

# Simulation Methods on Virtual Laboratories for Characterization of Functionalized Nanostructures

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## Introduction:

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.

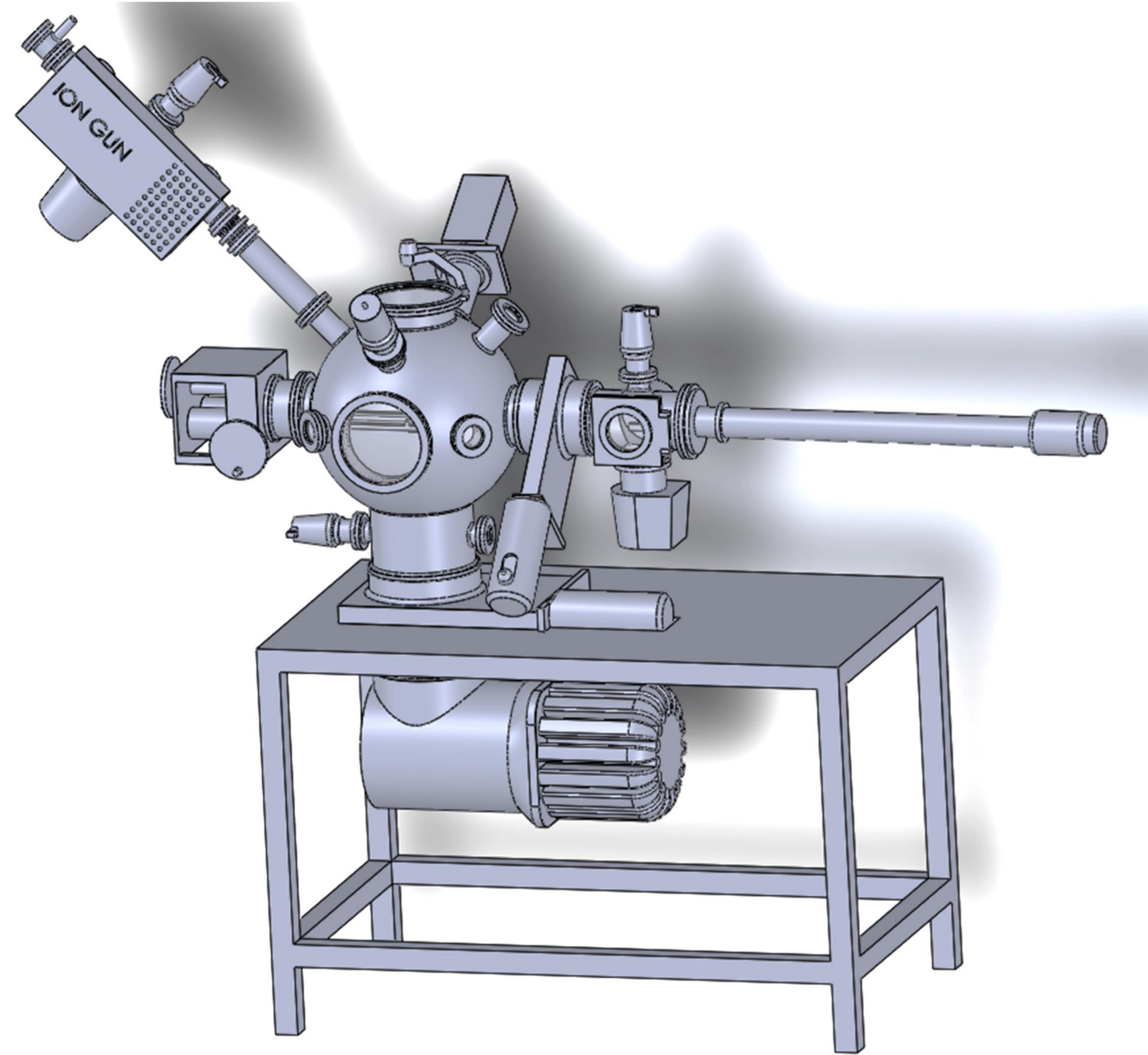


Figure 1. Mass Spectrometer- SW model

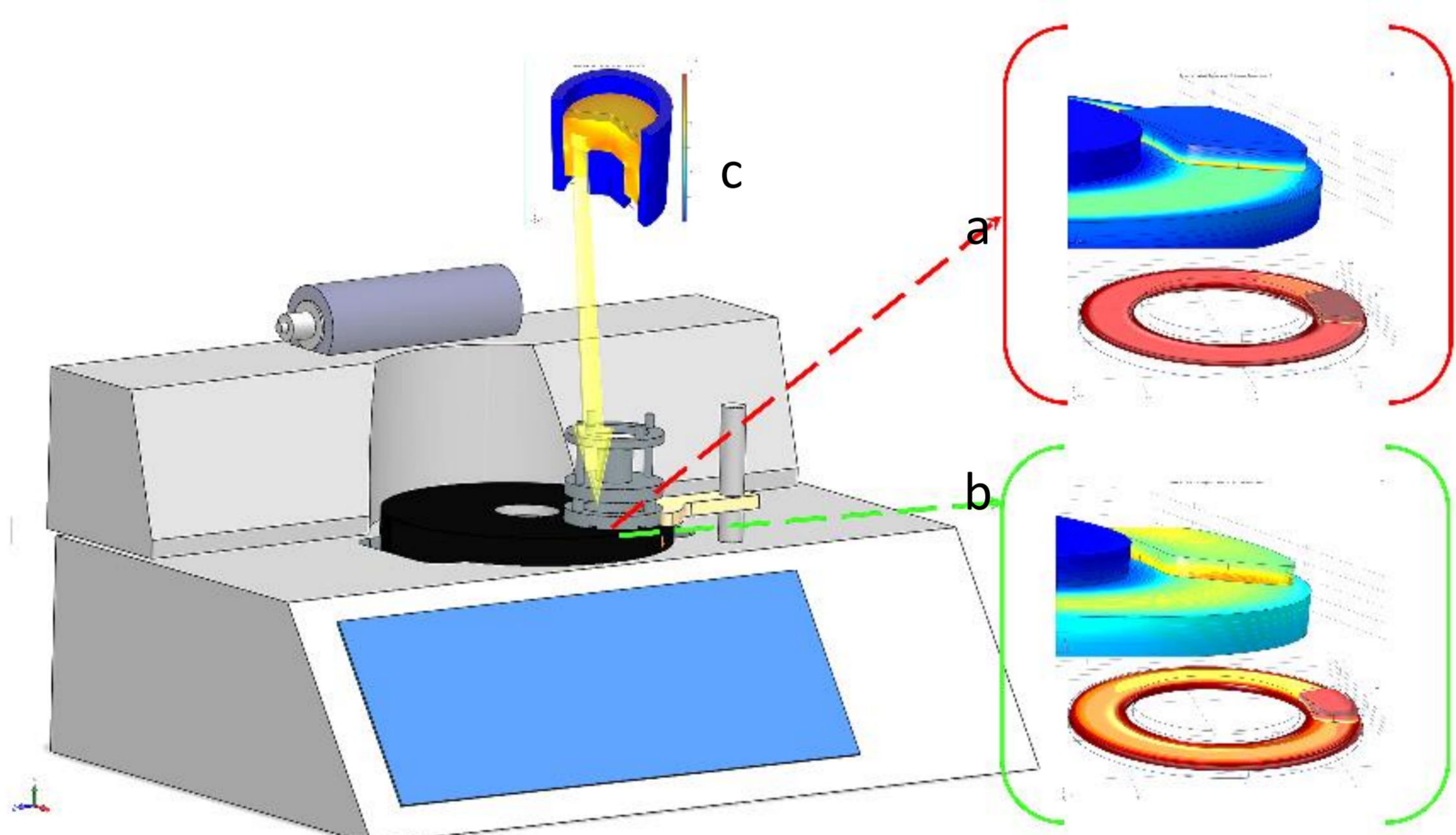


Figure 2 Crystal Polishing Equipment

(a , b) Polishing dynamics' and thermal effects; (c) Powder sintering

## Computational Methods:

For the description, characterization and process simulation phases the main modules of COMSOL Multiphysics® and its add-ons (LiveLink™ for SolidWorks®, LiveLink™ for CATIA, LiveLink™ for Excel, LiveLink™ for MATLAB®) were used.

## Results:

The main physical processes related to lab installation (Mass Spectrometer, Crystal Growth Installation, Crystal Polishing Equipment) were described adapting the existing COMSOL Multiphysics® models [1,2,3] to the “in place” lab equipment data (fig.1-4).

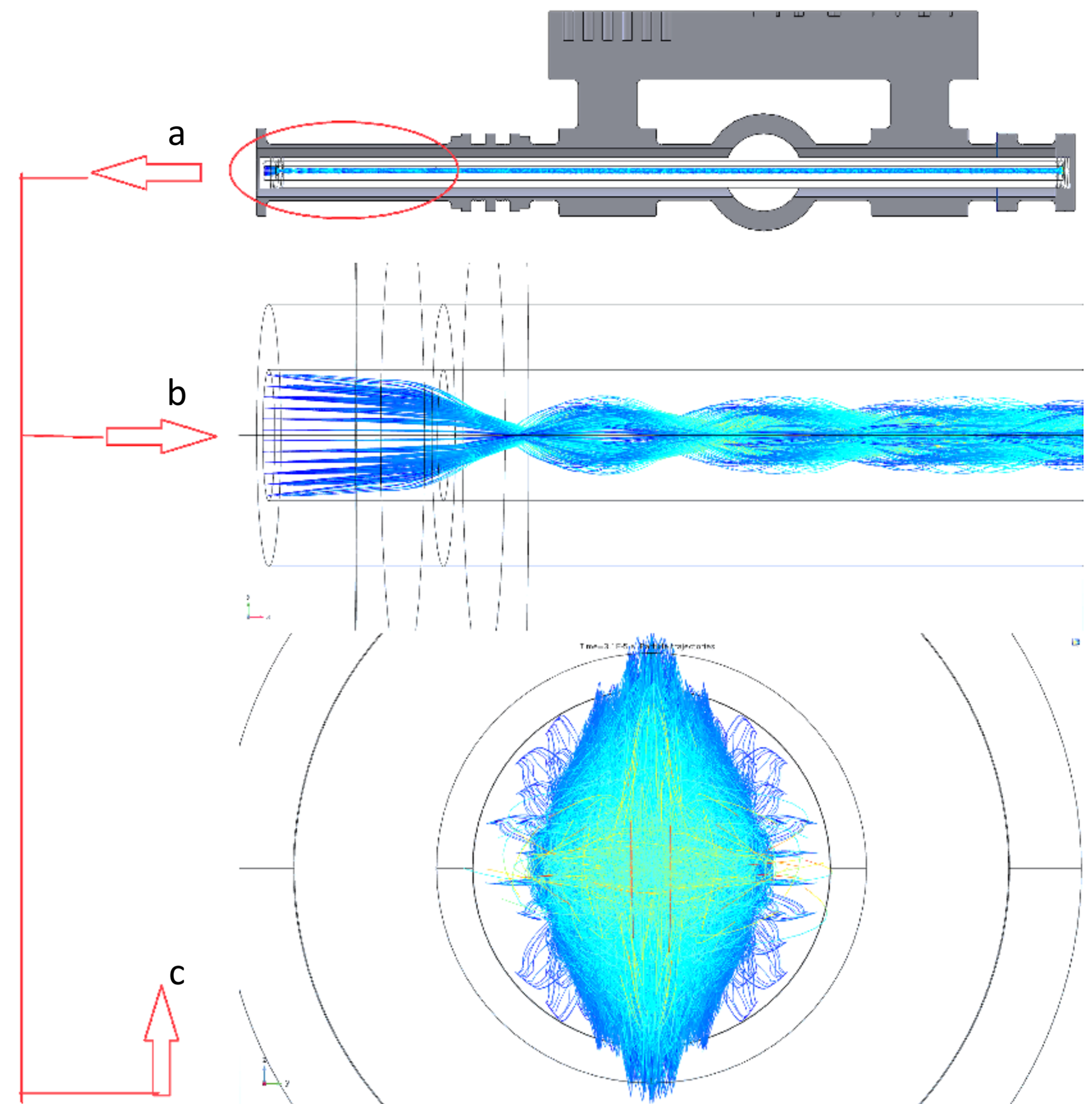


Figure 3. Ion source for mass spectrometry

(a) Ion Gun longitudinal section (SW) ;  
(b ,c) particle trajectories – COMSOL [1]

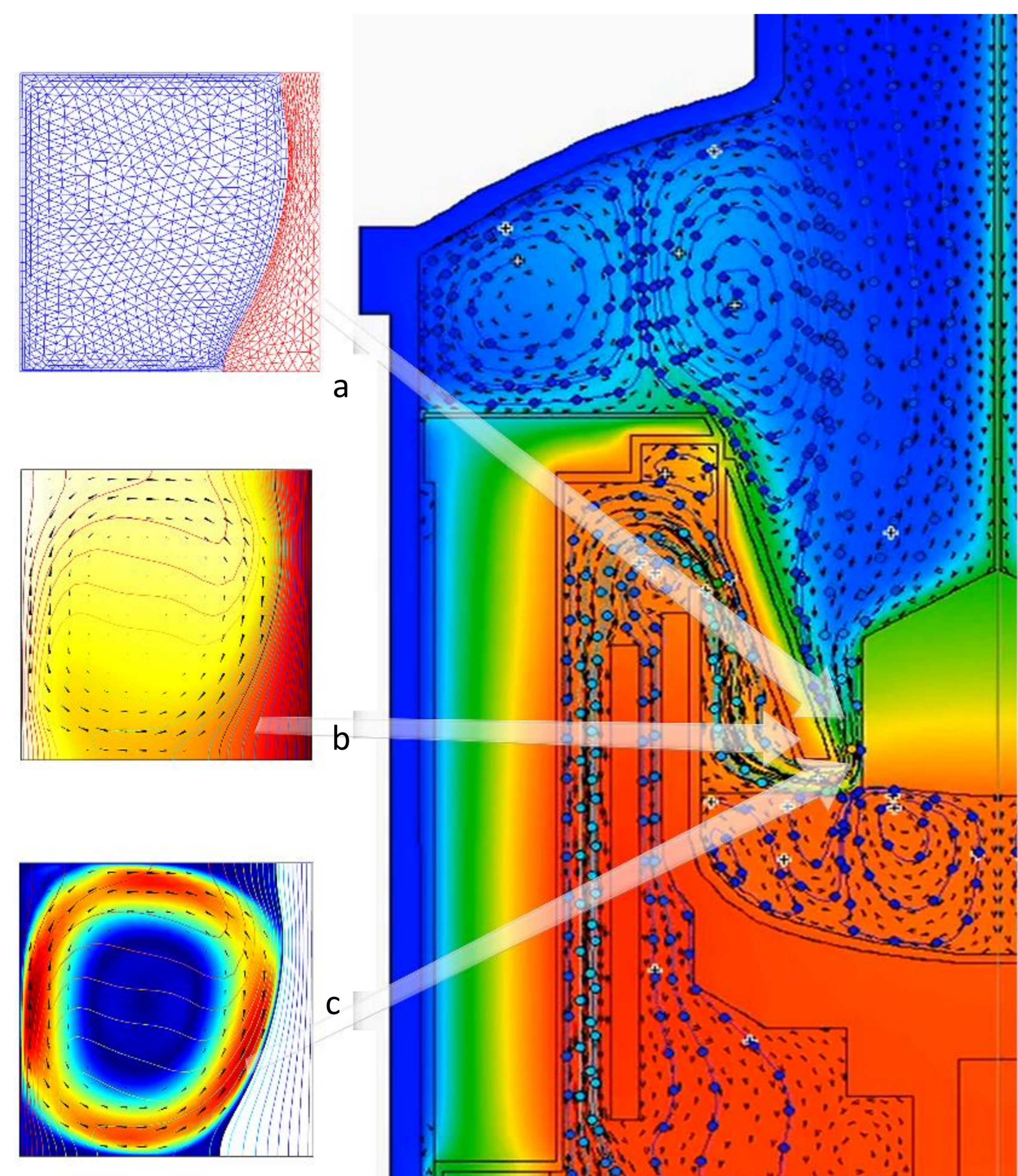


Figure 4. Crystal growth process

(a, b, c) Salt melting and crystal growing models – COMSOL [2,3]

## Conclusions:

All experimental data related to the processes were archived on dedicated modules for each specific installation. These will be further on adapted to the different experimental setups.

## References:

1. COMSOL- Quadrupole Mass Spectrometer
2. COMSOL- Marangoni Effect
3. COMSOL Melting Front