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

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This talk addresses three aspects pertinent to the progress in materials modelling: model developments, their validation against laboratory experiments, and last but not least, dissemination and popularisation via EMMC activities and open research platforms.

The EMMC assembles groups active in the developments of different material model types and even more such models are available on the European research area. Typically, each model comes with its own user interface, and in many cases the model cannot be practically used by anyone except its authors. This is especially true in the case of emerging technologies and new materials, such as energy materials, where the scientific progress in the models is much faster than computer interface developments may reasonably follow. This hinders the models' validation, interoperability, and general use. Herein, we consider a solution alleviating some of those obstacles, while seeking a compromise between the open innovation and the commercial interest of the European software companies.

- In the first part of this talk, we discuss our physics-based modelling approach, which originates from the electromagnetic modelling algorithms, subsequently coupled to thermal solvers and amalgamated in QuickWave software [1], for which industrial impacts have previously been shown [2].
- In the second part, we present how our modelling helps design material test-fixtures and experiments for energy materials' testing at GHz frequencies. We illustrate this part with selected results of dielectric resonator measurements organic semiconductors and graphene anodes.
- In the third part, we present our Open Platform initiated in H2020 MMAMA [3][4] and currently developed in the NanoBat project [5]. The Platform is based on a common, interoperable, licence-free GUI and a built-in expandable library of User Cases. The GUI invokes licence-free solvers relevant to teaching and basic research as well as commercial solvers appropriate for larger-scale industrial applications.

With this talk, we seek collaborations on extending the Open Platform with new multiscale models and linking-coupling procedures, for which purpose a Task Group is being proposed with the EMMC Focus Areas #1 and #2.

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