Modelling of energy materials and electrical test-fixtures: developments and Open Platform implementation linking MODAs and CHADAs

M. Olszewska-Placha, J. Rudnicki, M. Celuch

QWED Sp. z o.o.

Model Development FA

Outline

- Continuum modelling
- Continuum modelling for material test-fixtures
- Open Platform Environment
  - Concept
  - Multiscale modelling solvers & examples
  - Linking MODAs and CHADAs
- Concluding remarks

Continuum EM and Multiphysics modelling with QuickWave software

- *Electromagnetic modelling* = *physics-based modelling*
- *Electromagnetic* modelling means *solving Maxwell equations with boundary & initial conditions* subject to *material constitutive relations*

- *Electromagnetic modelling for GHz and THz technology*
- *Electromagnetic simulation techniques successfully applied telecommunications*
- *Extending application spectrum by coupling phenomena and processes:*
  - *MW power applications (EM coupled to thermal solvers)*
  - *material modelling (EM coupled to PDD)*
- *Modelling became an important stage of the design process as it serves as virtual prototyping*

Differential form

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

Integral form

$$\oint_l \vec{E}\,\vec{dl} = -\frac{d}{dt}\iint_S \vec{B}\cdot\vec{n}\,dS$$
$$\oint_l \vec{H}\,\vec{dl} = \iint_S \left(\frac{\partial \vec{D}}{\partial t} + \vec{J}\right)\cdot\vec{n}\,dS$$
$$\oiint_S \vec{D}\cdot\vec{n}\,dS = \iiint_V \rho\,dV$$
$$\oiint_S \vec{B}\cdot\vec{n}\,dS = 0$$
$$\oiint_S \vec{J}\cdot\vec{n}\,dS = -\iiint_V \frac{\partial \rho}{\partial t}\,dV$$

Simple material relations

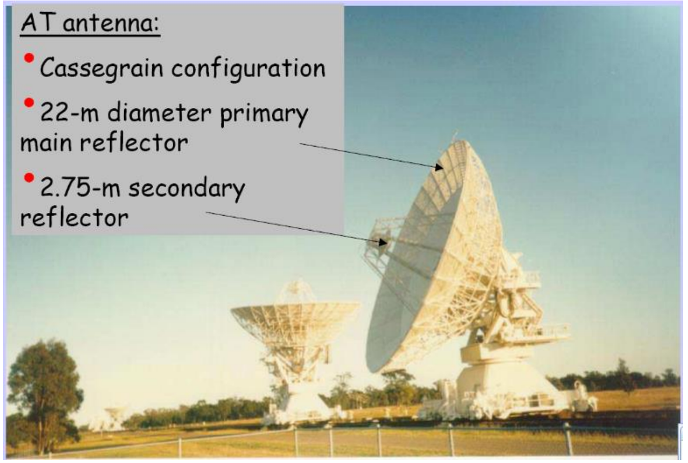
$$\vec{D}, \vec{B}, \vec{J} = \mathrm{F}(\vec{E}, \vec{H})$$
$$\vec{D} = \bar{\bar{\varepsilon}}\,\vec{E}$$
$$\vec{B} = \bar{\bar{\mu}}\,\vec{H}$$
$$\vec{J} = \bar{\bar{\sigma}}\,\vec{E}$$

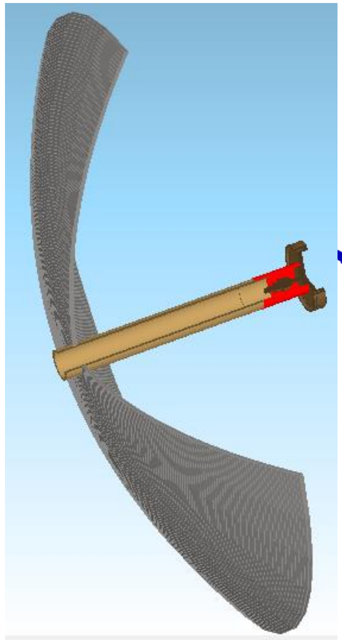
→ *Multiphysics and multiscale modelling*

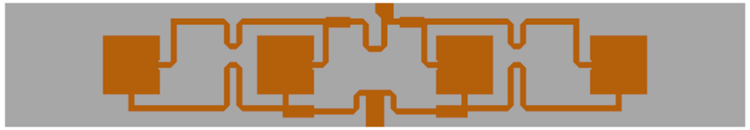
↓ **Complex material relations when coupling phenomena**

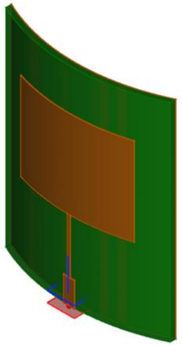
Continuum EM modelling with QuickWave software

Large dual reflector antennas: *Cassegrain, Gregorian, etc.*



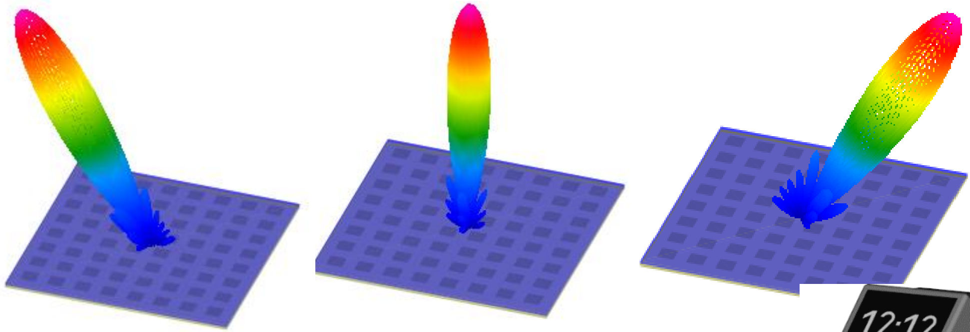


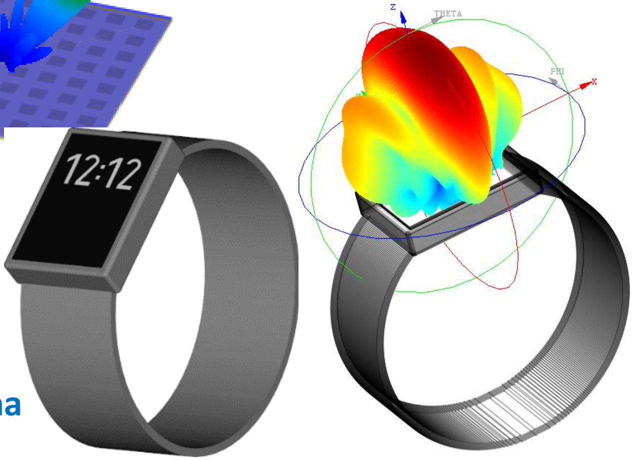




Planar antennas for smart bio-sensors

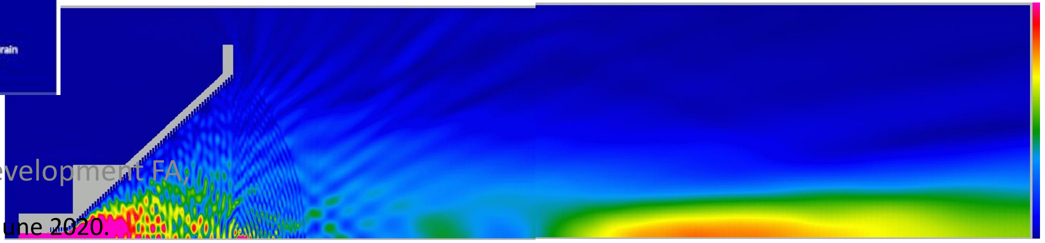
Antenna arrays for 5G and automotive radar application





Smartwatch with embedded patch antenna

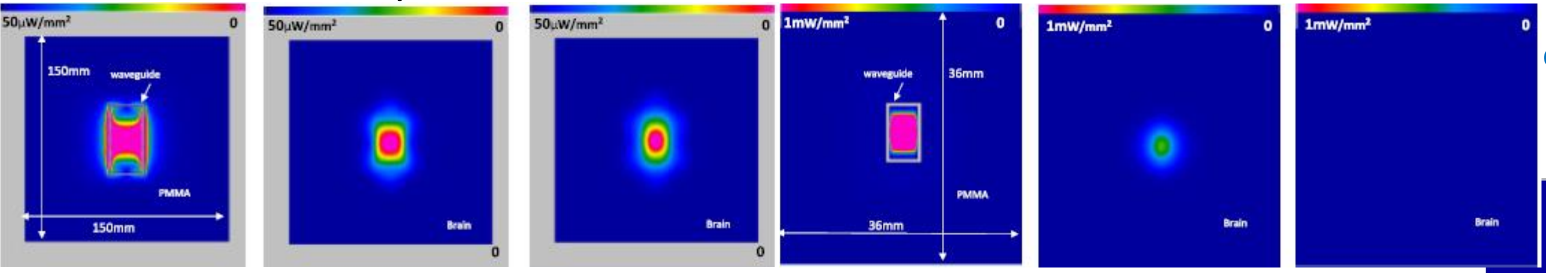
Corrugated horn antenna for material measurements



5G interactions with human tissues

Max 50μW/mm2

Max 1mW/mm2



surface | 1mm | 6mm | surface | 1mm | 6mm

4 GHz

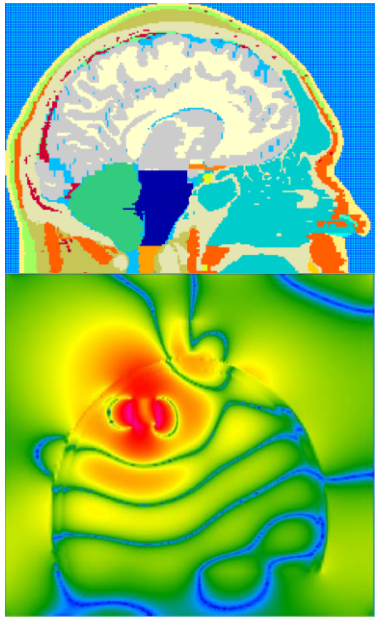
39 GHz

D. Gultekin, P. Siegel, „Absorption of 5G Radiation in Brain Tissue as a Function of Frequency, Power and Time", IEEE Access, vol. 8, June 2020.

Continuum Multiphysics modelling

Macroscopic modelling of biological problems

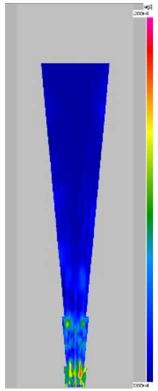
EM fields based medical systems



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

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

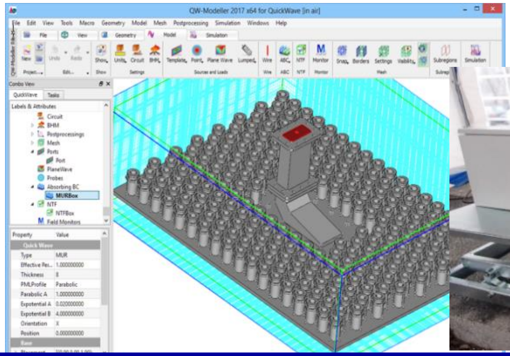
- ✓ **Tumours & haemorrhages detection**
- ✓ **Optimisation of multiantenna tomographic systems**

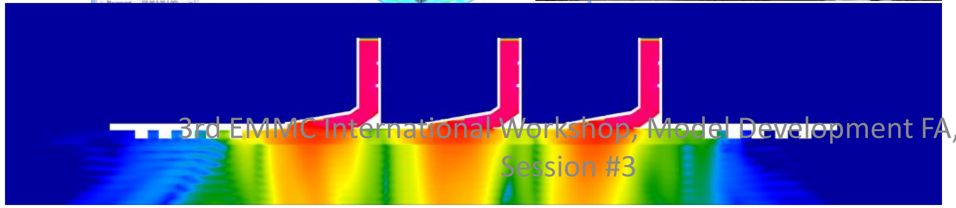


Free-fall waste processing systems on ships (Eureka FOODWASTE)

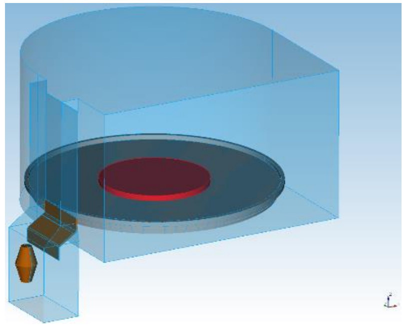
Microwave power systems for:

- ➢ **Food industry**
  - ❖ **Heating**
  - ❖ **Drying**
  - ❖ **Lyophilisation**
  - ❖ **Sterilisation**
  - ❖ **etc.**
- ➢ **Waste treatment**
- ➢ **Wood treatment**
- ➢ **Chemistry systems**
- ➢ **etc.**

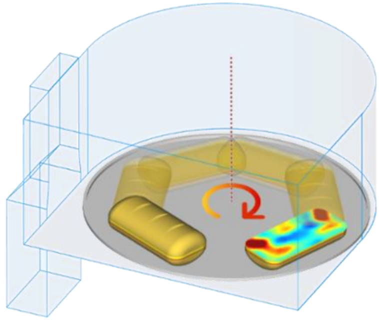




High power applicator for MW treatment of bituminous surfaces (road repair)



Whirlpool Max oven**



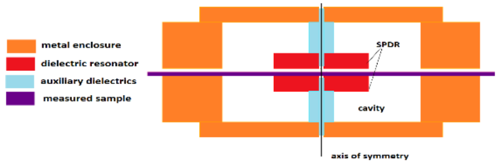
** Considered by M.Celuch, P.Kopyt & M. Olszewska-Placha in eds. M. Lorence, P. S. Pesheck, U. Erle, *Development of packaging and products for use in microwave ovens*, 2nd Ed. by Elsevier.

Modelling of MW heating effects in domestic oven

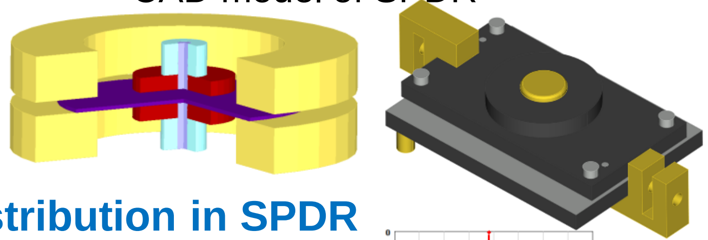
- ✓ Delivering microwave power
- ✓ heat transfer
- ✓ load dynamics (Load rotation during heating)
- ✓ temperature dependence of material parameters
- ✓ etc.

Modelling-assisted design of GHz material test-fixtures

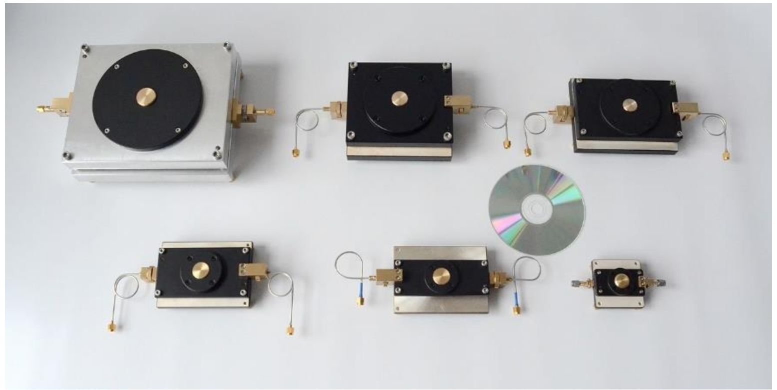
Split-Post Dielectric Resonator method for characterisation of lossy dielectrics and semiconducting materials (energy materials)



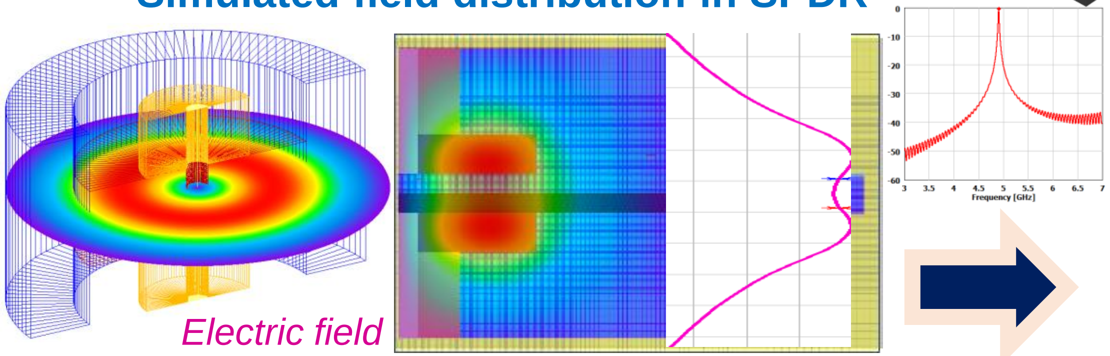
CAD model of SPDR



Family of SPDR test-fixtures



Simulated field distribution in SPDR

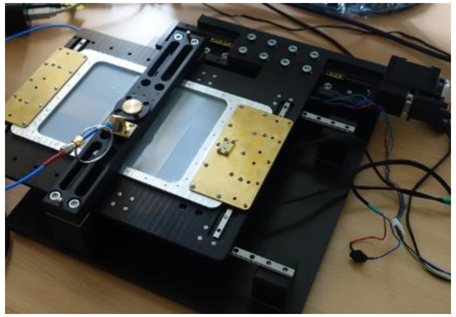


Electric field

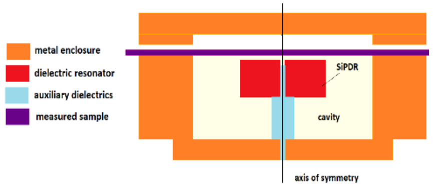
Material sample interacts with strong electric field, which facilitates parameters extraction of highly-resistive semiconductor materials with application to e.g. photovoltaic cells

Enhanced capabilities

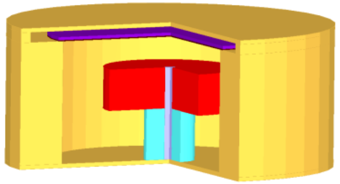
2D surface imaging scanner



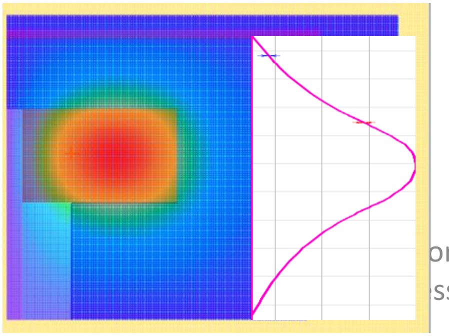
Single-Post Dielectric Resonator method for characterisation of thin conductive sheets



CAD model of SiPDR



Measurements of graphene anodes of battery cells



Simulated E-field distribution in the half cross-section

Material sample interacts with weak electric field, which facilitates extraction of conductive materials with application to e.g. battery electrodes

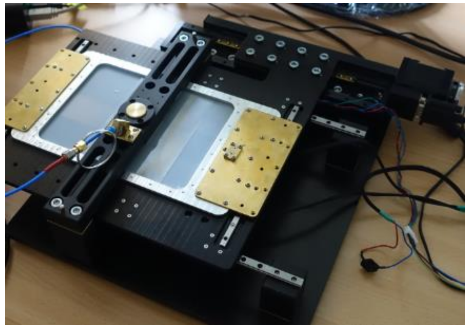
Macroscopic dielectric and electric properties

Characterisation of energy materials - examples (1)

Split-Post Dielectric Resonator method for characterisation of semiconducting materials for e.g. photovoltaic cells

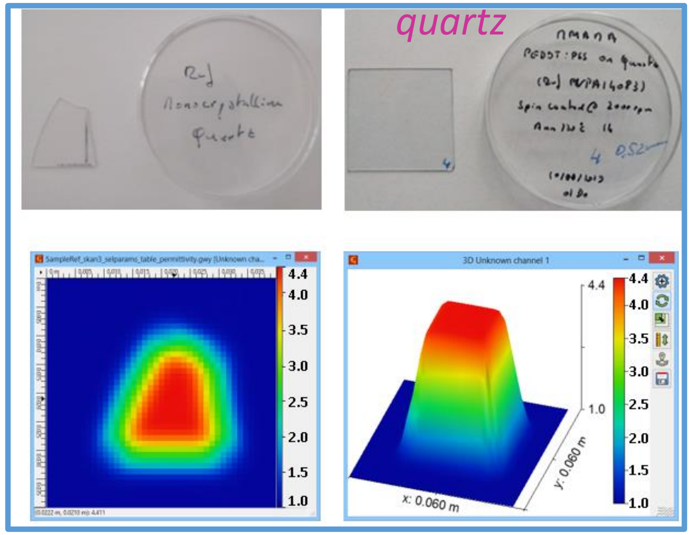
- ✓ Point-wise measurement for parameters’ values extraction
- ✓ 2D surface imaging for inhomogeneities detection

QWED’s SPDR 10GHz device



QWED’s SPDR 10GHz scanner

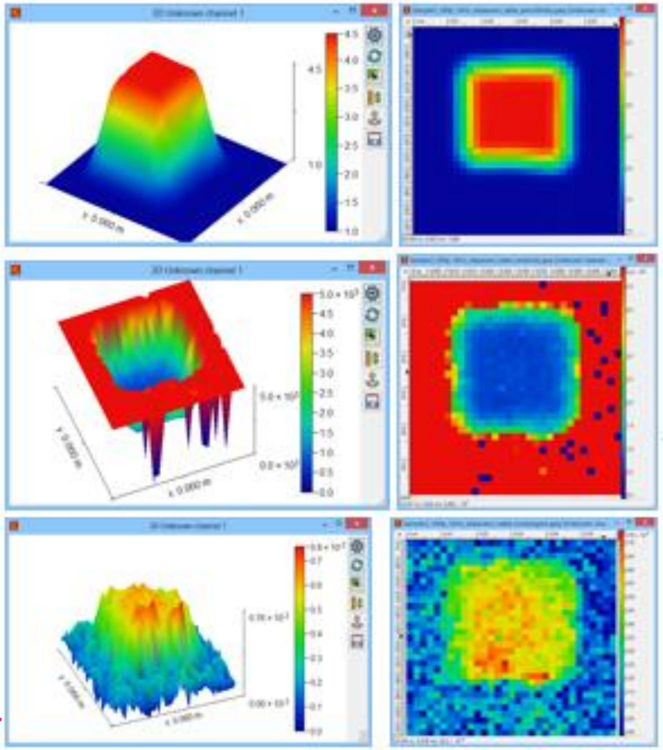
Semiconductor sample: PEDOT:PSS deposited on quartz



M.Celuch et al., IEEE IMS 2020.

MMAMA

2D surface maps with SPDR scanner



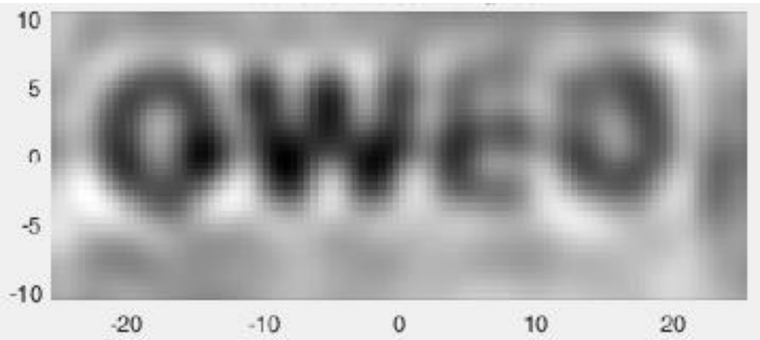
Permittivity

Resistivity: expected 500-5000 Ω.cm

Loss Tangent

PEDOT:PSS pattern deposited on quartz

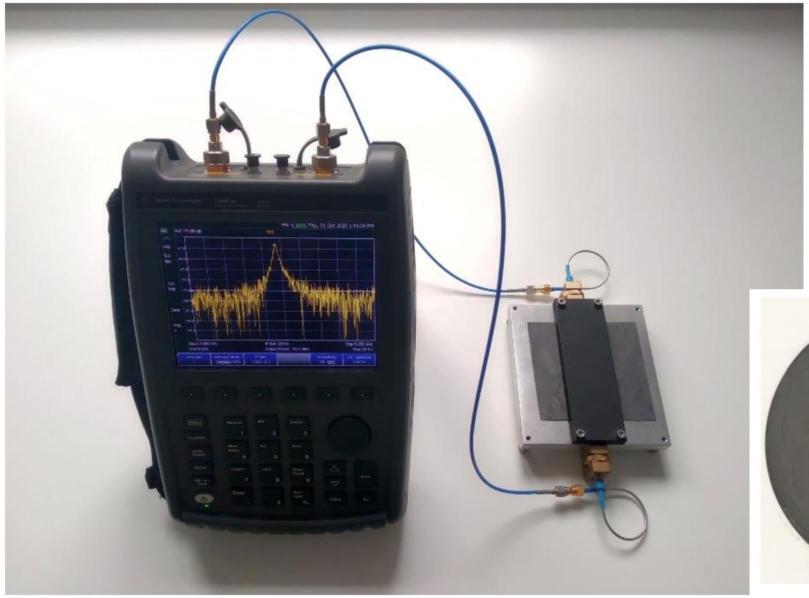
Courtesy: Materia Nova, Belgium



2D surface map with SPDR scanner

Characterisation of energy materials – examples (2)

Single-Post Dielectric Resonator method for characterisation of graphene anodes



QWED's SiPDR and Keysight's FieldFox measurement setup

Graphene anodes
(*PLEIONE, Greece*)

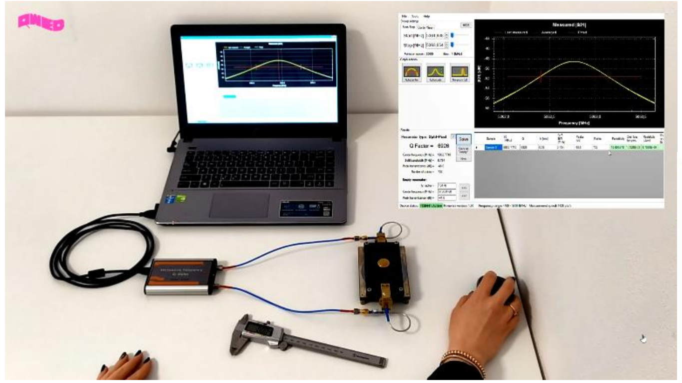
Manual surface scanning with QWED's SiPDR

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

To be developed

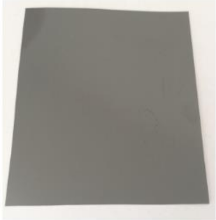
NanoBat

SiPDR 2D scanner for electric parameters imaging



SPDR characterisation of substrate materials

Dielectric substrates
(*PLEIONE, Greece*)



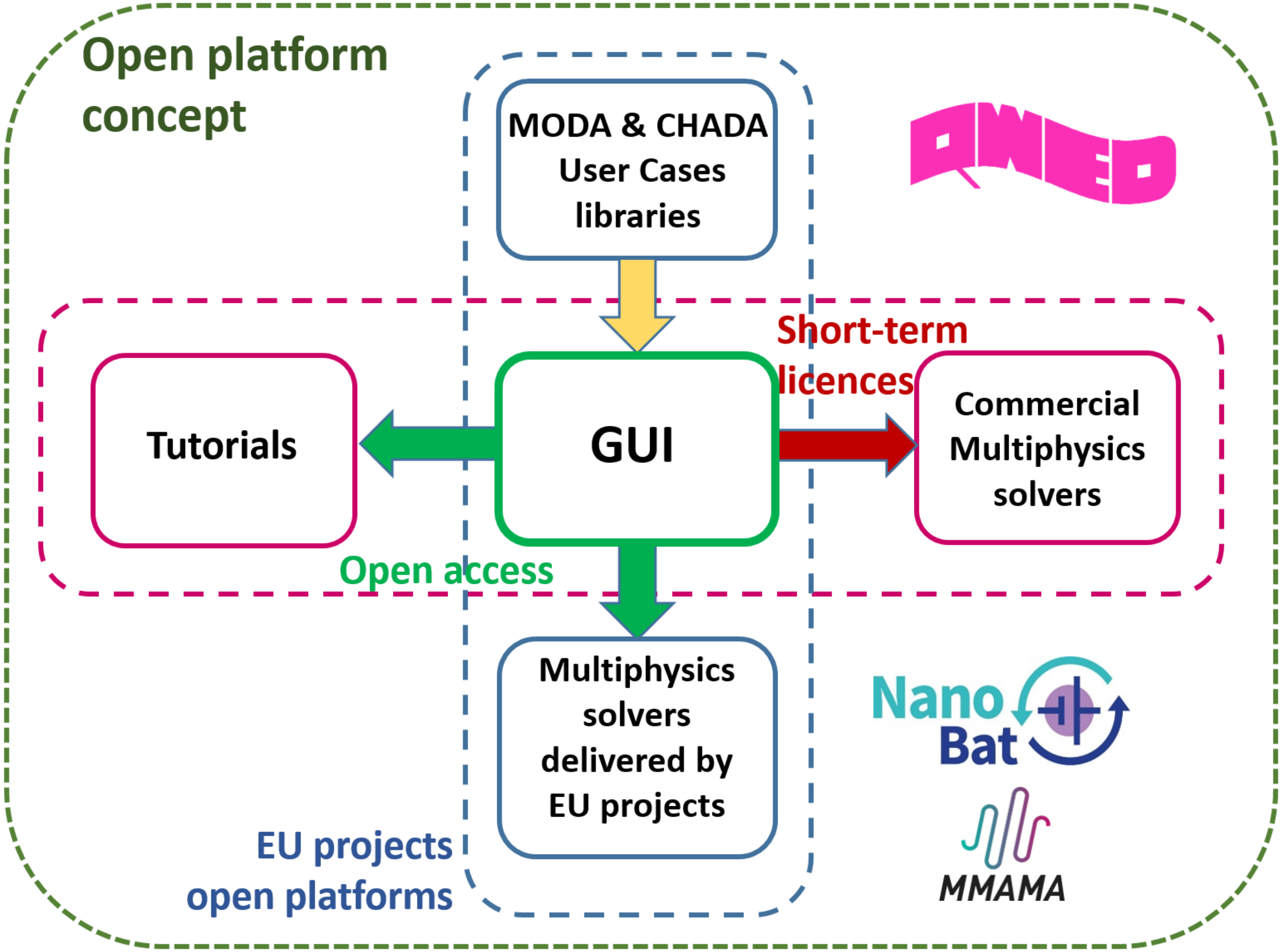
Sample	2.45 GHz		10 GHz	
	Dielectric constant	Loss tangent	Dielectric constant	Loss tangent
Quartz	4.42	0.000202	4.41	0.000164
Polymer	4.90	0.27403	5.49	0.091955

Overview on materials modelling in European research

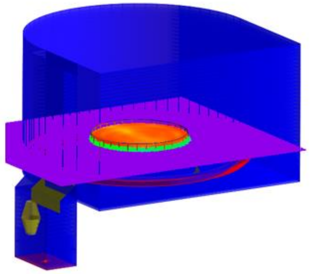
- The EMMC assembles groups active in the developments of different material model types
- Even more such models are available on the European research area
- Each model comes with its own user interface
- Scientific progress in the models is much faster than computer interface developments may reasonably follow
- This hinders models' validation, interoperability, and general use

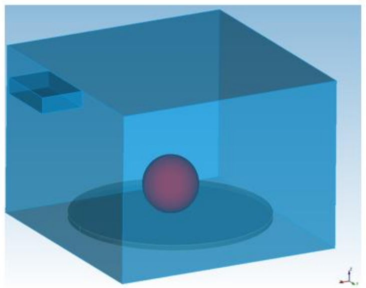
- A need for solution:
  - ✓ *alleviating those obstacles*
  - ✓ *providing compromise between the open innovation and the commercial interest of the European software companies*

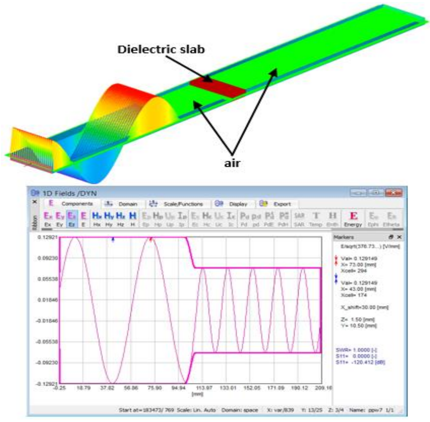
Open Platform concept



- ✓ **Interoperable, licence-free, time-unrestricted CAD-based GUI**
- ✓ **Tutorials** – teaching and project's results dissemination
- ✓ **Library of modelling examples** – documented in MODA format, incl. related CHADAs
- ✓ **Physics-based solvers** - solvers coming from EU projects or other initiatives, willing to provide their tools as open-access.
- ✓ **Commercial solvers** – linked through reading and processing the data in text files exported by GUI. This creates a unique capability to run full-power simulations of examples created in the free-to-use GUI.





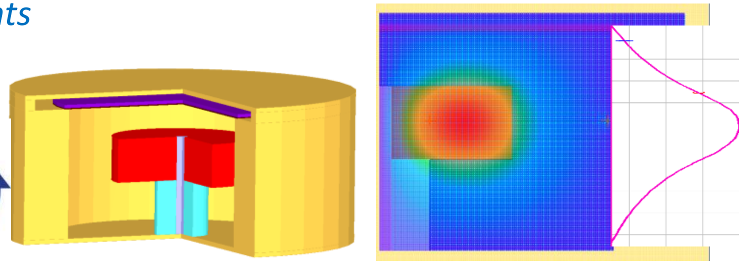


* Commercial microwave oven model courtesy of Whirlpool Sweden AB simulated with QuickWave software via Open Platform

Open Platform solvers & examples

- ✓ Initiated within EU H2020 MMAMA project
- ✓ Microwave microscopy of materials e.g. organic semiconductors
- ✓ FDTD and FEM EM solvers by QWED and ETH Zurich
- ✓ Further development and enhancements run under EU H2020 NanoBat project
  - ❖ Launching open-access solvers concerned with battery modelling
  - ❖ Simulation-based calibration of measurement test-fixtures dedicated to battery materials, e.g. solid electrolyte interphase (SEI), graphene anodes, etc.
  - ❖ Heat transfer analysis in battery cells, incl. reversible heat
  - ❖ Coupled EM and Poisson-drift-diffusion analysis for electrolyte in battery cells (but also semiconducting materials)

SiPDR for measurements of graphene anodes of battery cells.



Drift-Diffusion in semiconductors

$$\boldsymbol{j_p} = q_p \mu \boldsymbol{E} - D_{c_p} \nabla q_p$$

$$\boldsymbol{j_n} = q_n \mu \boldsymbol{E} + D_{c_n} \nabla q_n$$

$$\frac{\partial q_p}{\partial t} = -\nabla \boldsymbol{j_p}$$

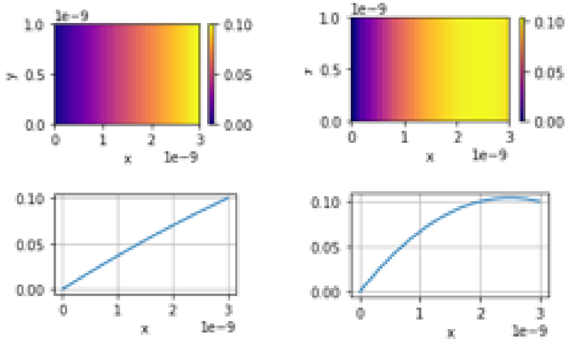
$$\frac{\partial q_n}{\partial t} = \nabla \boldsymbol{j_n}$$

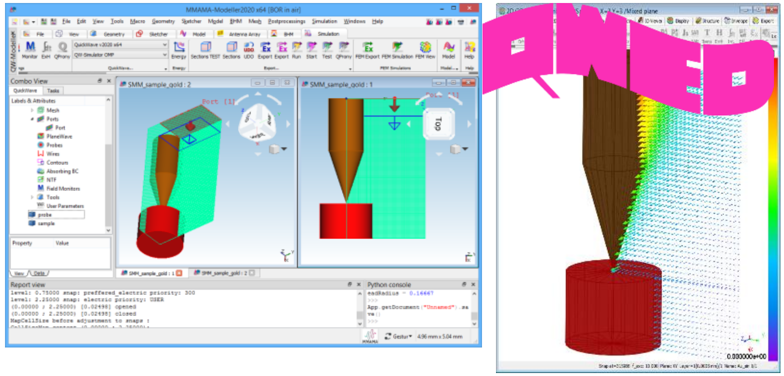
Nernst-Planck and continuity in electrolytes:

$$\boldsymbol{J} = -z_i u_{m,i} F c_i \nabla U - D_i \nabla c_i$$

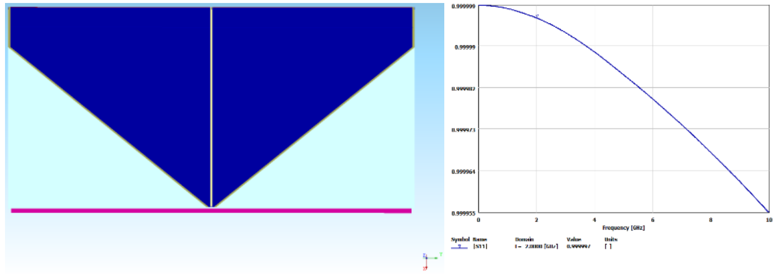
$$\nabla \cdot \boldsymbol{J_i} = R_i$$

Potential distribution between two electrodes for low and medium concentration of charged species in electrolyte

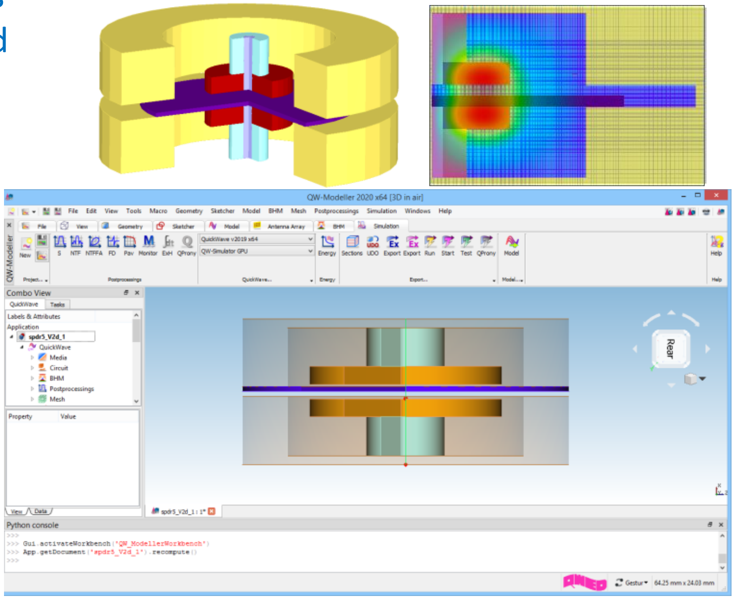




Scanning Microwave Microscopy (SMM) tip applied to dielectric material analysis with FDTD solver



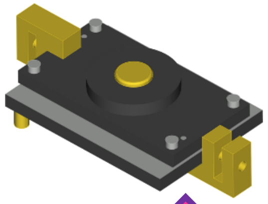
SMM tip in contact with battery SEI layer

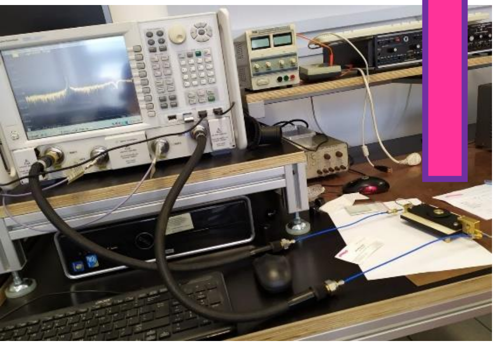


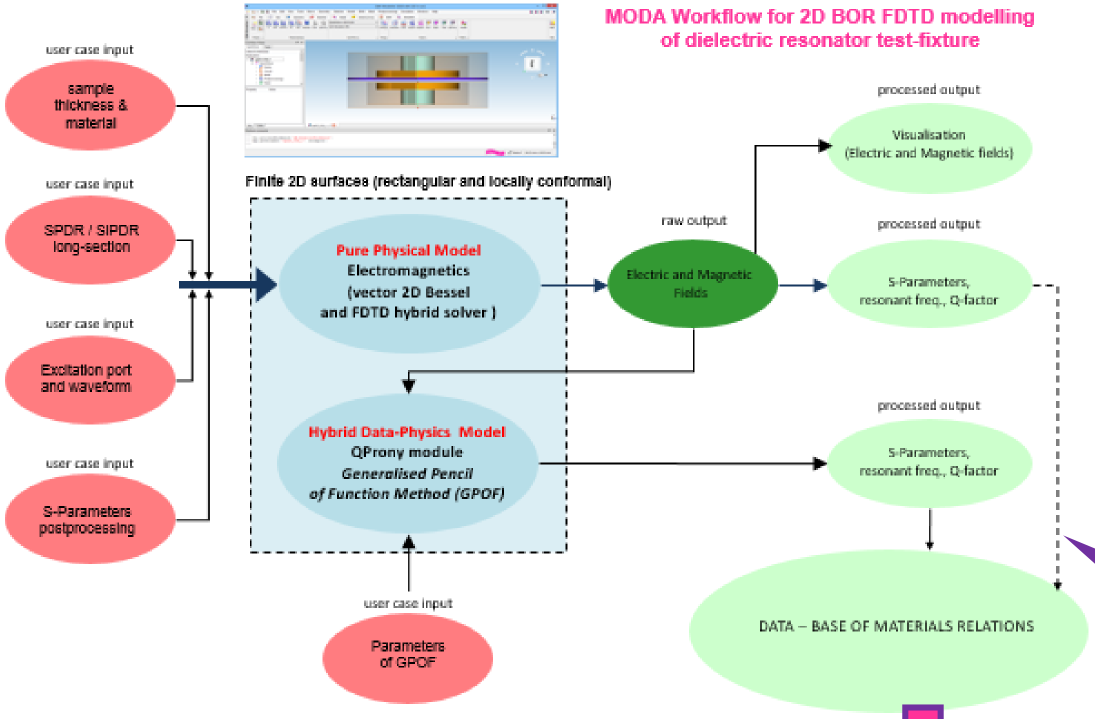
SPDR resonator for characterisation of e.g. semiconducting materials, battery separators, etc.

Open Platform – MODAs & CHADAs libraries

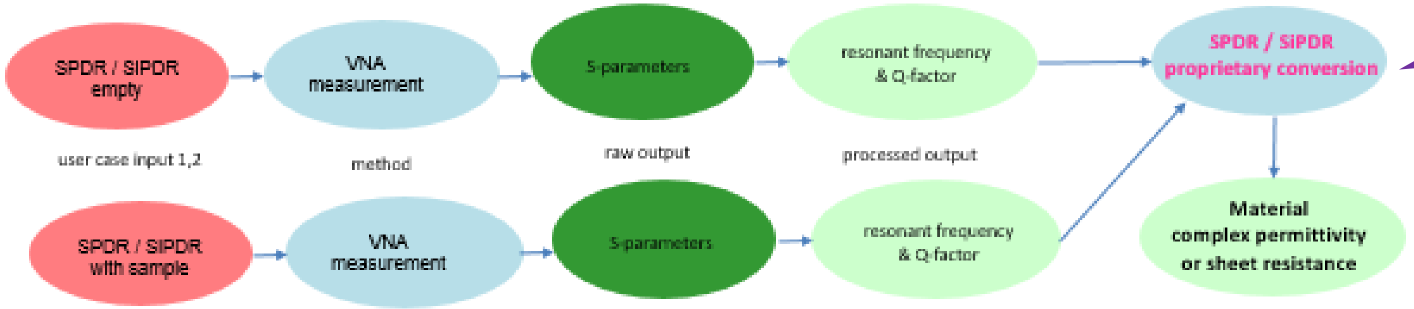
MODA







CHADA Workflow for material measurement with dielectric resonator test-fixture



CHADA

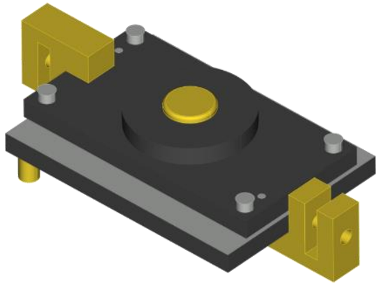
input from MODA
is ESSENTIAL
to complete CHADA!

Open Platform – MODAs & CHADAs libraries

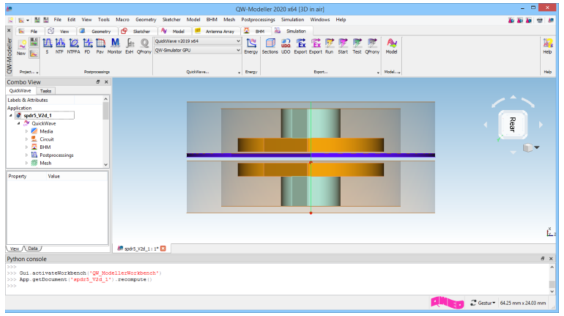
QWED's SPDR material characterisation device

MODA

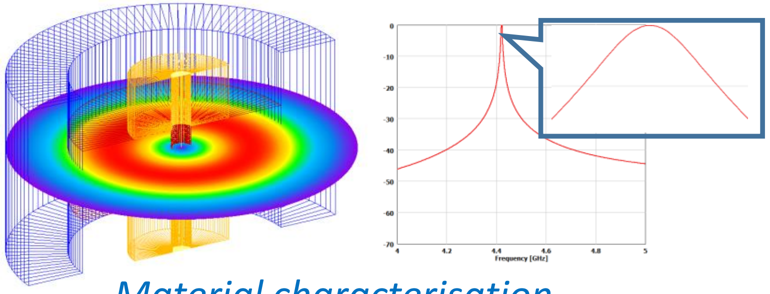
Simulation model



Simulation scenario

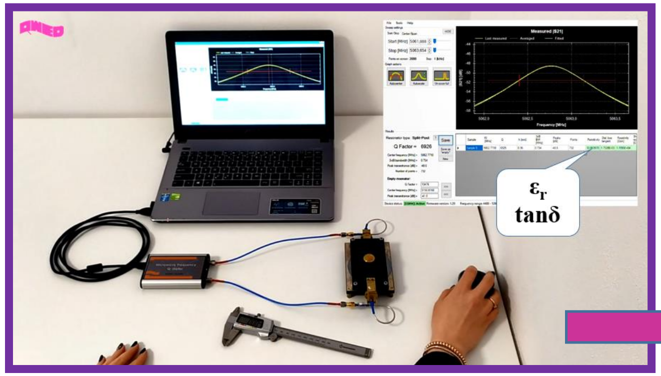


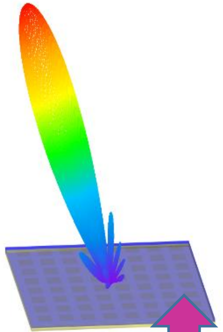
Continuum modelling results



Modelling-based calibration software

Material characterisation



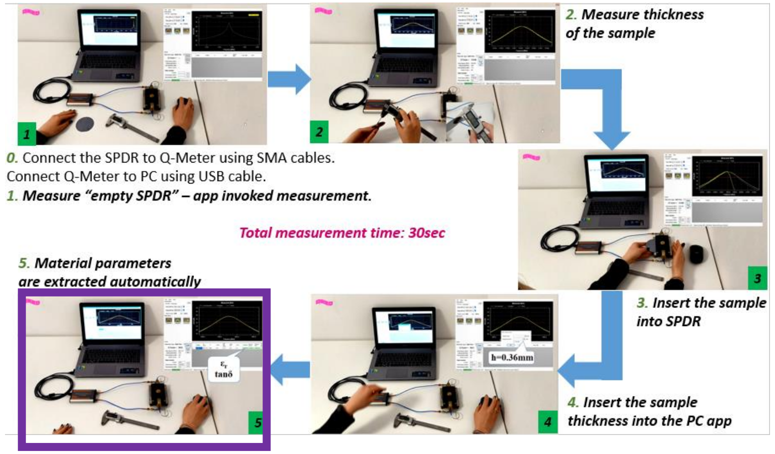


Macroscopic EM material parameters (dielectric constant and losses)

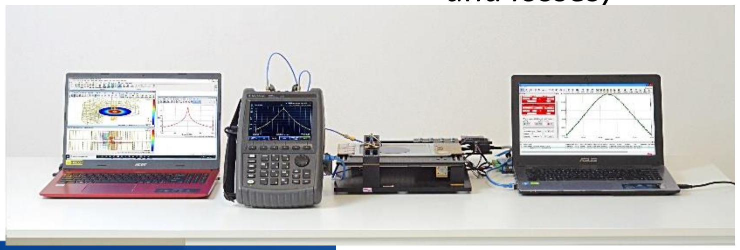
CHADA

Real-life device

Laboratory procedure



European Commission



European Commission > Horizon 2020 > Innovation Radar >

Discover Great EU-funded Innovations

QWED's SPDR scanner & Keysight FieldFox

Open Platform concept

Open platform concept

MO... DA

Tutorials

EU

op

✓ ... licence-free, ti... e-unrestricted CAD-

...hi... ...ect's results dissemination

...ples – documented in MODA

... from EU

...ing to provide their

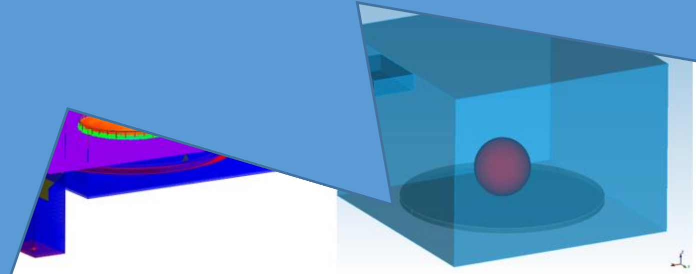
...rough reading and

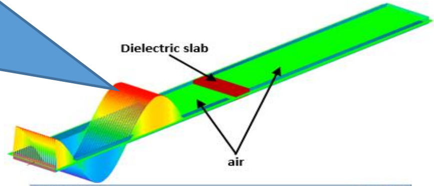
...xported by GUI. This

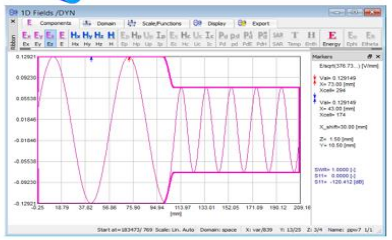
...bility to run full-power

...ed in the free-to-use GUI.

- ❑ **We seek collaborations on extending the Open Platform with new multiscale models and linking-coupling procedures**
- ❑ **Task Group is being proposed with the EMMC Focus Area #1 and #2**







* Commercial microwave oven model courtesy of Whirlpool Sweden AB, simulated with QuickWave software via Open Platform

Conclusions

- Promoting the concept and developing Open Platform with open and commercial access rights
  - Access to European research results
  - Linking models
  - Coupling solvers
  - Fostering interdisciplinary collaboration

- We seek collaborations on extending the Open Platform with new multiscale models and linking-coupling procedures

- Task Group is being proposed with the EMMC Focus Area #1 and #2

- Exploring and stimulating synergies between materials modelling and characterisation

Acknowledgement

The work presented has received funding from the

European Union's Horizon 2020

research and innovation programme (H2020-NMBP-TO-IND-2019)

under grant agreement *n°861962*.

(website: www.nanobat.eu)

Thank you for your attention!!!