

# Simulation Methods on Virtual Laboratories for Characterization of Functionalized Nanostructures

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## 1. Introduction

Within the emerging integrative concept of IoT (Internet of Things) and IIoT (Industrial Internet of Things) that are paving the way towards Digital Manufacturing Technologies and the next paradigm shift of Industry 4.0, R&D Laboratories have to be at the forefront of the transformation.

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. Thus, the necessary multidisciplinary-transdisciplinary expertise for running on the Digital Manufacturing Era to come will be properly achieved. 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.

## 2. Experimental Set-up

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.

## 3. Methods - Use of Simulation Apps

During the description, characterization and process simulation phases for different R&D Laboratory equipment and installations (fig.1,4,8,10) the main modules of COMSOL Multiphysics ® were extensively used, as well as its add-ons (LiveLink™ for SolidWorks®, LiveLink™ for CATIA, LiveLink™ for Excel, LiveLink™ for MATLAB®).

The main physical processes related to the lab installation (e.g., Mass Spectrometer) were described adapting the existing COMSOL Multiphysics ® models [1] to the installed lab equipment data (fig.1,2) 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.

## 4. Simulation Results

Teaching “Research Process Mapping” using the principles of scientific methods within Research Labs could be a challenge and an opportunity, equally.

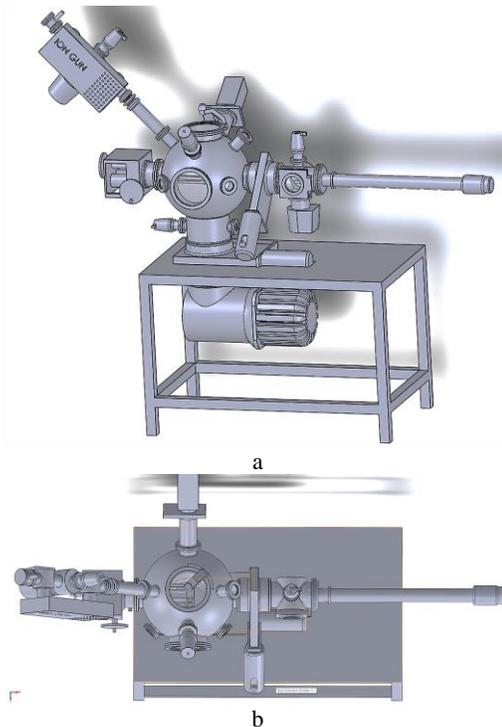
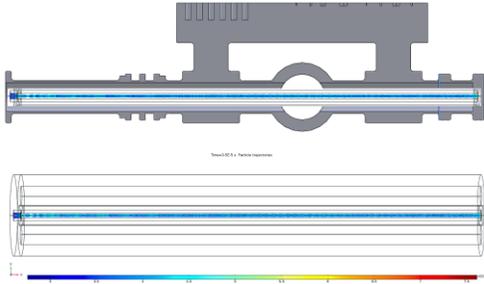
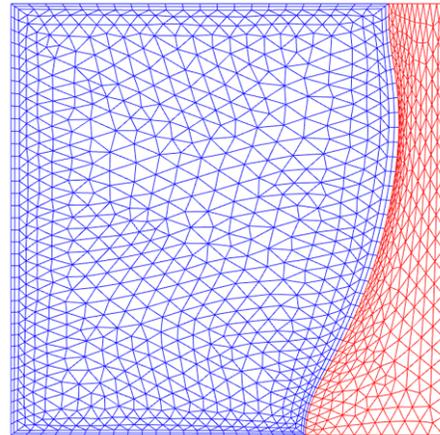


Figure 1. Mass Spectrometer- SolidWorks model

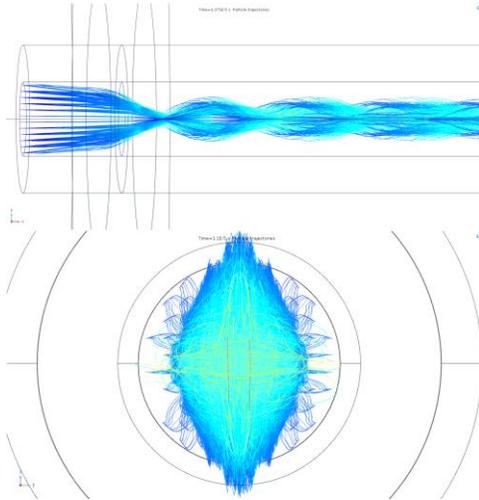
Nevertheless, students attending experimental research need to have some knowledge and skills before starting to do technical and scientific observation, measurements or experiments.



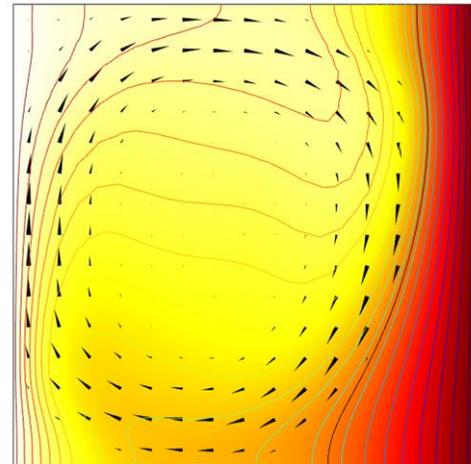
**Figure 2.** Longitudinal section view within the ion source (SolidWorks model and COMSOL Apps Gallery –CAG [1])



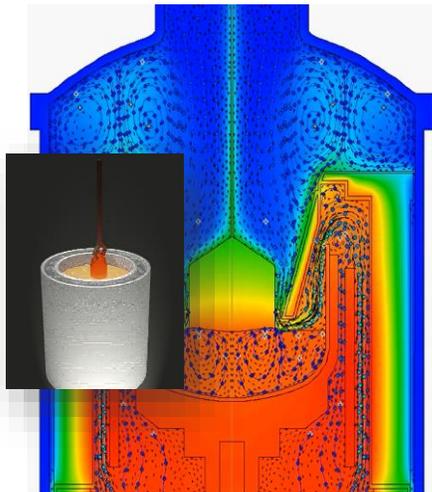
**Figure 5.** Mesh of the salt melting and crystal growing model (CAG [2])



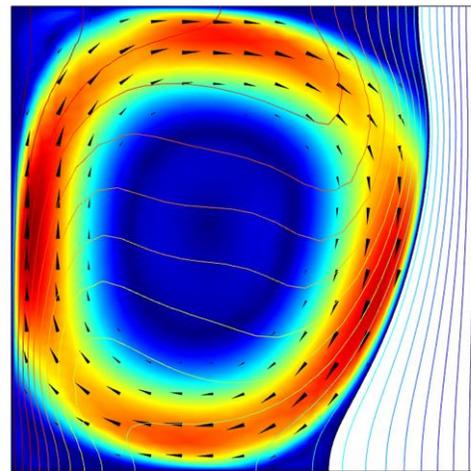
**Figure 3.** Transversal section on ion gun ( adapted CAG [1] with lab configuration)



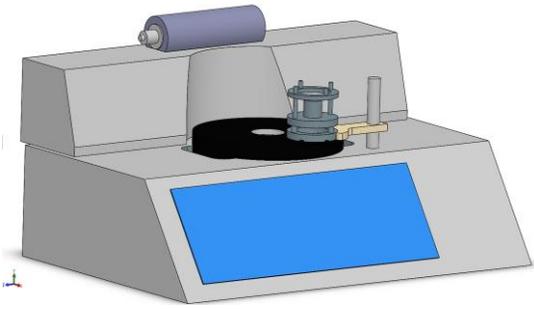
**Figure 6.** Thermal field dynamics during crystal growth (CAG [2,3])



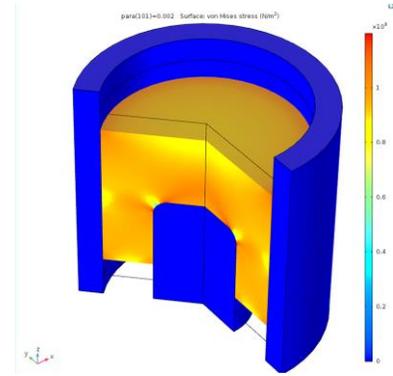
**Figure 4.** Crystal growth process (5)



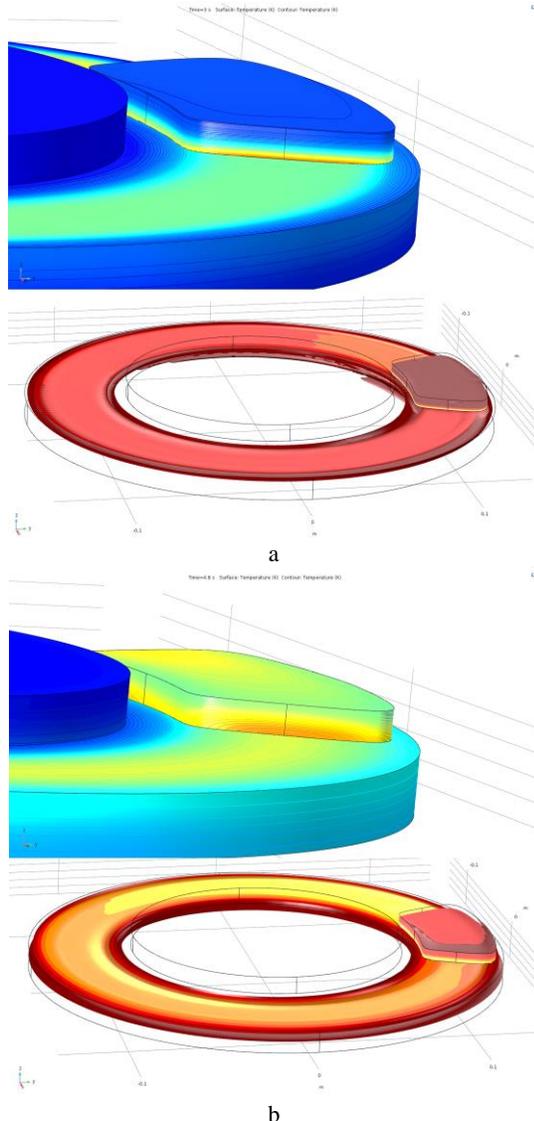
**Figure 7.** Figure 6. Thermal field dynamics during crystal growth (CAG [2])



**Figure 8.** Crystal Polishing Equipment. CATIA model (5)



**Figure 10.** Powder sintering (adapted model CAG [4])



**Figure 9.** Polishing dynamics' and thermal effects Time dependent (a, b) thermal flow and material thermal stress studies adapted form CAG [5]

## 5. Conclusions

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

For these R&D lab equipment and processes examples (fig.1,4,8) the Apps Gallery models were used to understand the experiments path and each parameter's influence on overall process.

## References

COMSOL Multiphysics ® App Gallery models (CAG)

1. Mass Spectrometer –ID: 10653
2. Melting Front - ID:6234
3. Marangoni convection – ID: 20329
4. Powder compaction – ID: 46931
5. Heat in a Disk Brake – ID: 102

## Note

During the time, former (2, 3, 4) and present (5) UPB students were working on the Virtual Lab dBs with the continuous support of UPB, INFLPR and CETAL researchers.

(5) A.D. Cotofana; G.M. Ene; E.A. Barbulescu; F.A. Cazanaru