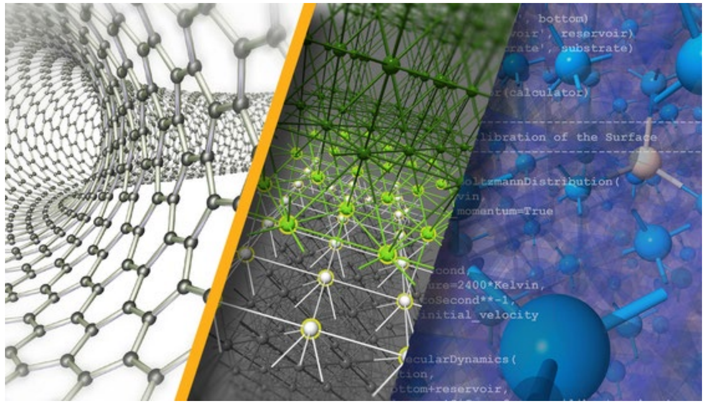
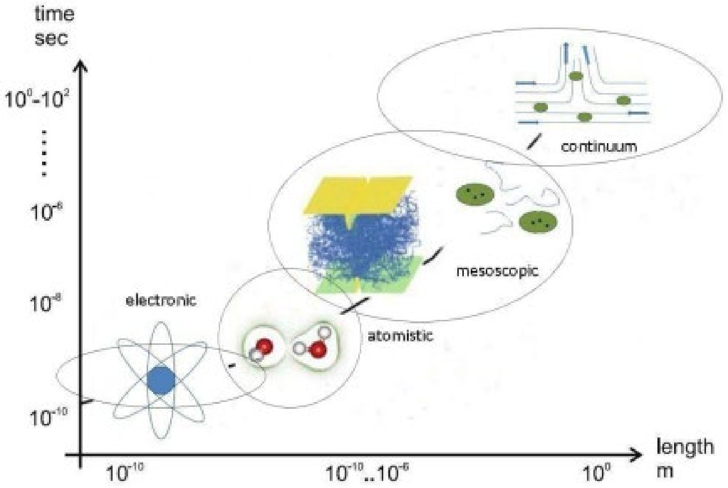
Capabilities of Materials Simulation

EMMC Demonstrator Activity

Anne de Baas, Erich Wimmer,
Ilian Todorov, Kersti Hermansson,





Outline of the activity

<u>*Purpose*</u> *Inspire industry*

to appreciate and have confidence in the capabilities of ***discrete*** *materials simulation*

Controlling expectations by building knowledge of simulation capabilities
Enabling a choice of (a combination of) e/a/m/c models

<u>*Scope*</u> *Agree and Simulate Demonstrator Cases available on the EMMC website*

The simulated cases will give an impression of which type of model (e/a/m/c) (or combination thereof) can address what type of problems and show that a certain property of process can be simulated and trusted.

<u>*"USER experience"*</u>

An industry (eventually guided by an advisor *(Simulation Translator))* who wants to embark on discrete simulation could look at simulations of relevant, representative cases on the EMMC web.
The industry will know that the EMMC endorses the relevance of these demonstrators and the path to the solution will become clear.
The Industry will get confidence that the SWO can simulate similar problems for them.
The industry could then acquire the simulation technology or ask a selected SWO to simulate their own problem.

EMMC Role

The EMMC will guard its **neutrality** in the following way.

The EMMC approves of the list but will not run the demonstrator cases (DC).

Each SWO is welcome to run the DCs and present their results at the EMMC website with a disclaimer from the EMMC.

It will be the job of Translators to interpret the SWOs results. Competition between SWO happens thus outside the EMMC umbrella.

The EMMC can use the list to create awareness of simulation capabilities.

EMMC Task Group Work Plan

Step 1: European **SWO and modellers** at the EMMC workshop in June 2022 will start building a list of cases

This is an intermediate step.

TODAY

- **should ensure we do not to stand with empty hands when meeting with manufacturers to ask them what capabilities they would like to see demonstrated**
- **is necessary as discrete modelling is not as mature as continuum modelling**
- **is necessary to control expectations as knowledge on the capabilities is not yet wide-spread**

Step 2: **Industrial manufacturers** will be invited at a webinar in ***Sept 2022*** to change and add and prioritise cases on the list

Step 3: **SWO** will be invited to document and share their simulations on the EMMC website.

Step 4: EMMC **Organisational Members** (SMEs and their Advisors) can access the simulation information

Any comments on this way of working?

Aspects of the cases

- Demonstrator cases (DCs) are only part of the solution of industrial problems.

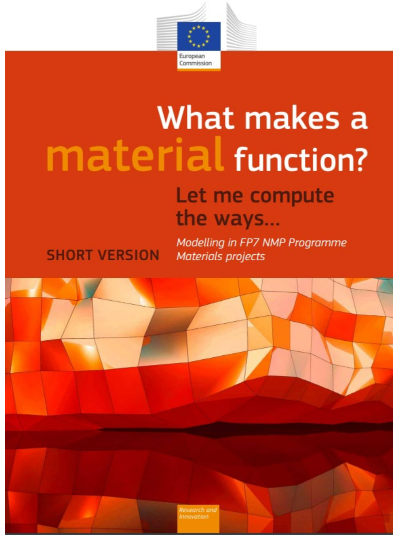
- The cases will span
  - from the lowest level of complexity
    - *Discrete modelling, even for "simple" cases, has today huge variety, veracity and speed*
    - *Introduction to newcomers to discrete modelling*
  - to State-of-the-Art research topics currently under investigation

- The simulated cases will give an impression of what each type of model (e/a/m/c) can produce on certain material science problems and as a consequence it will give an impression of what part of industrial problems can be handled, remembering that simulation is often used not to predict absolute values but to predict trends

- Reasons for the cases can be
  variety in model results
  problem that can not be handled by continuum models
  lack of experimental data

- The list of cases will be available to all, while the actual descriptions of the simulation (input parameters, model, results, PE , MR,….) will be available to EMMC Organisational Members.

Simulation Documentation



RoMM

Documentation :

The documentation has to be sufficient to be convincing, but not necessarily a blue-print for others to copy.

- The problem/property/mechanism/phenomenon in a nutshell description
- MODA (if chain of physics-based models)
  - PE+MR
  - Provision of input parameters (data base, physics-based simulation with data processing)
    - If acceptable, the parameter sweep (phase space) covered by the simulations and why – relationship with problem/property/mechanism/phenomenon
  - Post processing of raw data to get the post-processed data (the topic of the demo)
  - Software (version) used and accuracy of this exact set-up(s) or rather rooting out errors and pitfalls
  - If acceptable: validation and verification, and workflow issues like where to get the data and exemptions from licences for trials, scale of the problem and accuracy for crude explorations as well as for accurate representations
- Time to solution on example hardware (traffic lights)
- Skills level necessary (i) to set-up; (ii) to run; (iii) to extend to other materials (link to translators and other more accurate methods; link to specialised expertise SWO)
- Free format discussion of the results.

Is this information appropriate as industry attractor?

Topics on the list

I Materials properties

Structural properties
Mechanical and Thermomechanical properties
Thermodynamic properties
Electronic, optical, and magnetic properties
Transport properties
Chemical properties
Electric, electronic and magnetic properties
Optical properties:
Electromechanical and -chemical

III Phenomena and mechanisms

Time-dependant/happening at different scales (bridging))
Materials transformation under manufacturing or in-service behaviour

Mechanical and electrical materials transformation
Electrical materials transformation
Thermal materials transformation
Chemical materials transformation

II Understanding of phenomena and interpretation of experiments

Analytical and Characterisation Methods

X-ray diffraction spectra
IR and Raman spectra
UV/vis spectra
XPS, EXAFS, HREELS spectra
TEM images
AFM images
NMR spectra
STM images

Case examples
concerning material properties

Case 1 Simulation of Elastic Coefficient (in GPa)

System: polymer with complete cross-linking :

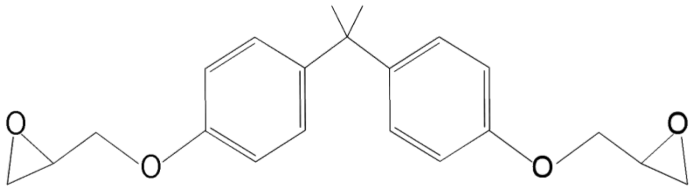
a) Resin: Diglycidyl ether of bisphenol A (DGEBA) resin cured with 4,4’ diaminophenylsulfone (DDS)
b) Resin: Tetraglycidyl diaminodiphenylmethane (TGDDM) cured with DDS

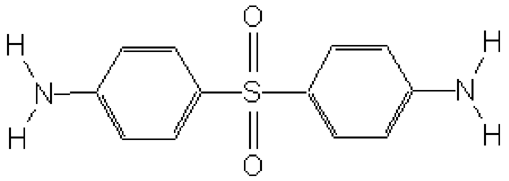
Conditions: ambient T and p

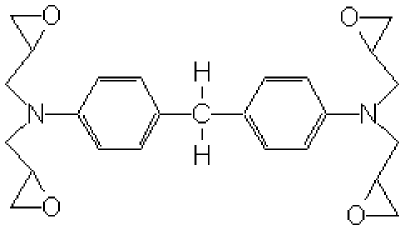
Experimental Data:

a) S. R. White, P. T. Mather, M. J. Smith, Characterization of the cure-state of DGEBA-DDS epoxy using ultrasonic, dynamic mechanical, and thermal probes, Polymer Engineering and Science, vol. 42 (1), 51-67 (2002) https://doi.org/10.1002/pen.10927

b.Shabnam Behzadi & Frank R. Jones (2005) Yielding Behavior of Model Epoxy Matrices for Fiber Reinforced Composites: Effect of Strain Rate and Temperature, Journal of Macromolecular Science, Part B, 44:6, 9931005, DOI: 10.1080/00222340500393881 https://doi.org/10.1080/00222340500393881







Type	Resin	Calculated Bounds (GPa)	Experiment (GPa)
RA_4+RB_2	DGEBA	3.49-3.53	2.4-3.2 [a]
RA_4+RB_4	TGDDM	5.18-5.19	5.103±.033 [b]

Case examples concerning material properties ctd

Case 2 **Simulation of solubility**

System: polystyrene soluble in ethyl-acetate

Conditions: ambient T, p, no stirring

Experimental Data: www.hansen-solubility.com

https://www.polymerdatabase.com/polymer%20physics/delta%20Table.html

https://chempedia.info/info/polymers_solubility_parameters/

Justification of this case: although solubility seems a straight forward materials property, it suffers from a large divergence in simulation results. The results depend on the exact procedure, the software used as well as on the Materials Relations (Forcefield) used. The industrial relevance would thus be to show reproducibility of the experiments.

Is the specification enough to make eventual simulations comparable?

Case examples concerning material properties ctd

Case 3 Piezoelectric Tensor

System: Hexagonal Aluminium Nitride (space group $P6_3mc$)
Conditions: ambient conditions
Experimental data:

Case 4 Thermal and transport properties

System: Lithium oxide, Li_2O
Properties to be simulated:

1. Density as a function of temperature between 0 and 2000 K in solid in liquid phases
2. Melting point
3. Diffusion coefficient of Li as a function of temperature between 750 and 2000 K

Case 5 Strength of Interfaces

System: Silicon nitride / Aluminium
Properties to be simulated:

Compute the strength of a Si_3N_4/Al interface, i.e. work of separation in J/m^2, as a function of crystallographic orientation and chemical composition (surface termination) at ambient conditions assuming a low-stress system.

Case 6 Refractive Index of Oxide

System: Yttrium oxide, Y_2O_3
Properties to be simulated:
At ambient conditions, compute the refractive index of cubic Y_2O_3 as a function of energy in the range between 1 and 10 eV. Before computing the optical properties, determine the equilibrium lattice parameters and internal atomic positions by energy minimization and compare with available experimental data and use the computed structural parameters for the computation of the optical properties.

Case examples
concerning understanding of experiments

Case 1 Degradation mechanism and products

Material: < *prototypical composite, microstructure, history*>

Conditions: Autoclave T=360°C during month

Experimental Data:

How can we select a part of this problem that can be handled by discrete modelling?

Case examples
concerning understanding of experiments ctd

Case 2 Interpretation of electron energy loss spectra

System: Surface of cubic SiC, 3C-SiC(001)-3x2, exposed to 50 Langmuir of hydrogen
Properties to be simulated: Experimental electron energy loss spectra
Conditions: measured between 500 and 3000 cm^{-1}.
Experimental Data: Soukiassian et al., Nat. Commun. 4, 2800 (2013).

Justification: The simulation should find a structural model of this surface and compute the vibrational modes that explain the experimental observations

Case examples concerning phenomena

Materials transformation under manufacturing or in service-behaviour

Case 1 Full curve of plasticity (stress strain curve)

Material : Mg and effect of 1% Al-alloy hcp single crystal random distribution of elements

Conditions: Ambient *T , strength and direction strain rate*

Experimental data:

Is the specification enough to make eventual simulations comparable?

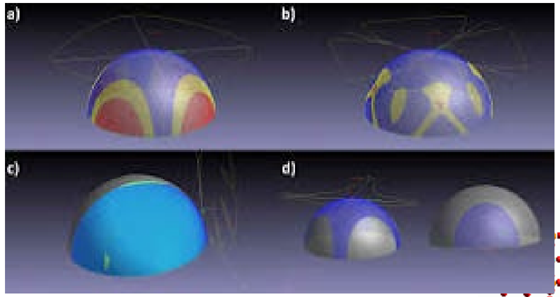
Case 2 Interlaminar/interply shear strength

Material: < *polymer, phase and curing, microstructure, geometry, fibres*>

Conditions: <*load, strain rate, T* >

Experimental data:

Case 3 Composite stiffness changes during manufacturing

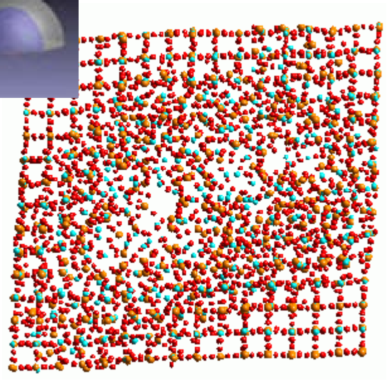


Material: <*specific material*>

Conditions: <*draping*>

Experimental Data:

Case 4 Radiation effects on glass during storage of nuclear waste



Material: glass BSi

Conditions: radiation

Experimental data: Geisler et al, J Phys.: Cond. Matt. 15, L597 (2003).

Actual List

Please add ideas to the list by sending your input to

debaas.anne@gmail.com

Please be **realistic** in specifying the case so that simulations can be done.
Focus on key mechanism!

Please be **precise** in specifying the case so that simulations can compared

Case Title:
Material:
Conditions:
Experimental Data:
Justification of the case :

Prioritisation of cases by Manufacturers Sept 2022

Result from one specific workshop

Properties of interest and digital twinning

Properties	Number of times selected	%
Chemical	67	17.3%
Thermodynamic	67	17.3%
Electrical	54	13.9%
Optical	42	10.8%
Magnetic	29	7.5%
Mechanical, elastic - stiffness	29	7.5%
Mechanical, elastic - strength	29	7.5%
Liquid-Vapour related	14	3.6%
Rheological - adhesion	13	3.4%
Mechanical, elastic - fatigue	12	3.1%
Rheological - wetting	12	3.1%
Mechanical, elastic - progressive damage	10	2.6%
Mechanical, elastic - damping	5	1.3%
Total times selected	388	

In the context of the comprehensive digital twin, with which disciplines should Materials Modelling software be integrated more closely?

- *85% - Experimental physical testing data (e.g., parameter identification process) and data management*
- *13% - the Manufacturing Process (e.g., build processors for agile manufacturing)*
- *2% - Both: Experimental physical testing data is the natural discipline, but if we achieve a proper and accurate multiscale protocol Materials modelling can have a huge potential in the manufacturing for materials and drug design.*