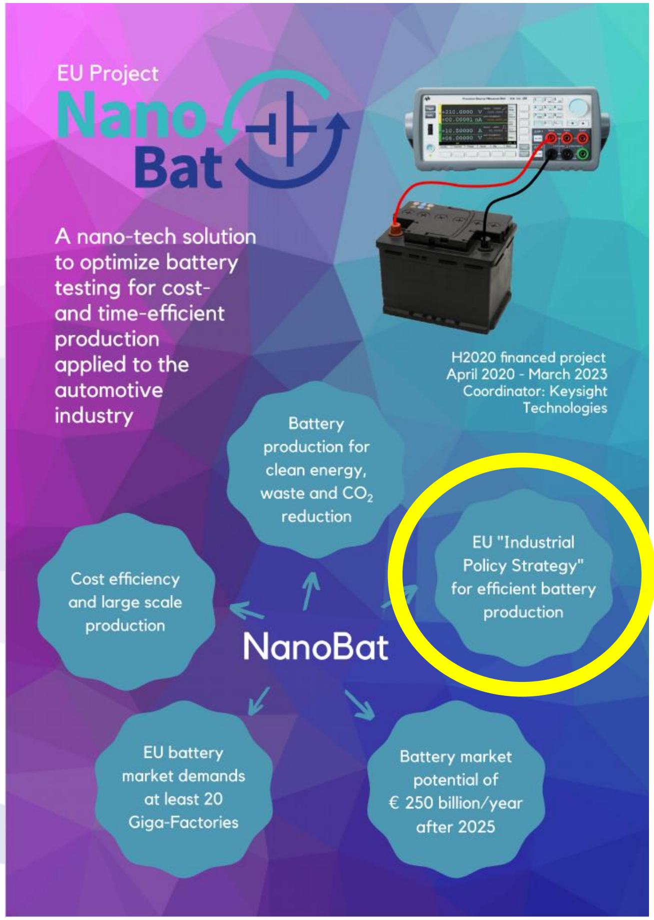
H2020 NanoBat project

13 NanoBat Partners:

- **Keysight** Technologies GmbH, Austria (Coordinator)
- **AIT** Austrian Institute of Technology GmbH, Austria
- **CRF** Centro Ricerche Fiat, Italy
- **EURICE** – European Research and Project Office GmbH, Germany
- **METAS** Federal Institute of Metrology, Switzerland
- **IMDEA** Energy Institute, Spain
- Universidad de **Burgos**, Spain
- **JKU** Johannes Kepler Universität Linz, Austria
- **Kreisel** Electric GmbH & Co KG, Austria
- **Pleione** Energy S. A., Greece
- **QWED**, Poland
- **RUB** Ruhr-Universität Bochum, Germany
- **TUBS** Technische Universität Braunschweig, Germany

- **4 Technology offers** (collaboration with **TEESMAT** OITB)
  - **Nano measurements – JKU, RUB, UBU**
  - **Battery test EIS – Keysight**
  - **Materials modeling – QWED**
  - **Pilot lines for battery materials – Pleione**
- **6 Advisory Board and 15 Stakeholders**
- **EMCC and EMMC councils, CHADAs and MODAs**
- **Public Workshops on Methods in battery testing (2 already done, >130 participants)**





Project Duration: April 2020-March 2023

Budget: 5M EUR

Call: H2020-NMBP-TO-IND-2019

Topic: DT-NMBP-08-2019 - Real-time nano-characterisation technologies (RIA)

NanoBat ambition & structure

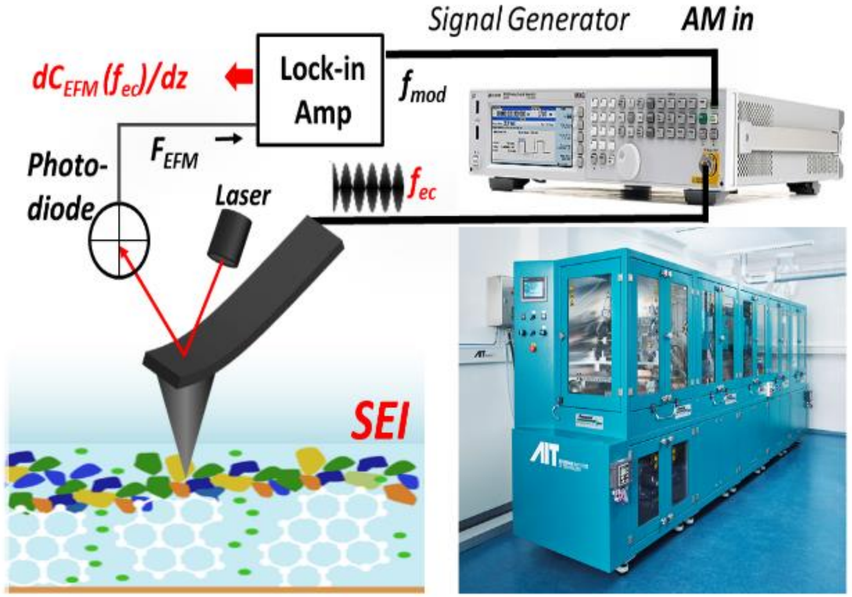
GHz nanoscale
electrical and dielectric measurements of the solid-electrolyte interface (SEI)
and applications in the battery manufacturing line

Optimised Battery Production through Nanotechnology

Instrumentation & Technologies

Microscopy & Imaging

Modelling & Simulation



CHADA = CHAracterisation DAta

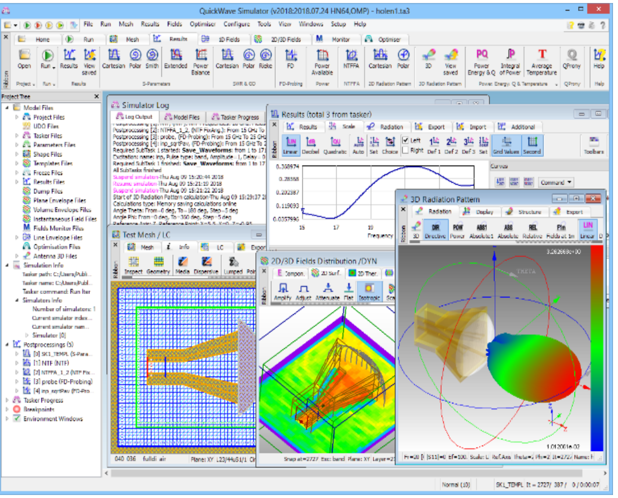
MODA = MOdelling DAta

QWED roles in NanoBat

- ✓ **modelling of materials interaction with EM waves**
- ✓ **material measurements in GHz resonators**
- ✓ **design of GHz devices**
- ✓ **dissemination & Open Platform**

Polish high-tech SME - 24 years on the world's market

Business branches *presented annually at IEEE IMS Show*



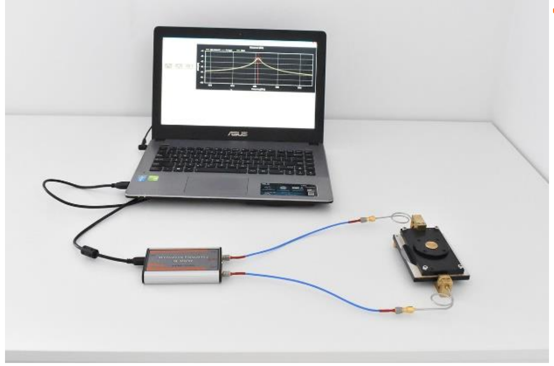
Electromagnetic simulation & design software, 3D & BOR 2D tools

based on 300+ publications by:

prof.W.Gwarek, IEEE Fellow, DML, Pioneer Award
dr.M.Celuch, President of QWED

THE EUROPEAN INFORMATION TECHNOLOGY PRIZE Winner

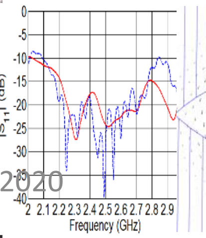
MISTRZ TECHNIKI WARSZAWA

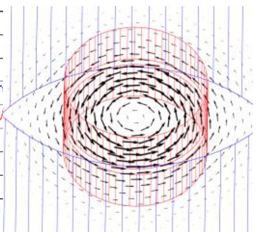


Test-fixtures for precise material measurements

based on 300+ publications

by prof.J.Krupka, IEEE Fellow



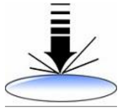


Consultancy & design services based on EM expertise & tools

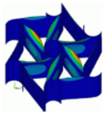
team of 10+engineers, 4 PhDs, 2 Profs
key areas: MW power appliances, customised resonators, antennas &feeds

R&D projects

started with: **COPERNICUS** 1994-1996



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

SYNTHETIC ENVIRONMENT RESEARCH PROGRAM HIRF

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

PBS Program Badań Stosowanych

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

MMAMA

MMAMA (Microwave Microscopy for Advanced and Efficient Materials Analysis and Production) – accelerating the development of high efficiency solar cells through application and enhancement of material measurement techniques

NanoBat

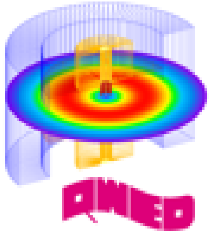
NanoBat - developing a novel nanotechnology toolbox for quality testing of Li-ion and beyond Lithium batteries with the potential to redefine battery production in Europe and worldwide.

QWED research, business, open innovation & standards at a glance

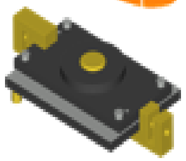
NanoBat

commercial since 1997
QuickWave Simulation Software
~1000 licences implemented

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

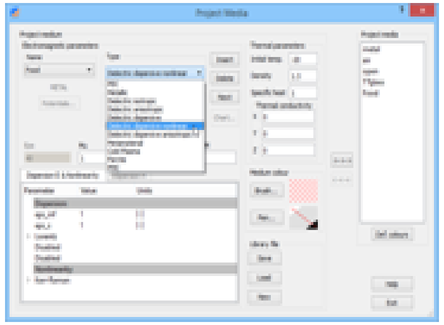


applicator design
& model
for parameter extraction

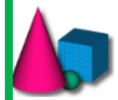


Material measurements

accurate material
parameters
(constitutive relations)



Open Platform Examples & Tools

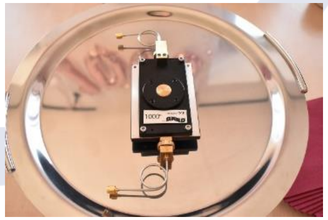


QW-Modeller for QuickWave
Free general purpose 3D CAD modeller for QuickWave

Open Platform Examples:

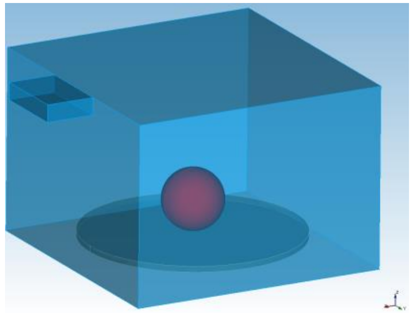
SMM tip presented at Numerical Electromagneti

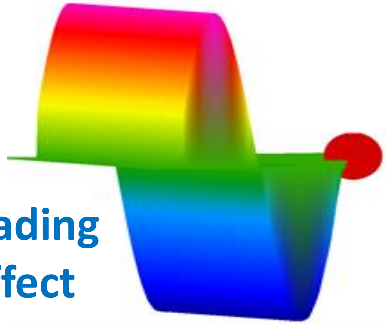
commercial resonator test-fixtures since 2001
1000th unit sold in 2020



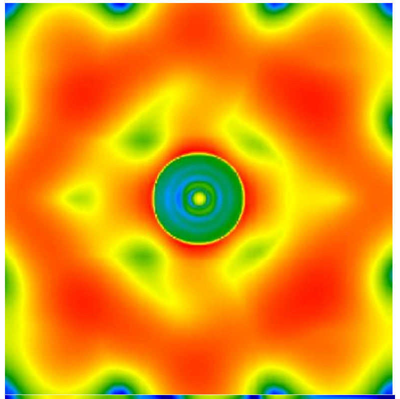
European Standard:
IEC 61189-2-721:2015

Electromagnetic wave interaction with materials

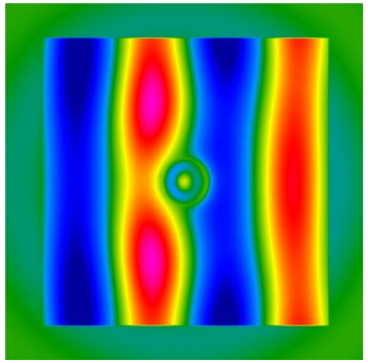


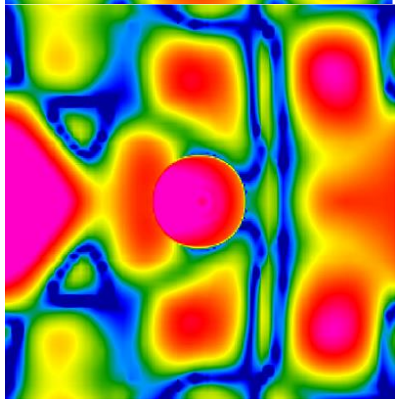


Exploding egg effect

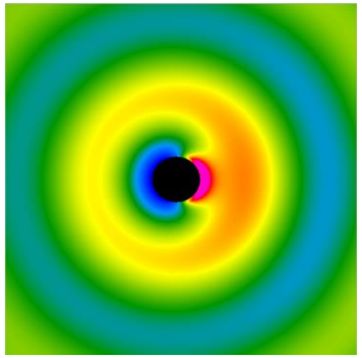


E-field





Scattered field



Physical Equations (Maxwell):

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

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

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

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

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

Material Relations:

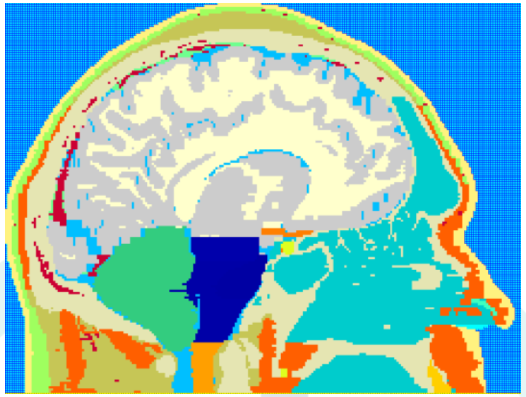
$$\vec{D}, \vec{B}, \vec{J} = F(\vec{E}, \vec{H})$$

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

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

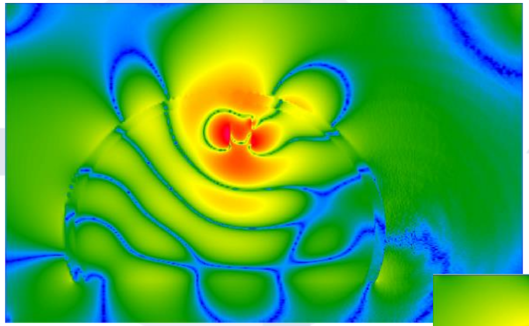
$$\vec{J} = \underline{\underline{\sigma}} \cdot \vec{E}$$

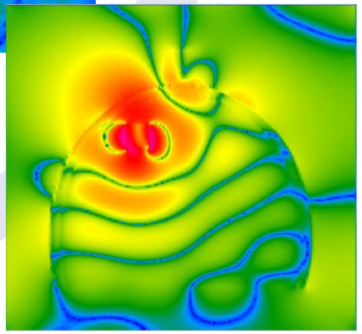
Detection of inhomogenities in tissues



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

Concepts & models by P.O.Risman



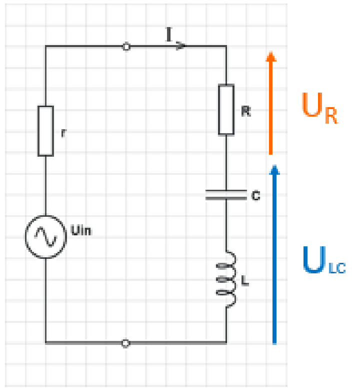


- ✓ **Detecting tumours & haemorrhages**
- ✓ **Optimising multiantenna tomographic systems**

Electromagnetic characterisation: resonant methods

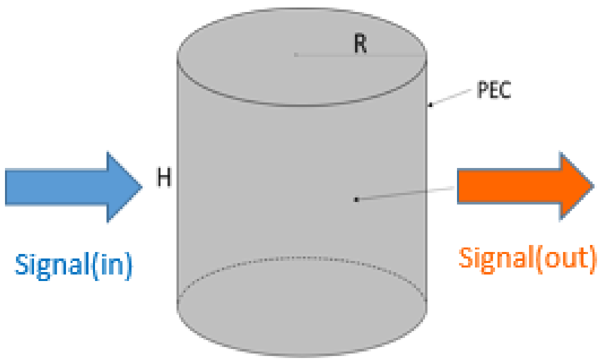
Methodology: design test-fixtures that provide a specific EM response to specific materials

Herein, we focus on resonator methods:

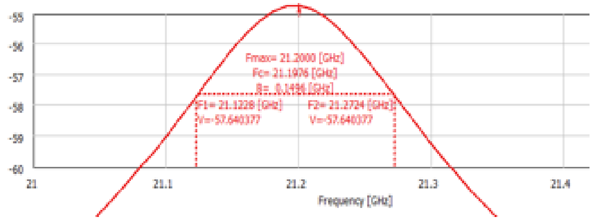


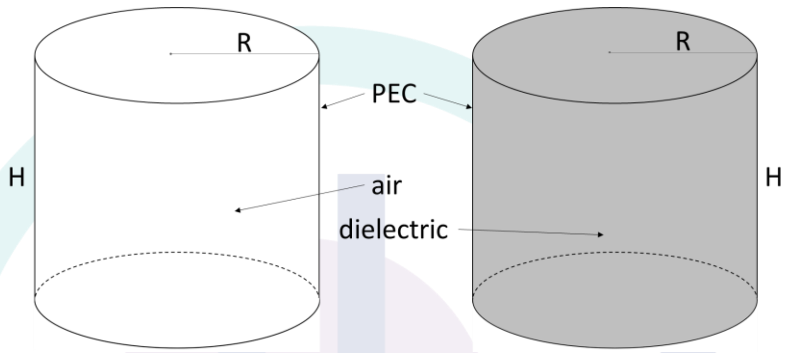
given fixed strength of Uin,
at resonance U_R is strongest (U_{LC} =0)

$$Q = 2\pi \frac{\iiint_V \varepsilon \vec{E} \cdot \vec{E}^* dv}{T \iiint_V \sigma \vec{E} \cdot \vec{E}^* dv} = \frac{\omega\varepsilon}{\sigma} = \frac{1}{Df} \approx \frac{fres}{\Delta f}$$

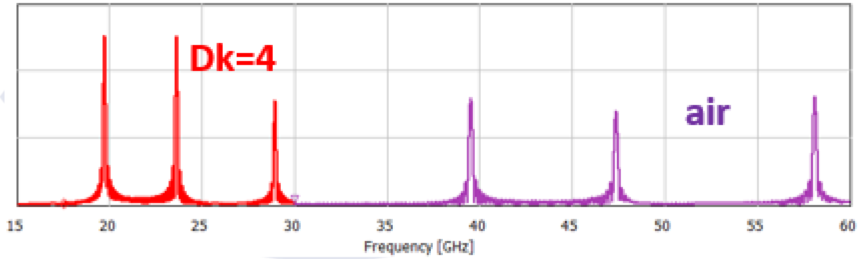


given fixed strength of Signal(in),
at resonance Signal (out) is strongest

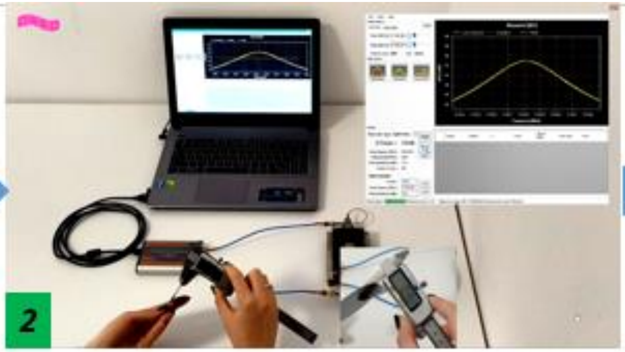




$$f_{r,mnp} = \frac{c}{\sqrt{Dk}} \sqrt{\left(\frac{\kappa_{mn}^{(,)}}{\pi R}\right)^2 + \left(\frac{p}{H}\right)^2}$$



Split-Post Dielectric Resonator (SPDR) – operation

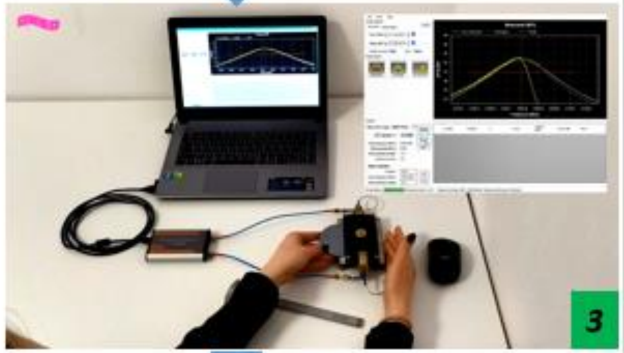


2. Measure thickness of the sample

0. Connect the SPDR to Q-Meter using SMA cables.
Connect Q-Meter to PC using USB cable.

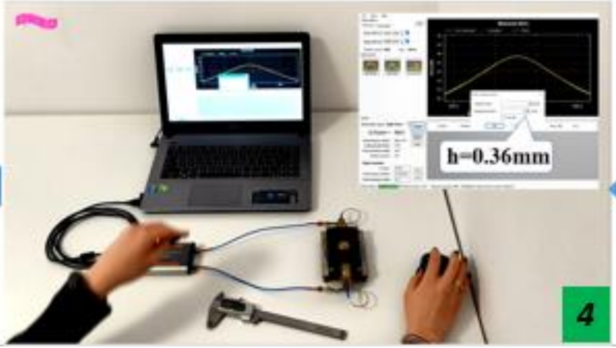
1. Measure "empty SPDR" – app invoked measurement.

Total measurement time: 30sec

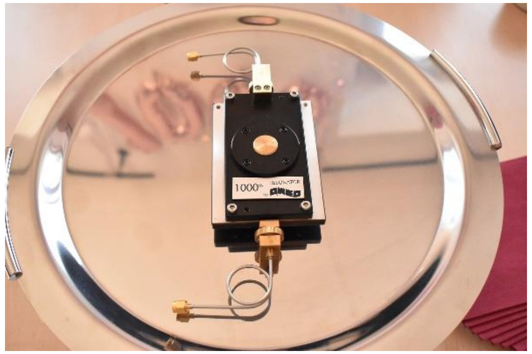


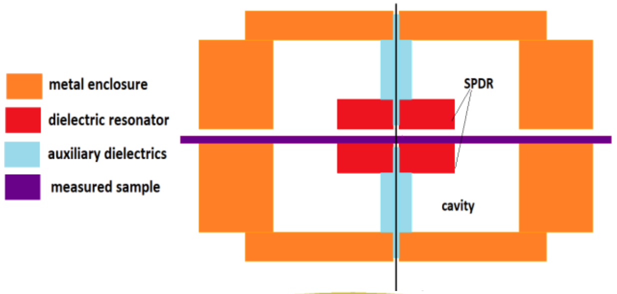
3. Insert the sample into SPDR

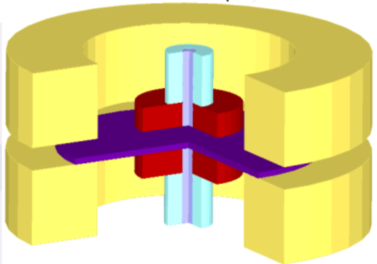
5. Material parameters are extracted automatically

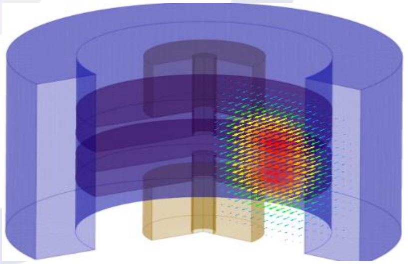


4. Insert the sample thickness into the PC app

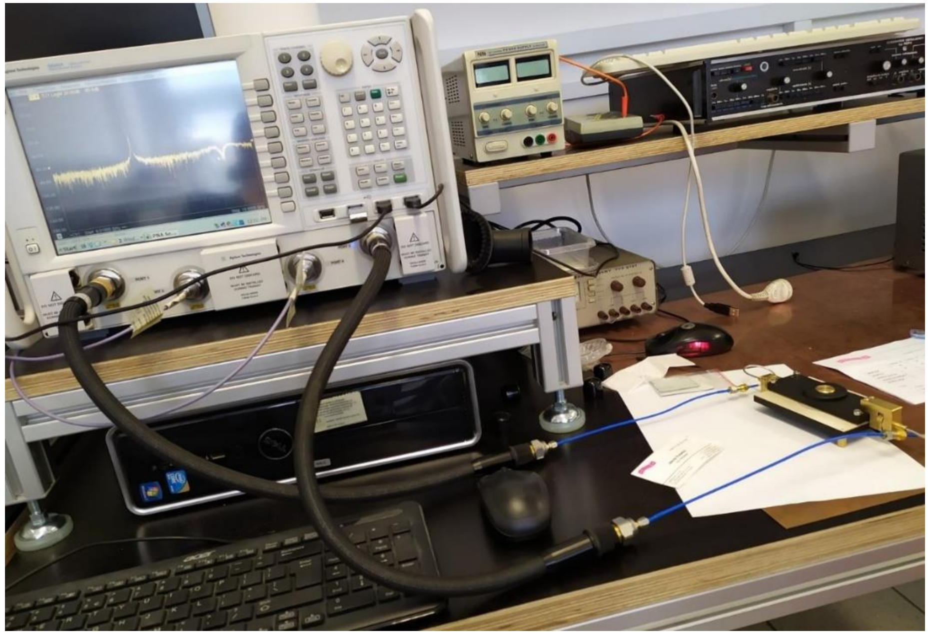






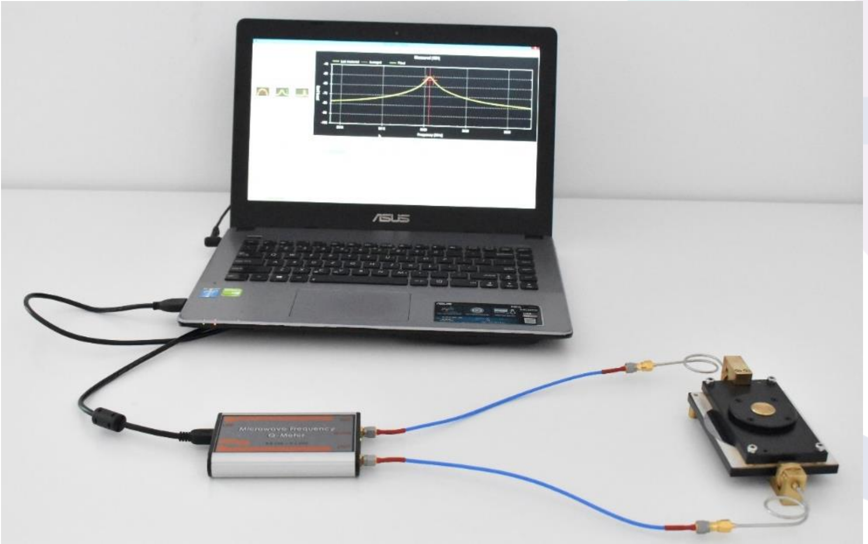


SPDR material characterisation in different setups



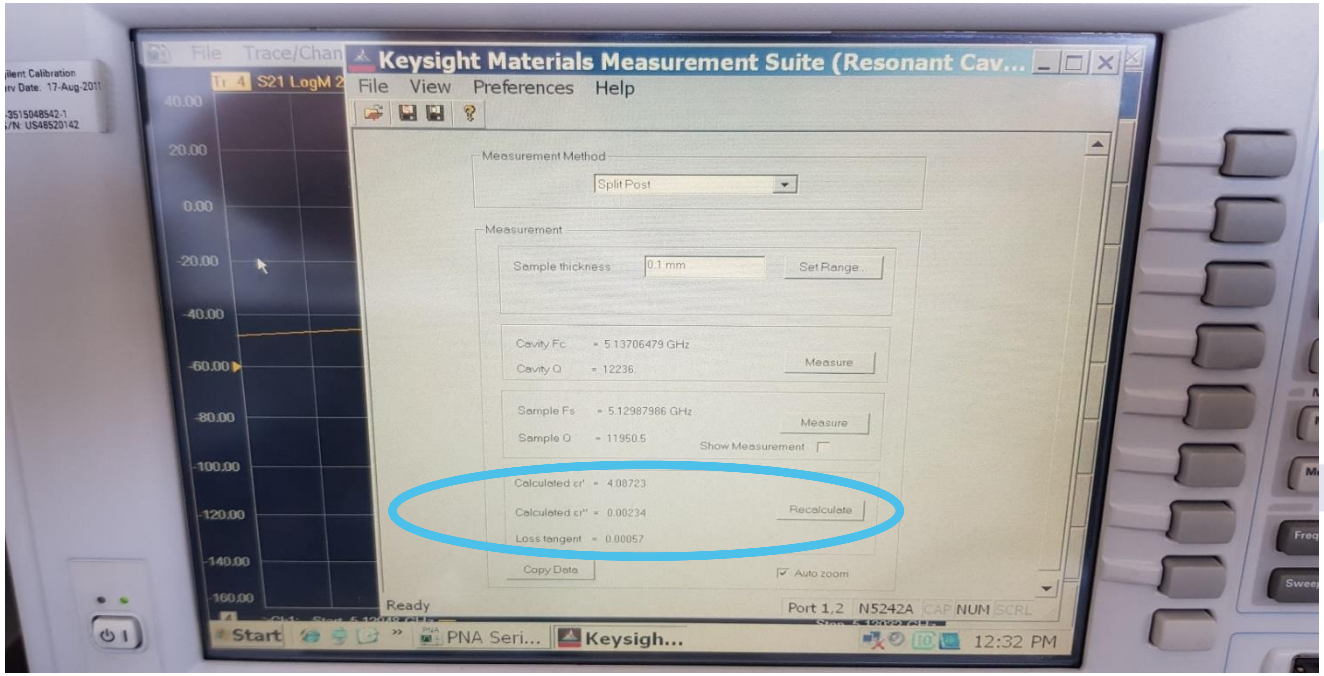
SPDR characterisation performed in labs...

...and at home office



A popular fallacy...

"Dielectric constant is measured by a VNA"



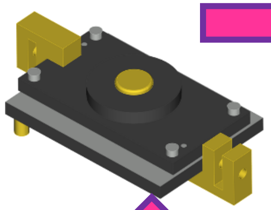
We get some numbers for our materials!

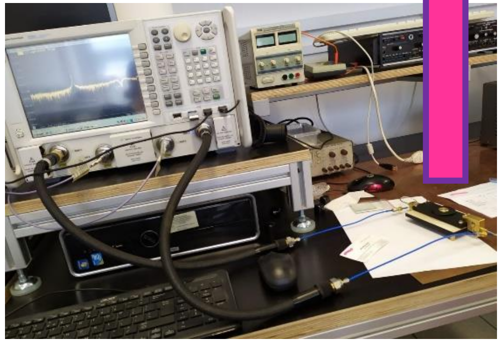
...but physics remains a black box...

Can MODA & CHADA enhance not just "the handling of numbers" but also understanding the physics behind?

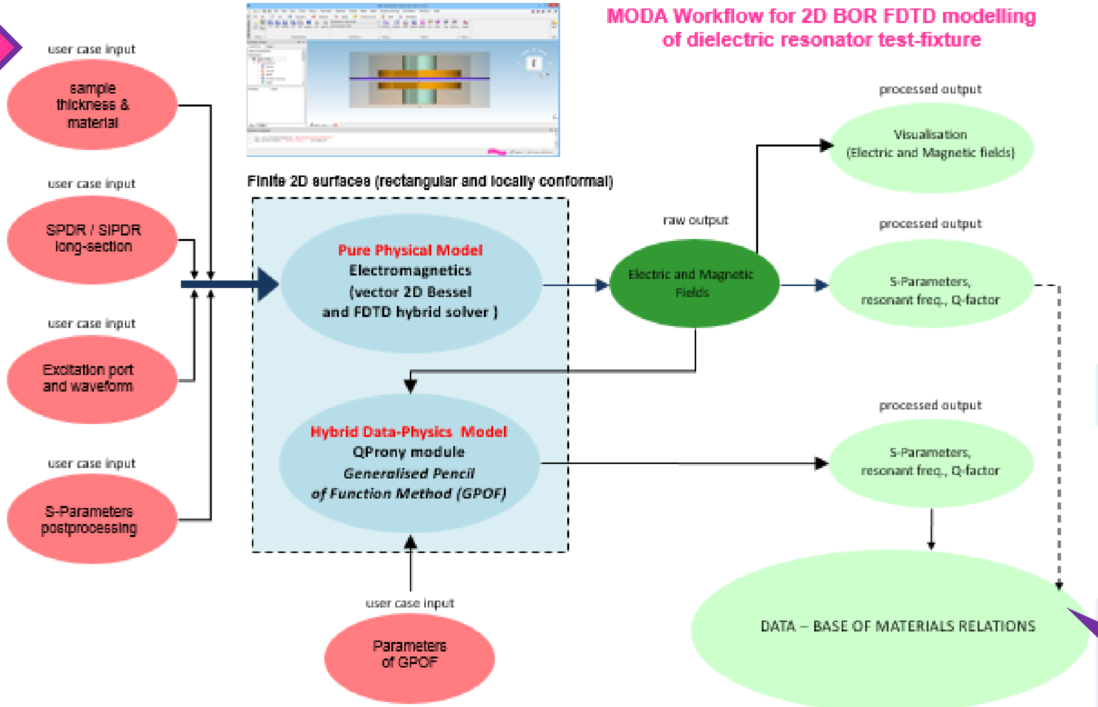
Twinned MODA + CHADA (electrical characterisation in resonator)

MODA



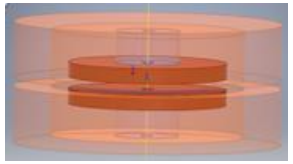


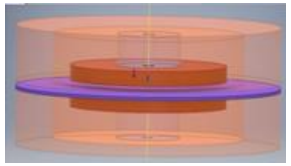
MODA Workflow for 2D BOR FDTD modelling of dielectric resonator test-fixture



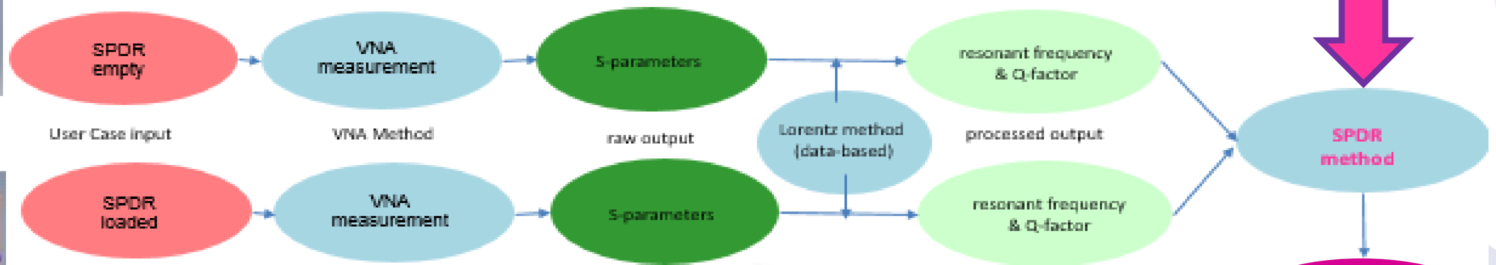
...more physics behind...

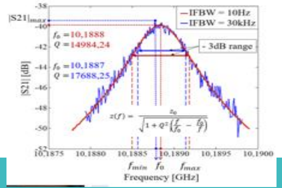
CHADA





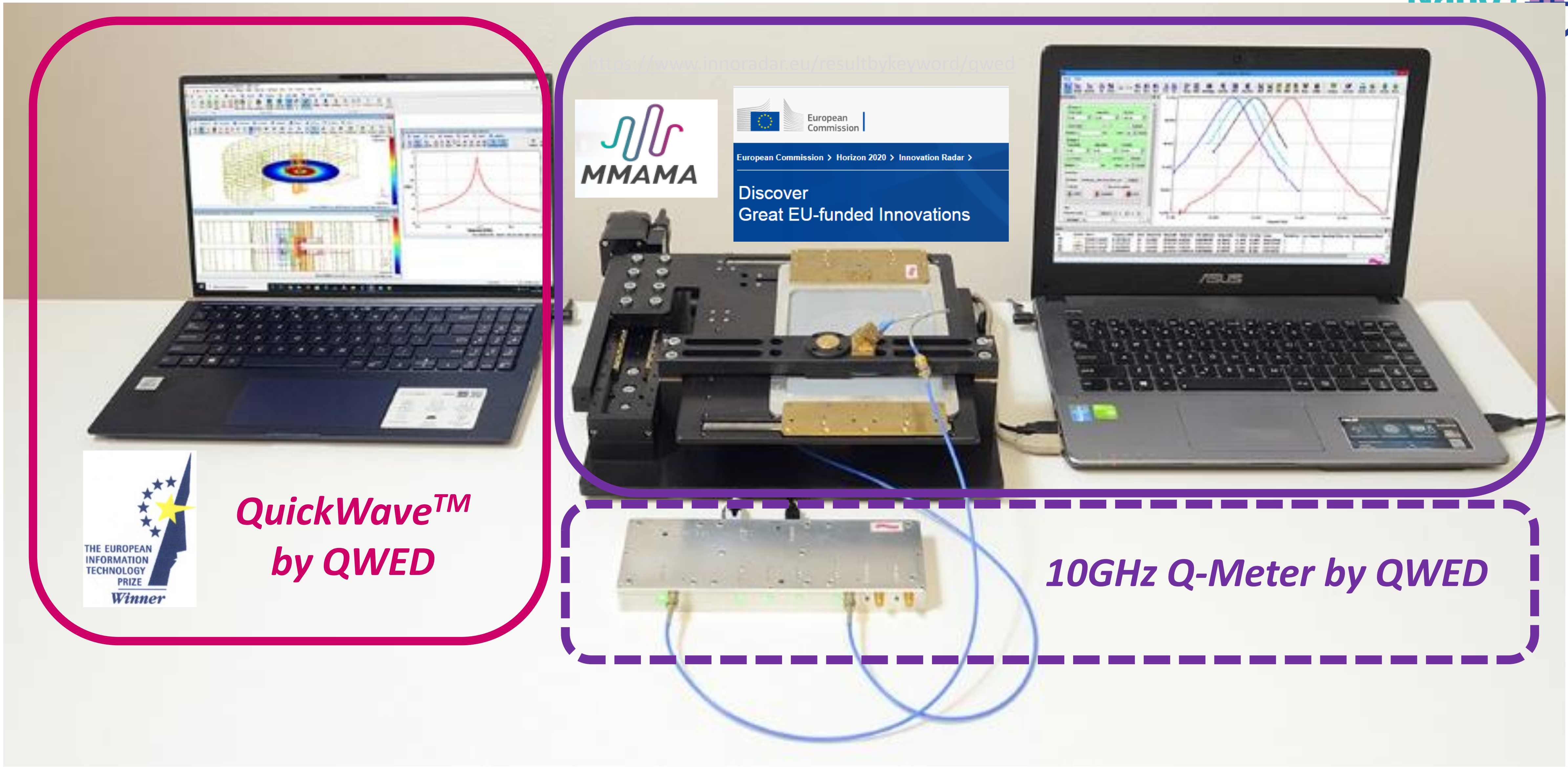
CHADA Workflow for material measurement with dielectric resonator test-fixture





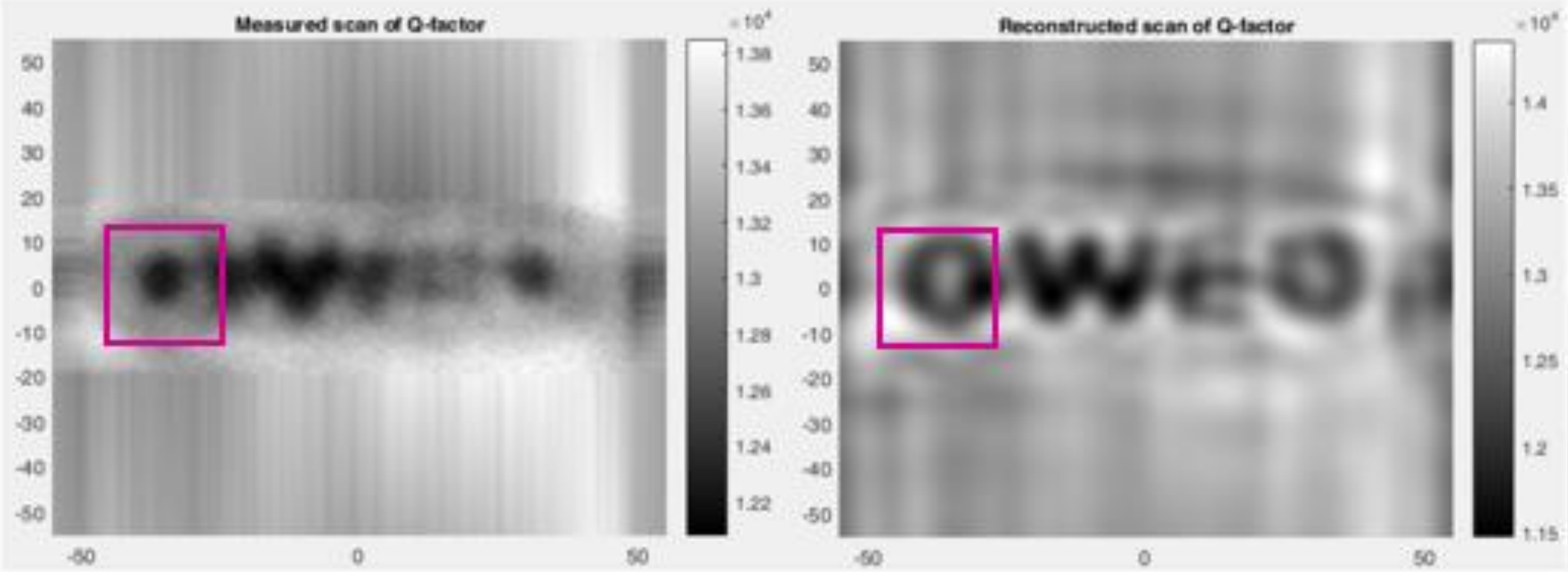
input from MODA is ESSENTIAL to complete CHADA!

Implementation of twinned MODA + CHADA



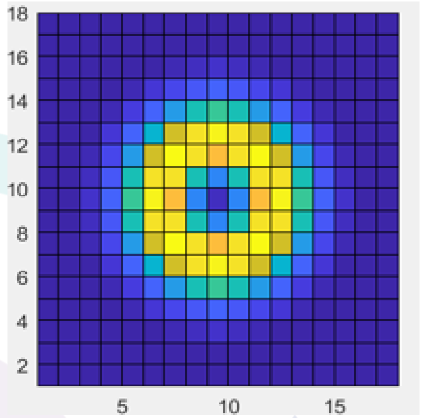
Example #1 of successful CHADA + MODA use

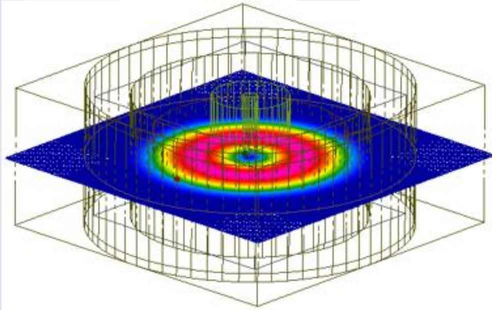
Application of SPDR scanner to patterned PEDOT:PSS (MateriaNova, Belgium) – imaging @ 10GHz, material used in photovoltaics



sample resistivity (measured Q-Factor) scan with QWED 10GHz SPDR scanner in H2020MMAMA project

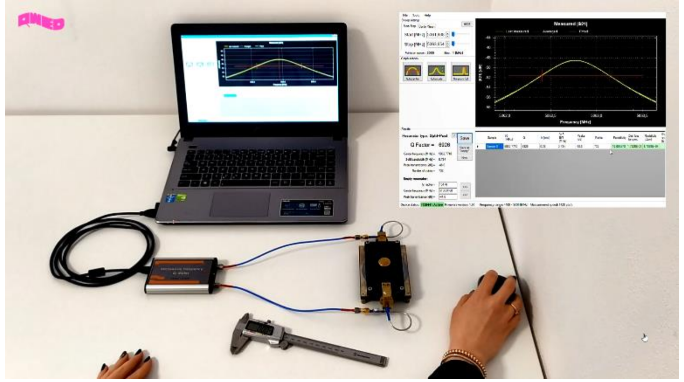
image further post-processed using SPDR field pattern simulated in QuickWave



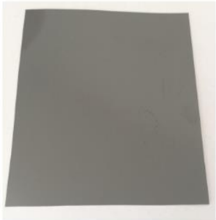


Example #2 of successful CHADA + MODA use

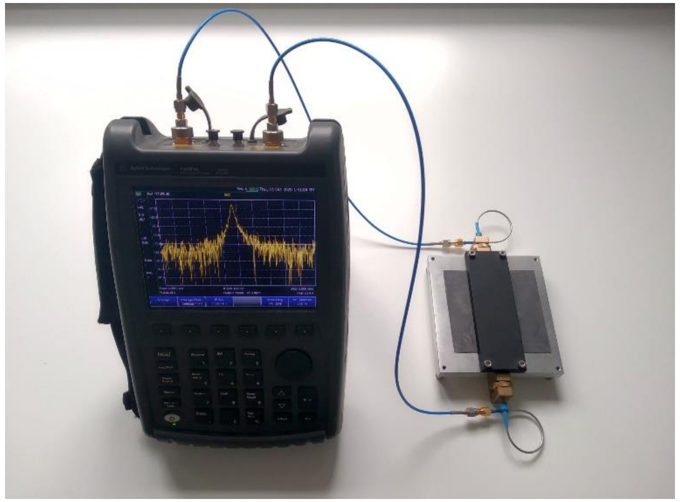
Application of stand-alone SPDR & SiPDR to graphene anodes & substrates from Pleione (Greece) – characterisation @ 2.45, 5, 10GHz; material used in batteries



Dielectric substrates
(*PLEIONE, Greece*)



Sample	2.45 GHz		10 GHz	
	Dielectric constant	Loss tangent	Dielectric constant	Loss tangent
Quartz	4.42	0.000202	4.41	0.000164
Polymer	4.90	0.27403	5.49	0.091955



Graphene anodes
(*PLEIONE, Greece*)

Sample		Surface resistance [Ω/□]
GNP on quartz	Edge	21.485
	Centre	21.020
GNP on polymer	Edge	90.167
	Centre	25.557

Take-away message:

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

4. **Unified MODA+CHADA will facilite:**

- 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,

- continuous improvements in materials characterisation, through the improvements in test-fixtures.

Thank you for your attention.

The NanoBat team will appreciate your further interest & collaboration!