

# PhD Thesis

in GRENOBLE (SIMAP) with periods in BORDEAUX (ICMCB)

## CONTEXT

The rare event searches in astroparticle physics by means of heat-scintillation cryogenic bolometers (HSCBs), the core of which is made of bulk crystals, is an emergent field that encompasses the quests for the basic particles of the dark matter (DM) halo of our galaxy and for the nature of the neutrino -that could possibly reveal a new type of matter- and the spectroscopic exploration of the rare fast neutrons being the ultimate background found on DM direct detection in underground sites. It turns out that large  $\text{Li}_2\text{MoO}_4$  single crystals, of mass in the range 300-500 g, would be excellent candidates to build such HSCBs able to address two kinds of rare events: neutrinoless double beta decays ( $0\nu\text{-DBD}$ ) and fast neutron backgrounds. We propose to grow not only larger  $\text{Li}_2\text{MoO}_4$  crystals, but also with unprecedented purity and quality, by means of combined Czochralski pulling and modelling, single crystal characterizations and exploratory bolometer tests. This project will break down the boundaries between crystal growers and astroparticle physicists and benefit from contributions of both communities converging towards a single interdisciplinary collaborative project. In the project, the feedback between scintillation measurements, detector performances (background) and crystal growth will enable the elaboration of one pilot natural  $\text{Li}_2\text{MoO}_4$  crystal of mass  $\sim 500$  g, and three other pilot  $\text{Li}_2\text{MoO}_4$  crystals of mass  $\sim 500$  g, one of which will be enriched with  $^6\text{Li}$  isotope (95 %) and the remaining two will contain a considerable amount of enriched  $^7\text{Li}$  (99.9 %). The CLYMENE consortium is based on a synergetic interaction between experimented scientists of complementary research teams: a crystal growth laboratory, a growth process simulation laboratory, a crystal technology platform and an astroparticle physics laboratory.



LMO single crystal (234 g) grown at ICMCB by the Czochralski process.

## PhD OFFER

A PhD thesis student will be recruited starting in summer 2017. This student will be co-advised by Professor Thierry Duffar and Dr. Matias Velazquez, for experimental crystal growth issues (furnace characterizations, materials bibliographical data, growth run preparation). (S)he will also be involved in the experimental developments at CristallInnov platform. The main tasks of this thesis will be divided in three parts:

### 1<sup>st</sup>: Crystal growth experiments

- Learning  $\text{Li}_2\text{MoO}_4$  Czochralski pulling at ICMCB (several visits and weeks in Bordeaux);
- Interact in the up scaling of the growth experiment at CristallInnov (close to Grenoble), using the experience gained in Bordeaux and the numerical simulation results;
- Participate in the optimization of the growth process (crucible filling and position, temperature gradients and screens, etc.).

### 2<sup>nd</sup>: Measurement of physical parameters

- Measurement of density, surface tension and possibly viscosity of the melt.
- Measurement of elasticity tensor coefficients at high temperature.

### 3<sup>rd</sup>: Numerical simulation

- Compute the temperature and hydrodynamic fields in the Czochralski growth process, on the basis of already existing models at SIMAP;
- Implement in COMSOL the optically participating media model (already done in various cases by SIMAP);
- Implement in COMSOL the model aiming to compute stresses (already done in various cases by SIMAP). In parallel to these rather classical developments, the research activity will focus on the numerical simulation of the behaviour of ions in the crystal growth process;
- Develop a model in COMSOL for chemical distribution, taking advantage from SIMAP's experience in the simulation of such problems;
- Bibliographic analysis of the chemistry and thermodynamics of ions in the liquid state;
- Derive a numerical model of ions distribution in the crystals: numerically solve the set of temperature dependant equations including diffusion, advection, chemical reactions and mass/charge conservations;
- Validate/adjust the code via comparison with experiments.

## POSITION

This work is well suited for a Master 2 or Engineer in Material Sciences with skills and inclination in both experimental work and numerical simulation.

Salary: 1465 €/month netto

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13

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56

