Multiscale Modelling of materials and test-fixtures – Open Platform development

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NanoBat project aims to develop 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. The targeted radio frequency **(RF)-nanoscale techniques** will be faster and more accurately calibrated than existing methods. The project will significantly reduce the costs of battery production thus greatly benefiting the evolving **clean energy and e-mobilit**y transition in Europe.

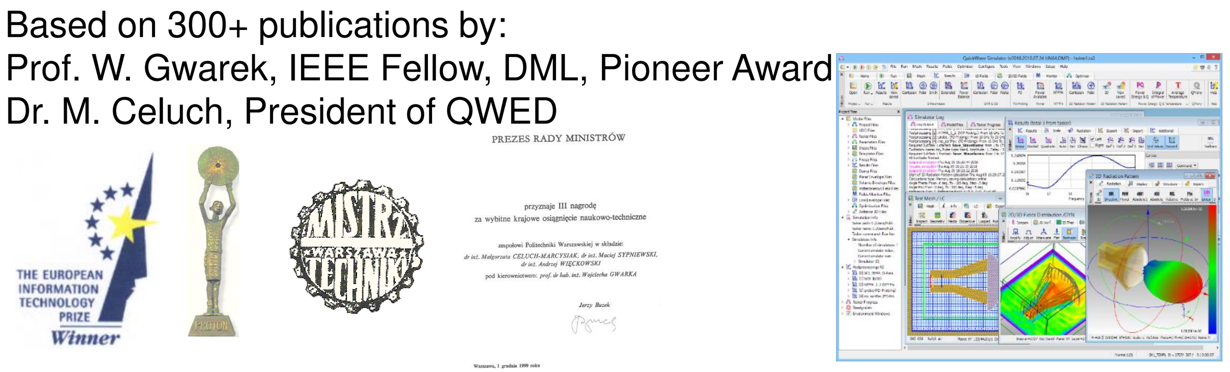
Motivation & Objectives

The modelling platforms are foreseen to implement research results of the projects' consortia and deliver them for the usage of a wide scientific community, including universities as well as industry.

Business branches & activities

Electromagnetic & Multiphysics modelling & design software, 3D & BOR 2D tools from QuickWave family

Based on 300+ publications by:
Prof. W. Gwarek, IEEE Fellow, DML, Pioneer Award
Dr. M. Celuch, President of QWED



Text-fixtures for precise material measurements

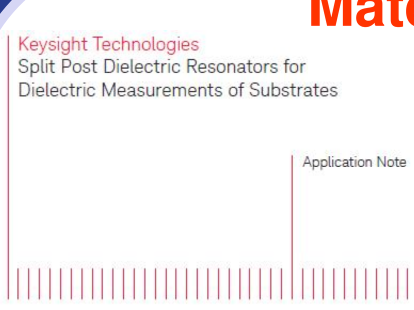
Based on 300+ publications by Prof. J. Krupka, IEEE Fellow

Consultancy & design services based on EM & material characterisation and measurements techniques

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

Public co- funded research projects

Material measurements

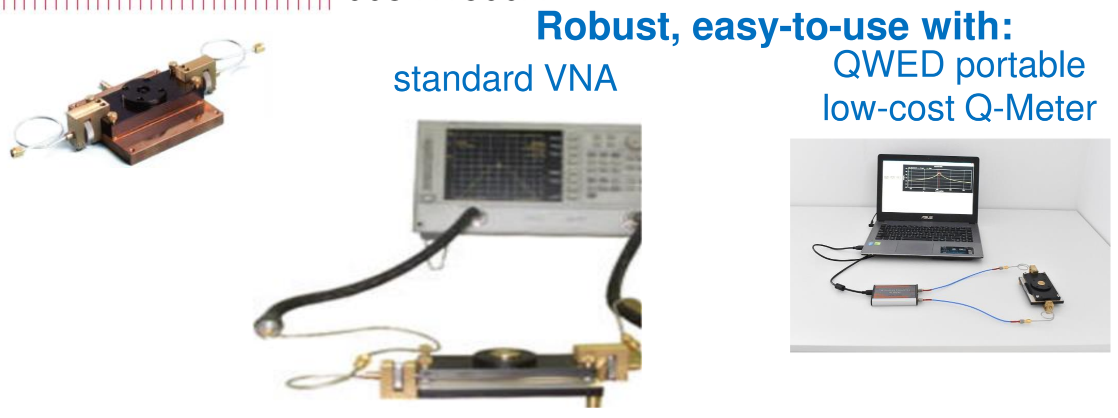


Split-post dielectric resonators for low-loss laminar dielectrics measurements subject of **European Standard IEC 61189-2-721:2015** endorsed by Keysight Technologies Option 003 N1500A

Robust, easy-to-use with:

standard VNA

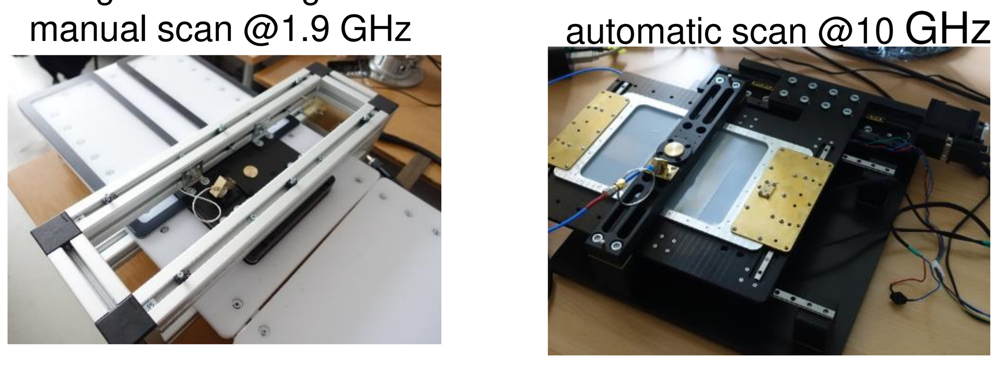
QWED portable low-cost Q-Meter



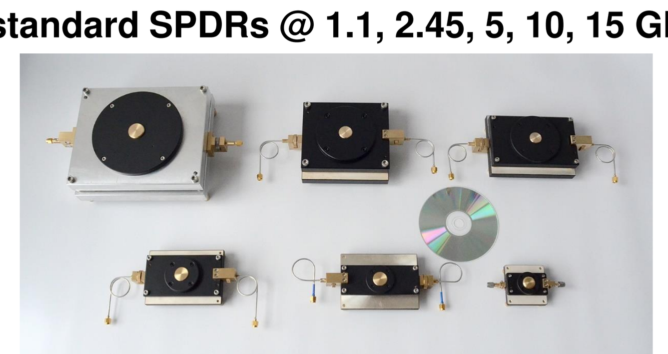
Recent SPDR-based designs for larger surfaces of:

large sheets of glass manual scan @1.9 GHz

semiconductor wafers automatic scan @10 GHz



QWED standard SPDRs @ 1.1, 2.45, 5, 10, 15 GHz

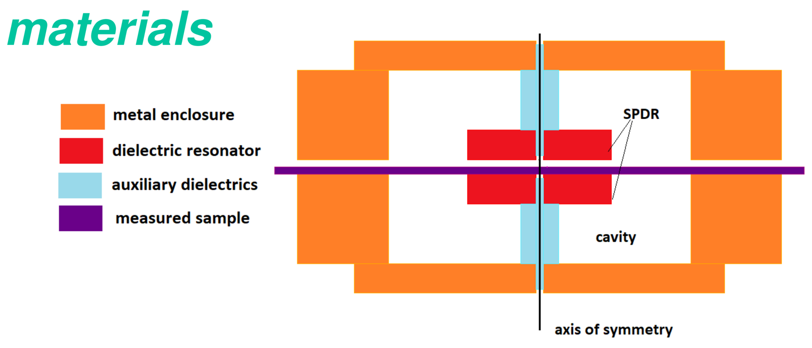


QuickWave

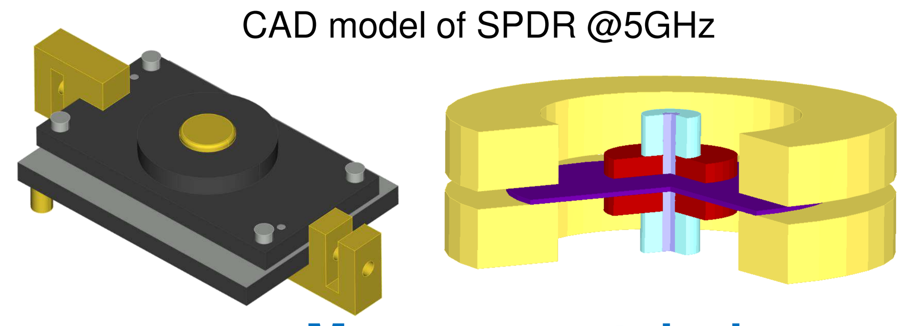
Electromagnetic & Multiphysics modelling software accounting for materials modelling at the continuum level.

Simulation – assisted design of microwave test-fixtures for material measurements

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



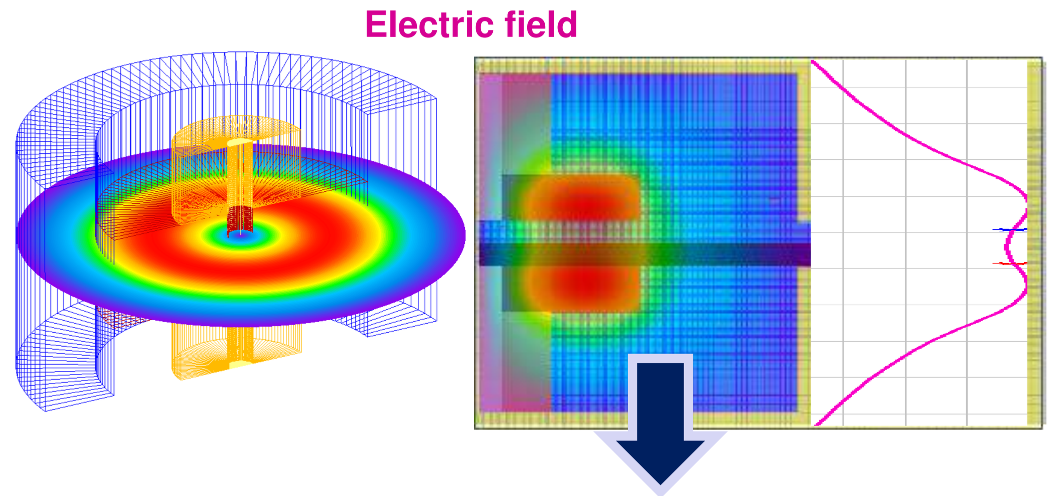
CAD model of SPDR @5GHz



SPDR 5GHz device

Simulated field distribution in SPDR

Electric field



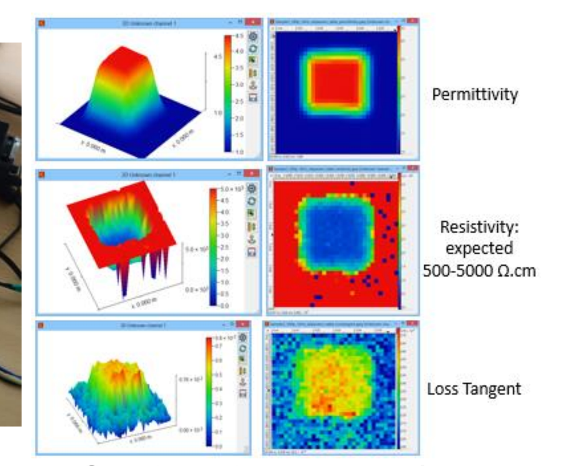
Material sample interacts with strong electric field, which facilitates parameters extraction of highly-resistive semiconductor materials with application to e.g. photovoltaic cells

Measurement device

Enhanced capabilities

semiconductor wafers automatic scan @10 GHz

2D surface imaging - Detection of parameters' inhomogeneities

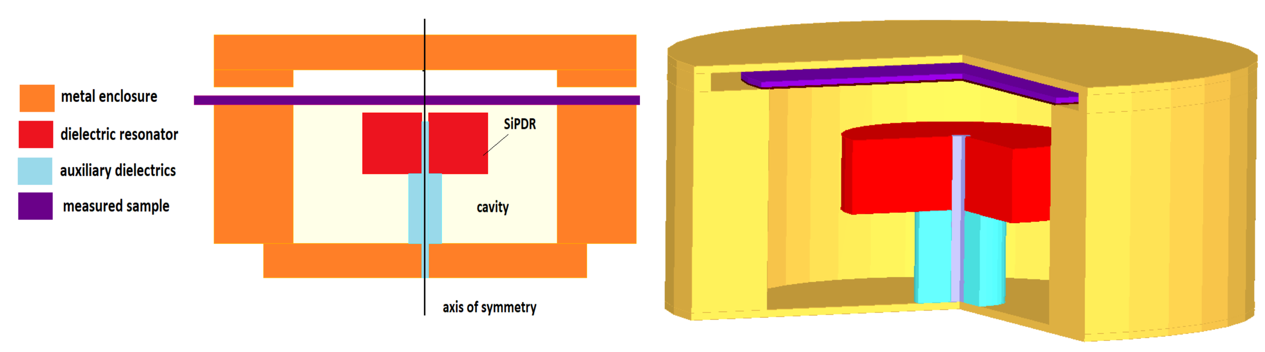


Semiconductor sample: PDOT:PSS deposited on quartz

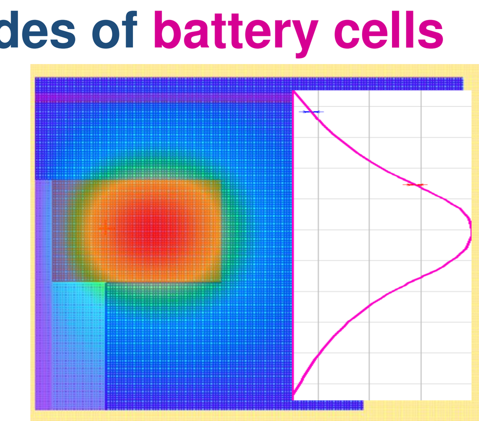
Single-Post Dielectric Resonator method for characterisation of thin conductive sheets

Challenges for the NanoBat project

Measurements of graphene anodes of battery cells



NEW SiPDR configuration for conductive materials



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

Multiscale modelling of battery cells and semiconductor junction

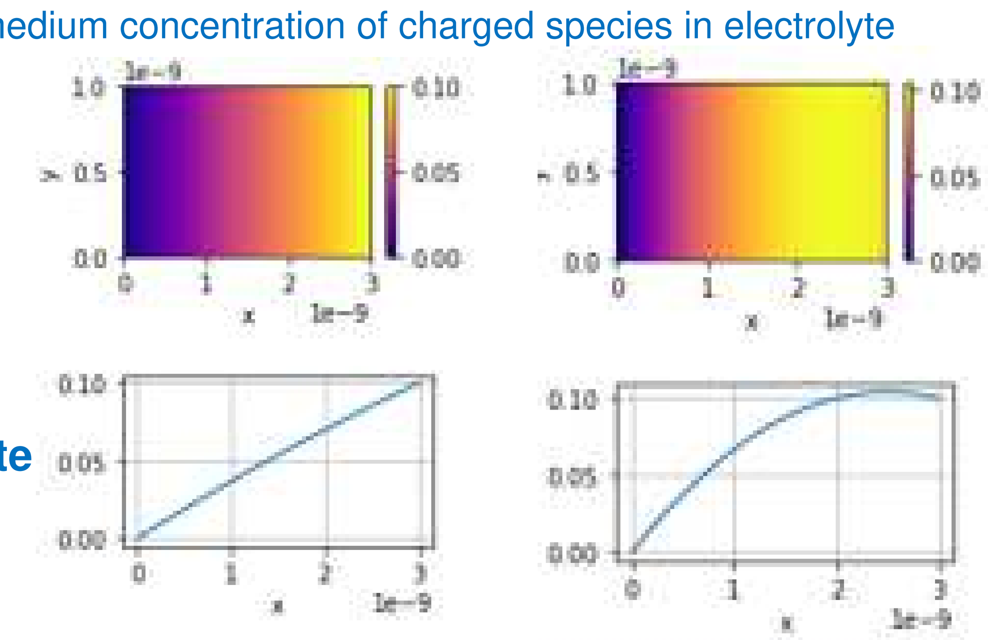
Drift-Diffusion in semiconductors

$$j_p = q_p \mu E - D_{c_p}\nabla q_p$$
$$j_n = q_n \mu E + D_{c_n}\nabla q_n$$
$$\frac{\partial q_p}{\partial t} = -\nabla j_p$$
$$\frac{\partial q_n}{\partial t} = \nabla j_n$$

Nernst-Planck and continuity in electrolytes:

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

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



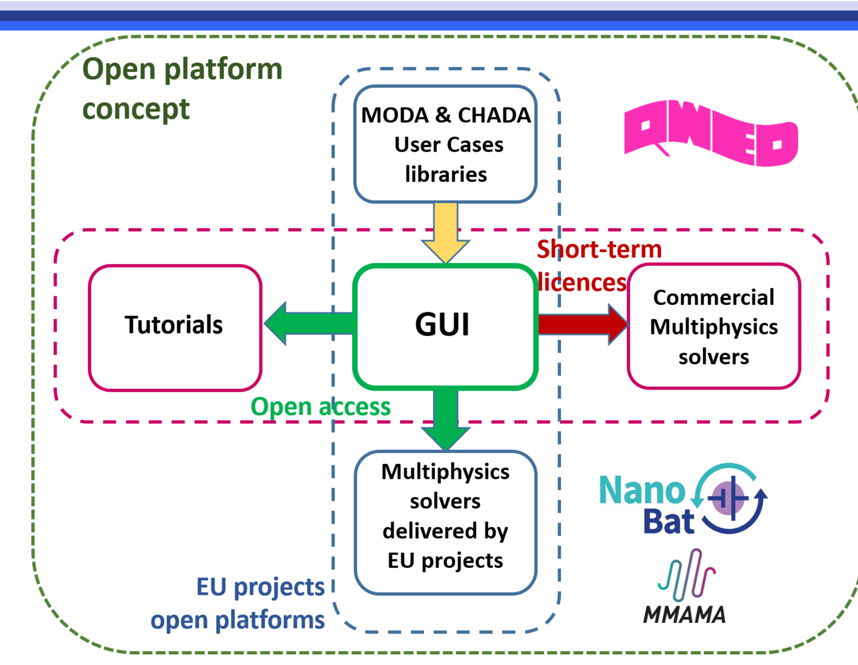
- ✓ **To be implemented in the Open Platform**
- ✓ **Modelling of species transport in electrolyte of battery cells**
- ✓ **Modelling of semiconductor junctions**

Open environment for modelling

- ➢ *Common GUI*
- ➢ *Interfaces to various solvers*
- ➢ *Assuring FAIR data*
- ➢ *Enabling modelling at different levels*

Such an approach will deliver a complete solution allowing for multi-scale multi-physics material analysis from the electronic level, through atomistics and mesoscale to continuum modelling (and possibly also data-based modelling), which eventually enables the analysis of device performance, being of high interest of industry.

Various access rights (open access, licensed access to commercial tools, etc.)



Modelling platform with exemplary commercial contribution of QWED tools

European modelling environment with common Graphic User Interface

Facilitating:

- ✓ *Interoperability*
- ✓ *Software deployment*
- ✓ *Model development*
- ✓ *Enhancing industry impact*

Acknowledgement

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