Simulation Methods on Virtual Laboratories for Characterization of Functionalized Nanostructures

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Overview

- o Virtual Lab Emergency

- o COMSOL Multiphysics Collaborative Modeling Environment

- o COMSOL Multiphysics Teaching Tool on Modeling & Simulation

- o Use of COMSOL Multiphysics

- o Mass Spectrometer

- o Laser Crystal Growth Process

- o Powder Sintering

- o Polishing Sintered Powder Blocks
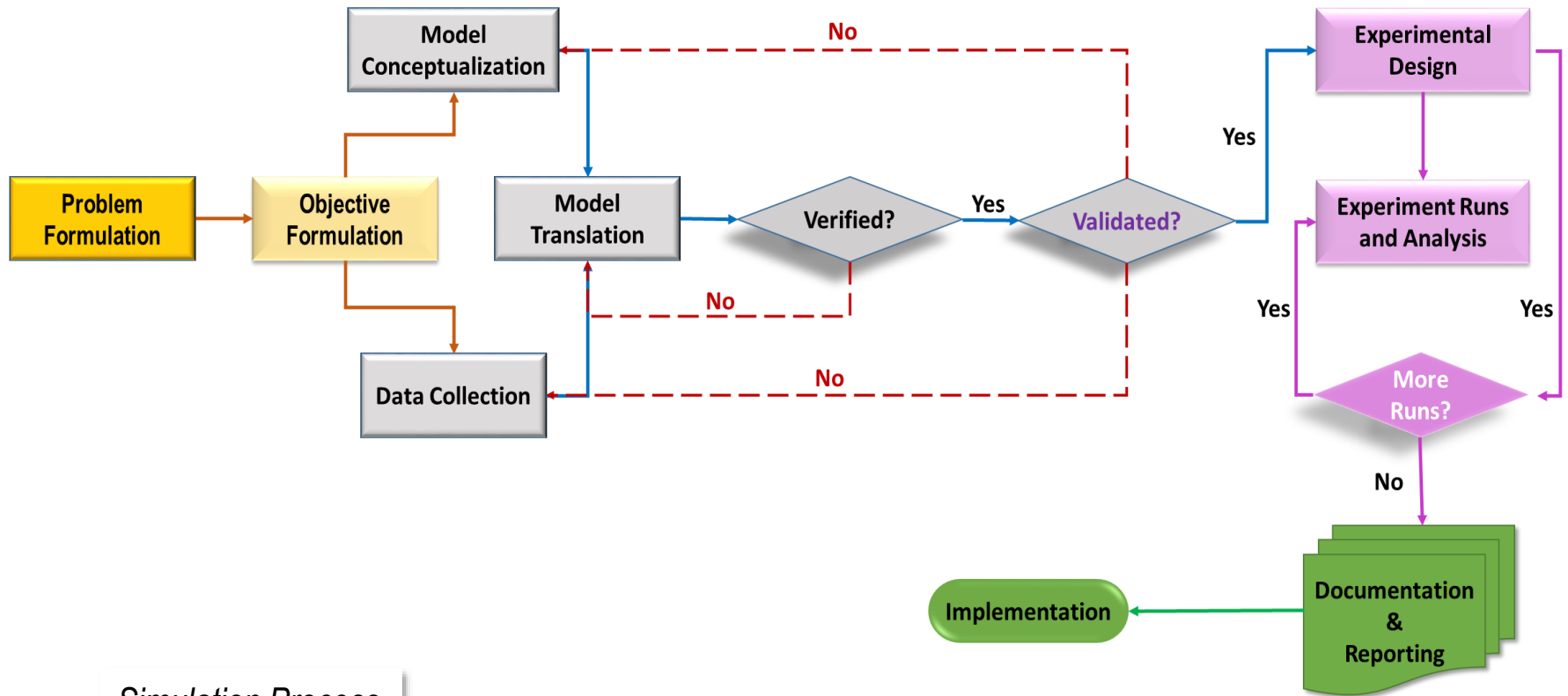
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Virtual Lab Emergency

- Using remotely the existing top R&D Laboratories facilities would become soon common practice, but for now basic training, teaching and R&D collaboration on specific issues can be successfully deployed.

- A first step on producing functionalized materials to be integrated on smart applications is to properly settle their multi-physical models as to adequately consider their properties during designing the processing, post-processing and controlling phases based on successive simulations.

- For settling the multi-physical models associated to R&D Labs installations and equipment, **COMSOL Multiphysics is a core-function software to be used** for a proper and deeper understanding of the complex-dynamic relationship existing among Physics, Processing and Controlling on experimental research.

- Teaching "Research Process Mapping" using the principles of scientific methods within Research Labs is a challenge and an opportunity, equally.

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COMSOL Multiphysics
Collaborative Modeling Environment
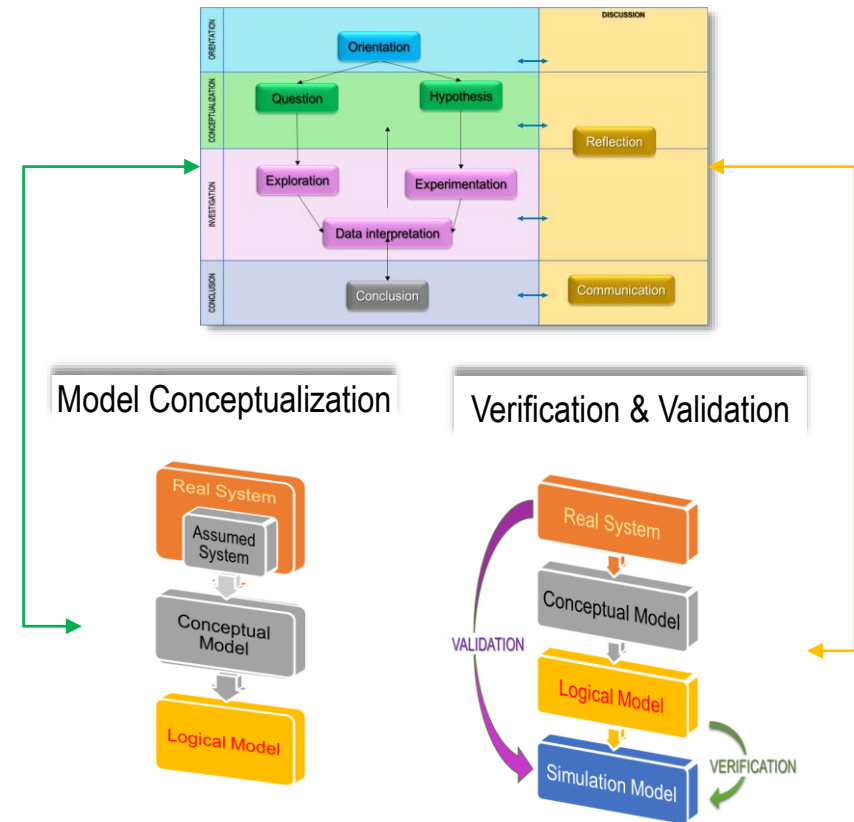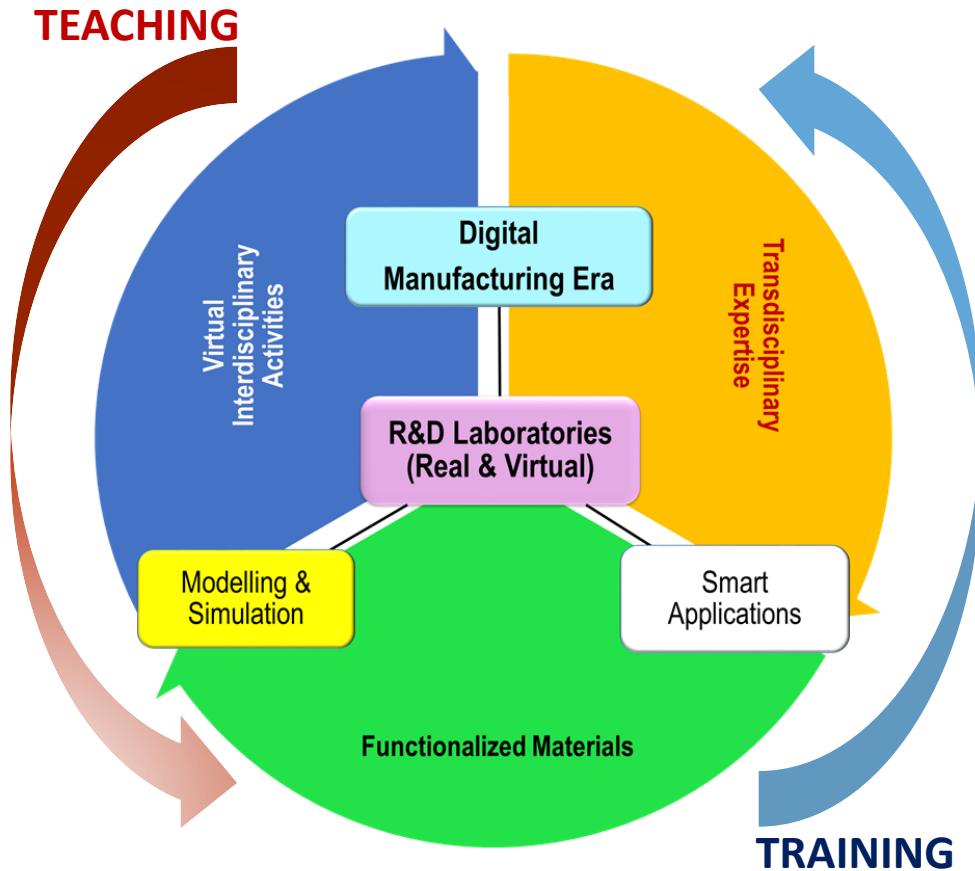
COMSOL Multiphysics
Teaching Tool on Modeling & Simulation

Simulation Process

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Use of COMSOL Multiphysics

COMSOL Multiphysics®

COMSOL Server™

ELECTROMAGNETICS	STRUCTURAL & ACOUSTICS	FLUID & HEAT	CHEMICAL	MULTIPURPOSE	INTERFACING
AC/DC Module	Structural Mechanics Module	CFD Module	Chemical Reaction Engineering Module	Optimization Module	LiveLink™ for MATLAB®
RF Module	Nonlinear Structural Materials Module	Mixer Module	Batteries & Fuel Cells Module	Material Library	CAD Import Module
Wave Optics Module	Geomechanics Module	Subsurface Flow Module	Electrodeposition Module	Particle Tracing Module	ECAD Import Module
Ray Optics Module	Fatigue Module	Pipe Flow Module	Corrosion Module		LiveLink™ for Inventor®
Plasma Module	Multibody Dynamics Module	Microfluidics Module	Electrochemistry Module		LiveLink™ for Revit®
Semiconductor Module	Rotordynamics Module	Molecular Flow Module			LiveLink™ for PTC® Pro/ENGINEER®
MEMS Module	Acoustics Module	Heat Transfer Module			File Import for CATIA® V5

Additional Interfacing column:
- LiveLink™ for Excel®
- Design Module
- LiveLink™ for SOLIDWORKS®
- LiveLink™ for AutoCAD®
- LiveLink™ for PTC® Creo® Parametric™
- LiveLink™ for Solid Edge®

COMSOL as a Teaching Tool

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Mass Spectrometer

The main physical processes related to the lab installation (e.g., Mass Spectrometer) were described adapting the existing COMSOL Multiphysics ® models to the installed lab equipment data.
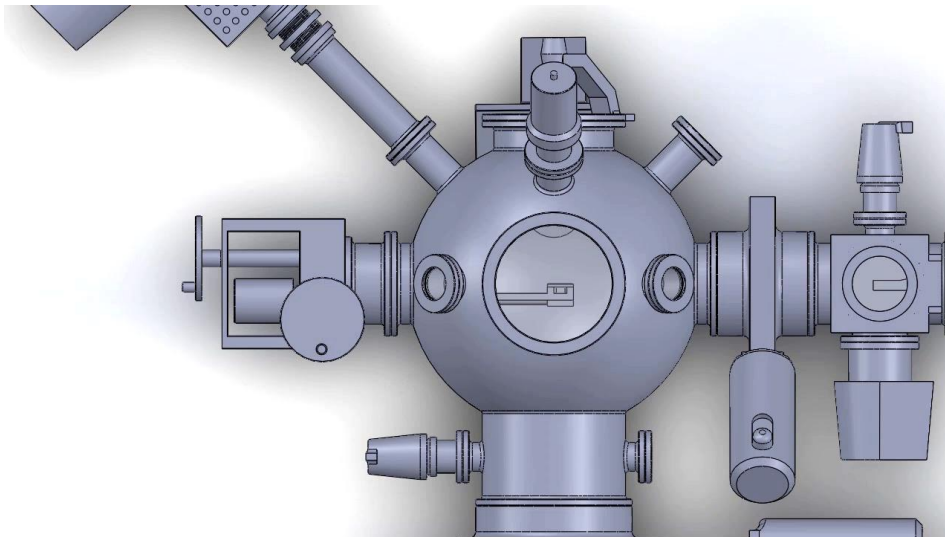
Mass Spectrometer- SolidWorks model

(a) Longitudinal section view within the ion source
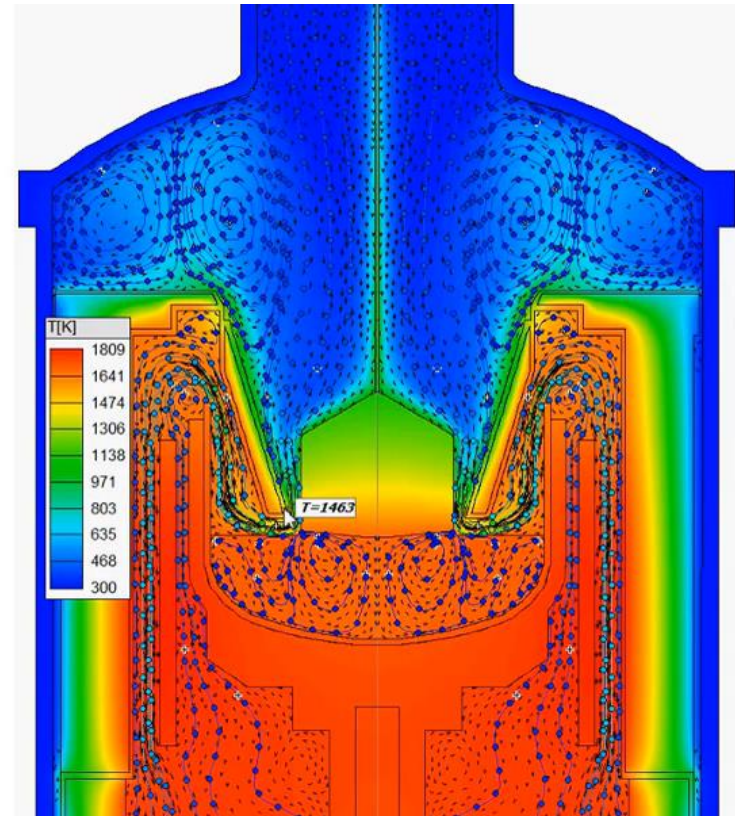   (SolidWorks model and COMSOL Apps Gallery)

a

b

b

(detail)
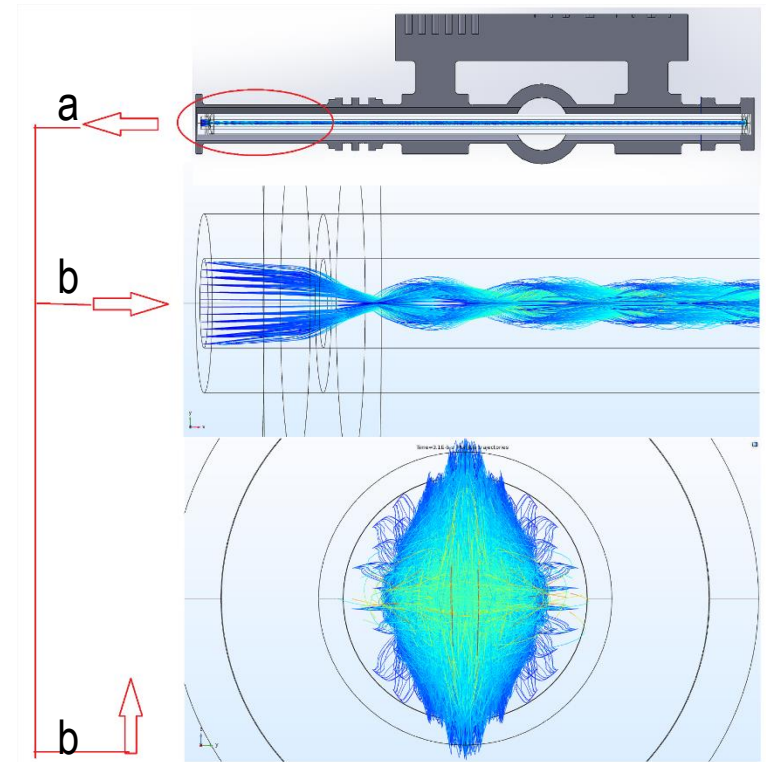
(b) Transversal section on ion gun
(adapted COMSOL Apps Gallery with lab configuration)

Laser Crystal
Growth Process

Crystal growth process dynamics

Salt crystal growth temperature related process
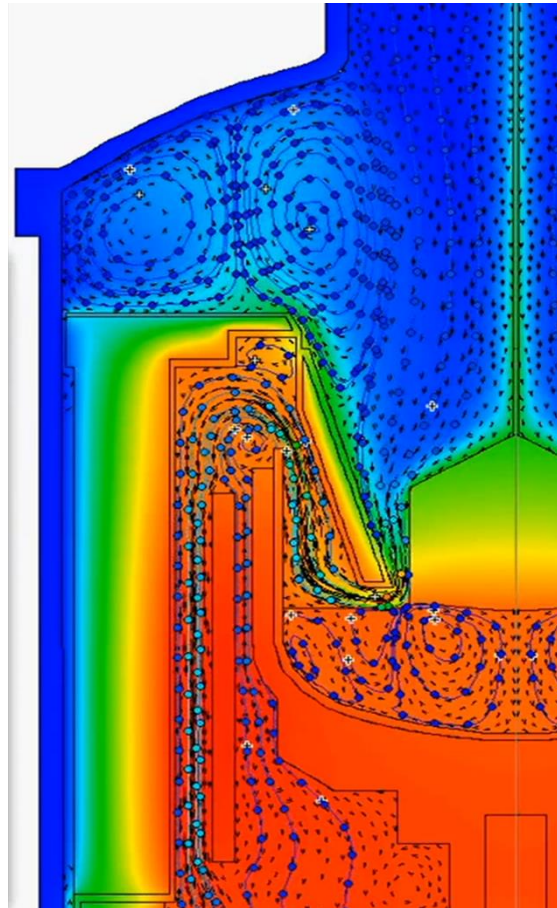
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Laser Crystal
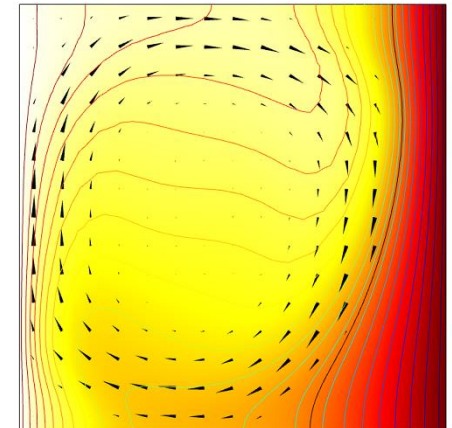## Growth Process (cont. I)
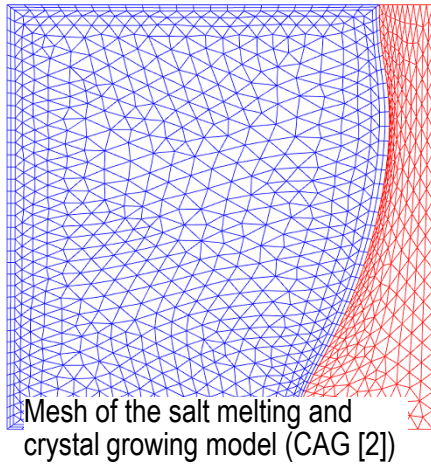
Mesh of the salt melting and crystal growing model (CAG [2])
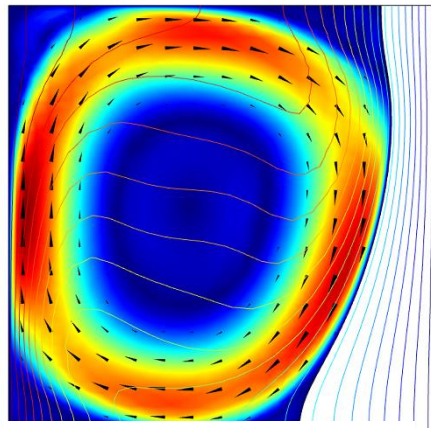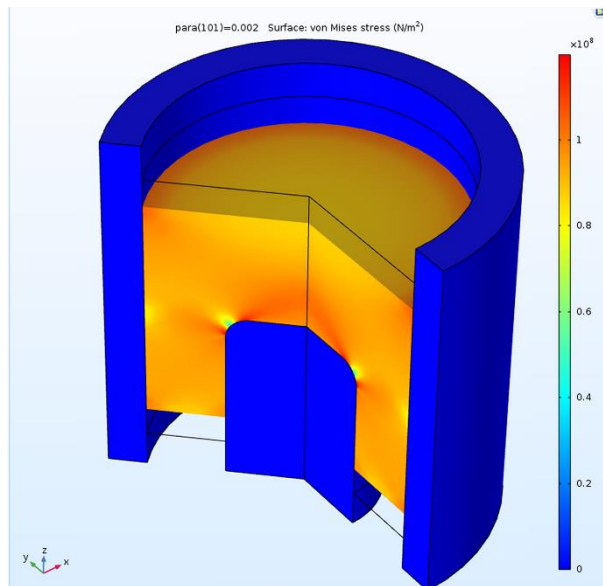

Thermal field dynamics during crystal growth (CAG [2])
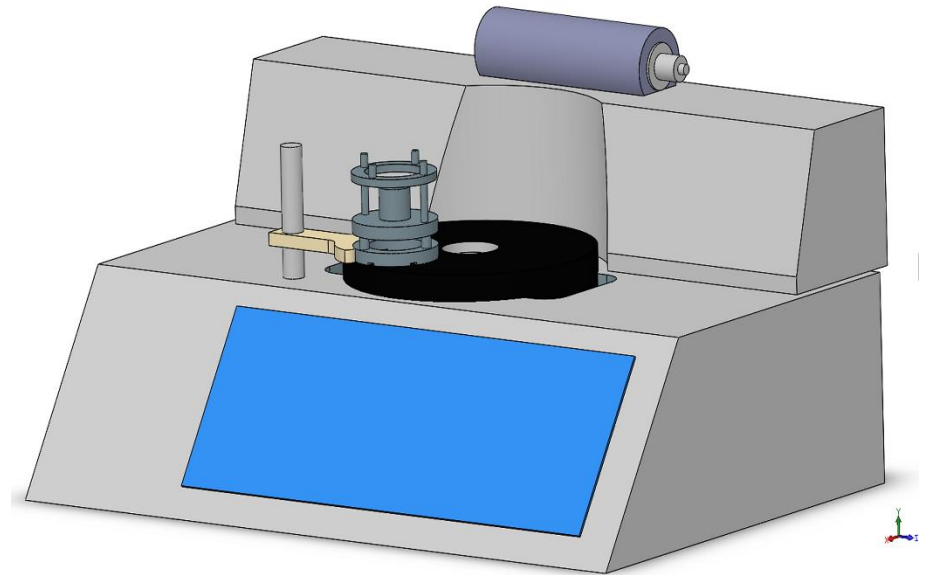

COMSOL used as an adaptive Teaching Tool

Thermal field dynamics during crystal growth (CAG [2,3])

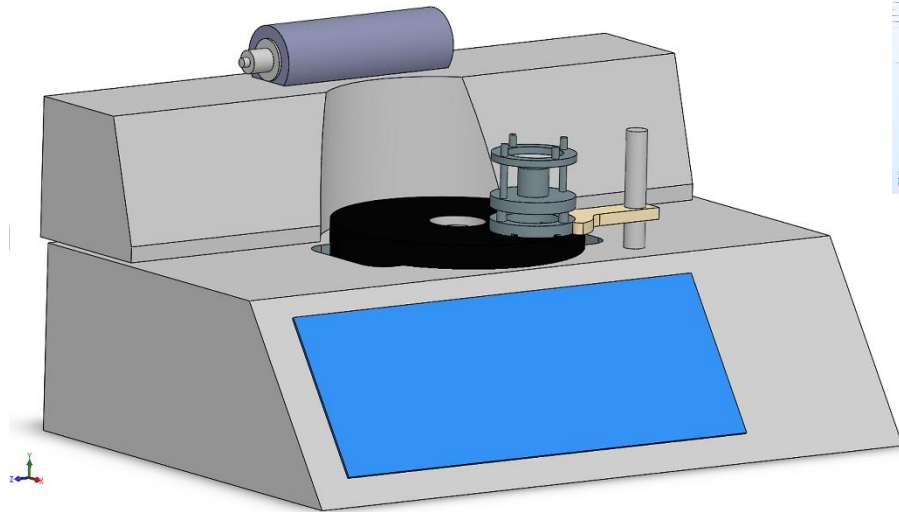**COMSOL CONFERENCE 2017 ROTTERDAM**

Powder Sintering

Powder sintering
(adapted model CAG [4])

Crystal Polishing Equipment
(CATIA imported CAD model)

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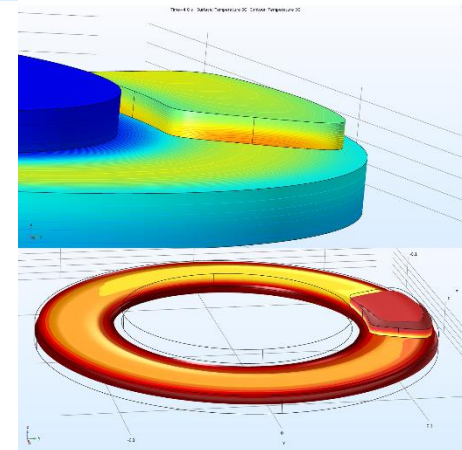
Polishing Sintered Powder Blocks

Polishing dynamics' and thermal effects
Time dependent (a, b) thermal flow and
material thermal stress studies adapted
form CAG [5]

a

b

Crystal Polishing Equipment
(CATIA imported CAD model)

Excerpt from Proceedings of the 2017 COMSOL Conference in Rotterdam
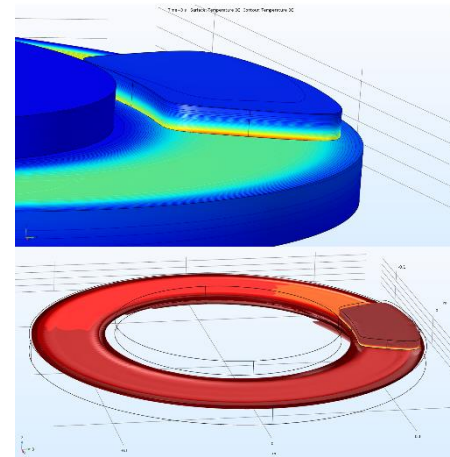
Conclusions

o COMSOL Multiphysics® software and COMSOL App Gallery were used as valuable teaching tools.

o Comparing the laboratory observations with the calculated/simulated data from the COMSOL App Gallery, understanding, adapting or redesigning an application is a first learning step on modeling and simulation.

o For real R&D lab equipment and processes the Apps Gallery models were used to understand the experiments path and each parameter's influence on overall process.

o The main physical processes related to the lab installation were described adapting the existing COMSOL Multiphysics ® models to the installed lab equipment data

o All experimental data related to the on-the-site process were archived in dedicated modules for each specific installation. These would be further on adapted to the different experimental arrays.

Thank you

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