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EMMC case study:

Multi-length-scale modelling in ferroelectric Materials

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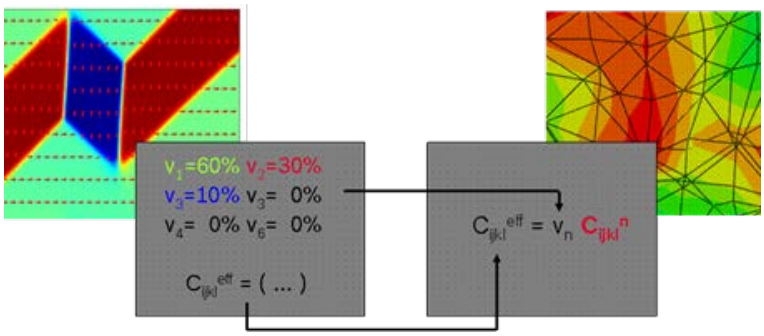

About the Company

The Robert Bosch GmbH, referred to as Bosch in the following, is a world leading multinational technology and services company headquartered in Germany. Bosch employs more than 400000 people worldwide of which about 64400 contribute to the R&D activities (04/2018).

Materials modelling is a core topic, applied for more than 15 years at the Bosch Corporate Sector Research and Advance Engineering as well as in product development. Among this, modelling projects are offered for internship at bachelor and master level and are part of PhD theses.

Internal training is provided for most commonly used software and theoretical approaches, while external training is used for very specific software and is outsourced to the software vendors.

About modelling – the nuts and bolts

The materials modelling groups at Bosch Corporate Research in Germany are familiar with various models including electronic (DFT), atomistic (molecular dynamics), mesoscopic (phase field), continuum (microstructure reconstruction, continuum mechanics and fluid dynamics), data-based statistical, and machine learning models. Multiscale modelling is also used, for example to link molecular dynamics to phase fields models, phase field models to continuum mechanics models and electronic density functional models to continuum mechanics with discrete element solvers.

Modelling is applied for structural analyses, prediction of material properties at a continuum scale, virtual material and component design. In the design process, modelling is used for the prediction of functionalities, reliability and mechanical loading analyses as well as component optimization.

The modelling engineers use both commercial and open-source software. Commercial software is used mostly for continuum models (e.g. FEM solvers, microstructure reconstruction, parameter optimization) and also for ab initio simulations, while open-source software is used more frequently for discrete models and solvers.

In the materials modelling groups at Bosch Corporate Research, modelling is widely used and the modelling type is chosen depending on the project objectives. If needed, new tools and methods are investigated and tested, also in collaboration with external resources. External resources are typically academic, but can also be research institutes and software vendors. Collaborations with academics are mostly started when there is an in-house lack of specific expertise regarding methods and approaches. These collaborations are both bilateral or in public-funded projects with various partners. Large collaboration, such as EU projects, are particularly relevant for interdisciplinary problems with the need for a wide range of expertise.

About the Case Study

The case study is based on Bosch's contribution to the German public funded project "Multi-length-scale modelling of ferroelectric materials". It was presented at the MRS Fall Meeting 2009 (Boston, USA) and the Multiscale Materials Modeling Conference MMM 2010 (Freiburg, Germany). The report on the project is available (in German) at the following link https://www.tib.eu/de/suchen/id/TIBKAT%3A651803438/Computergest%C3%BCtzte-Multiskalenmodellierungzur-virtuellen/. The effort in the project also lead to many publications by all partners involved.

For this particular case, which were your objectives as an industrial consumer of modelling?

The objective was to develop a method to predict materials properties with the intention to reduce time for development as well as materials and components related costs. This was achieved by using multiscale modelling to speed up the optimization of the material. Experimental tests were included for validation purposes.

How did materials modelling play a key role in problem solving?

Materials modelling played a key role in achieving a better understanding of failure mechanisms in materials and parts, and to derive quantitative measures for improvements.

In addition, modelling was used for reliability and lifetime assessment under specific loading conditions for selected ceramic designs. Then, simulations were performed to guide the selection of ceramic variant for maximizing reliability or function.

In the specific case was materials modelling replacing experiments or was there a special need for modelling?

In principle it could all be done by experiments, but for instance to predict reliability experimentally would be extremely costly and time consuming.

What tools and methodologies have been applied?

Continuum mechanics modelling was used with the Finite Element Analysis codes Abaqus and Ansys in combination with COMSOL Multiphysics.

What were the expected improvements of the material behaviour simulation?

Bosch expected improvements in the design of ceramics with respect to mechanical load and functionality. It was further intended to develop a better understanding of ageing effects and derive methods to reduce it, and to improve functionality by engineering the microstructure.

For this particular case, did modelling affect your value chain?

The understanding of properties of known materials were improved by linking the microstructure with the material behaviour under electrical and mechanical loadings. Piezoelectrics were screened to find new variants by modifying ceramic compositions, and the performance of these variants under electrical and mechanical loading was investigated.

In other projects, modelling supports the setting up of manufacturing processes.

For this particular case, how did you measure the impact of Materials Modelling as a tool to assist in problem solving, process optimisation, product development?

The impact was clear since modelling was used to solve a specific problem. In other cases, the definition of clear performance indicators allows to give a measure of the impact of material modelling on the targets we want to achieve.

What sort of obstacles or barriers did you have to overcome to use modelling?

A typical obstacle is the availability of characterization data regarding materials properties. For many modelling activities it is paramount to have well determined material data, which at Bosch are often obtained by in-house characterization. Because of this, before starting any project involving materials modelling, it is fundamental to create awareness of the need to involve characterization.

Do you also use reference data or do you rely on in-house characterization mainly?

Generally, data from available public sources (literature, databases, etc.) or pre-existing in-house data are taken. In case of differences to literature data, in-house data are preferred. Public databases are particularly useful when it comes to discrete modelling, because there are many available and we managed to get access to them.

Are there other obstacles or barriers you had to overcome to use modelling?

Another typical obstacle is the computational infrastructure. Requirements in terms of computational power have been increasing in the last years, thus raising the need to move from personal computers to HPC facilities, which Bosch now has available in-house.

Regarding the infrastructure. Is the storage of results also a barrier?

Simulation creates large volumes of data, so storage costs, data safety and security requirements have to be balanced in order to find the appropriate solution.

How do you think the barriers you experience could be overcome?

Generally, obtaining materials data is time consuming because the data are normally sparse over various resources. New simulation platforms being developed (e.g. H2020 MarketPlace) will help to search for standard materials data in a very efficient way, since these platforms will be able to access different data sources and aggregate information.

Do you think Marketplace could help also in terms of computational resources?

Yes, a marketplace platform with access to computational infrastructure, simulation tools, materials data and structured workflows available would be the ideal solution.

Do you see as a problem for a company to run simulations outside the company firewall?

It depends on how these platforms will be able to protect confidential data. Today, we do not use external resources for confidential projects, but with appropriate data security ensured, this may change.

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