EMMC case study:

First-principle simulations of electronic structure in semi crystalline polyethylene

Interview of Dr Mikael Unge, ABB

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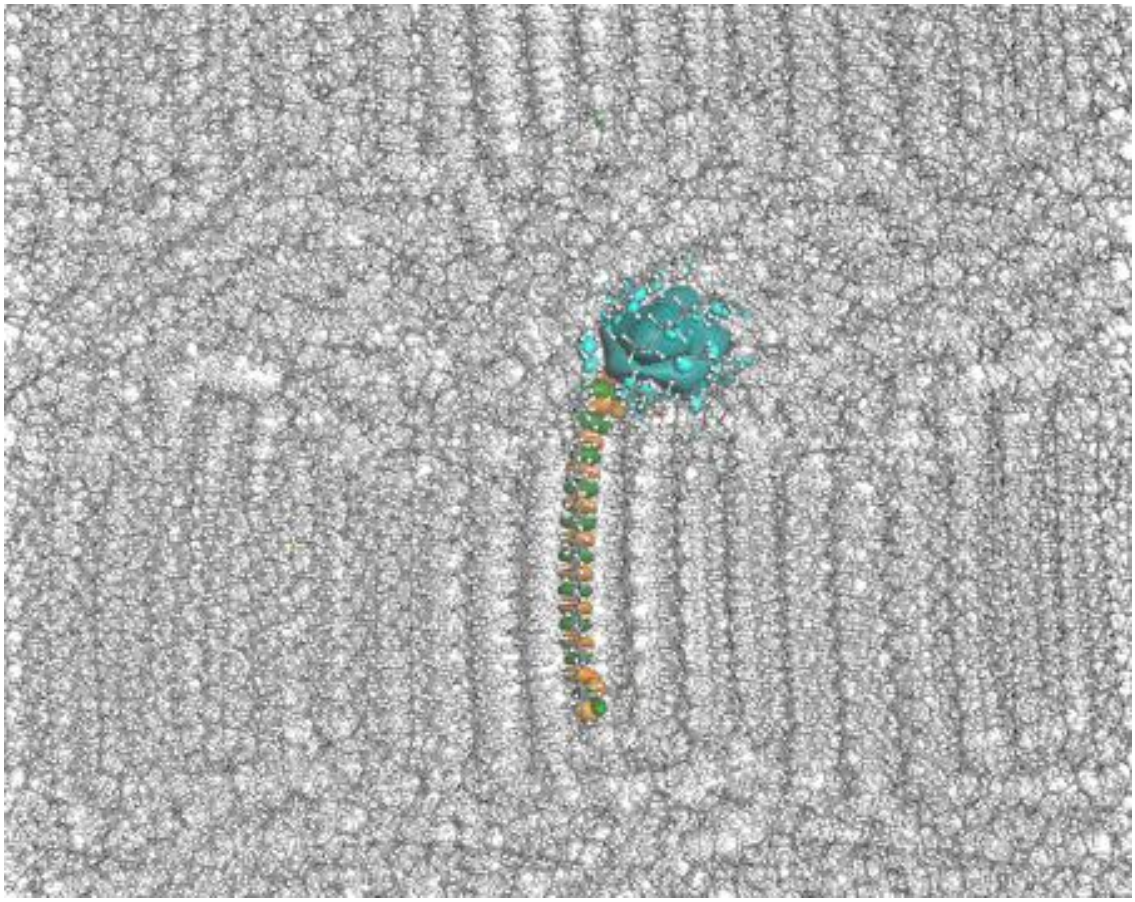


About the Company

ABB is a pioneering technology leader in power grids, electrification products, industrial automation and robotics and motion, serving customers in utilities, industry and transport and infrastructure globally. ABB's value propositions are "Bringing electricity from any power plant to any plug" and "Automating industries from natural resources to finished products" which makes them partner of choice for Power Grids, Electrification Products, Industrial Automation, and Robotics and Motion.

Their headquarters are in Switzerland and they employ over 147 000 people worldwide. In seven research centres worldwide and several Division Technology centers, more than 8000 technologists contribute to their R&D effort and an annual investment of $1.5bn feeds into these efforts.

The ABB Corporate Research Center in Sweden is located in Västerås, and employs two modellers at a PhD level. They started ten and five years ago, respectively, and keep enhancing their skills by attending courses provided by 3rd parties such as software owners.

About modelling – the nuts and bolts

The modellers in Västerås are familiar with electronic, atomistic and continuum models and they also use some mesoscopic modelling. Data-based modelling is on the verge of becoming more important. They work with multiscale modelling and can link electronic, atomistic and continuum models. The modellers use commercial software, open source/free software and in-house software on at least a weekly basis. In their projects, they are looking at a specific application/problem which they address with different types of modelling.

Occasionally, they use external services like support from software vendors and they entertain a network with academia and would sponsor PhD students. Their main reason to do this is to complement their knowledge in specific topics.

ABB works with very complex materials, and their modelling has to cover more than one particular type of material. They will have to translate quite carefully how materials modelling can address a well-defined problem. Often, one software tool cannot describe the complexity required or could not deliver in the timeframe required – hence, these are situations where modelling would definitely not be used.

About the Case Study

The case is based on ABB's work in studying electrical insulation materials and their publication, which was a joint effort with KTH, "First-principle simulations of electronic structure in semi crystalline polyethylene", A. Moyassari, M. Unge, M. S. Hedenqvist, U. W. Gedde, and F. Nilsson; J. Chem. Phys. 146 (2017) 204901 (DOI: 10.1063/1.4983650)

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

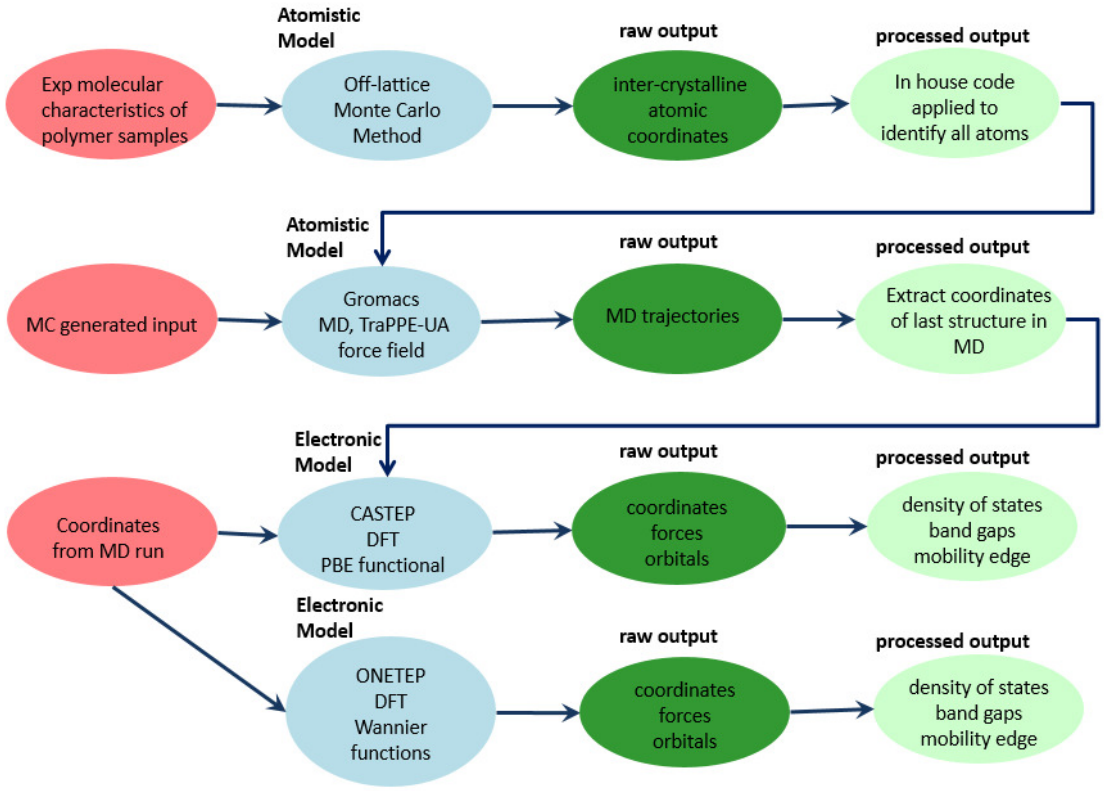
Polyethylene (PE) is currently used as the preferred electrical insulation material in extruded high voltage cables. Besides representing PE realistically (i.e. as amorphous, crystalline, semi crystalline, branched, and crosslinked), another problem was that PE can trap charge carriers such as electrons and holes that impact the mobility/conductivity and thus the leakage current. The current literature is limited of work describing which chemicals and structure that can create which sort of electron traps, so the objective was to use modelling to fill the gap.

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

Materials modelling can aid in measuring the traps, i.e. if they are shallow (within a range of about 1 eV from the band edges) or deep, and also to describe which chemicals can generate such a trap.

What tools and methodologies have been applied?

ABB and KTH used electronic (CASTEP, ONETEP) and atomistic models (GROMACS) and a commercial GUI to create and pre-process the input structures and post-process the results (Materials Studio).



What were the expected improvements of the material behaviour simulation?

It is an accepted fact that the flow of leakage current through an insulator is correlated to the chemical and structural composition. If one can now describe with materials modelling the chemicals and the structure that cause these traps and how deep they are one can move from guessing to evidence.

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

The modelling used allowed a better understanding of known materials and also allowed to study formulations (i.e. pure PE plus chemical defects).

For this particular case, what was the quantitative value of materials modelling?

Materials modelling can aid to speed up the materials selection, reduce development costs and also reduce failure of an insulating material.

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?

ABB uses materials modelling on a regular basis to solve problems, so there were already high expectations that it will make an impact when applied to this particular case.

What technical and technological benefits resulted from the project?

A better understanding of the material performance leads to a better product and in understanding how to predict level of leakage current, the case contributed to ABB's value proposition of "*Bringing electricity from any power plant to any plug*".

What where the economic benefits/impacts when you did use modelling?

The modelling project was part of a long-term R&D venture so cannot be seen as an isolated attempt.

What was the business impact versus previous approach?

The outcome of this materials modelling application cut down on trial and error experiments as the role of chemical defects and structure was better understood. Hence, saving costs was a big impact on business.

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

The modellers had to learn how to use an open source code (GROMACS).