



18-months post-doctoral fellowship – Open position

"Microfluidic study of plasma-induced nucleation of perovskite"

Context

Crystallization is a separation and purification process widely used in industry for drug synthesis, purification of battery-grade metals, food manufacturing, etc. Although the technique is mature, industrial crystallization still faces two main challenges: (1) controlling the crystal size distribution (CSD) to improve the efficiency of downstream processes (filtration, washing, drying), and (2) controlling the polymorphic phase in order to optimize the physico-chemical properties of the product -e.g. solubility of active pharmaceutical ingredient (API).

A better control of these features is hindered by undesired nucleation in the crystallization reactor. Nucleation is a stochastic phenomenon producing solid crystalline seeds from a supersaturated solution. In the development of crystallization processes, scale-up is often an issue because solution stirring (required for homogeneity) induces shear stress that strongly impacts the nucleation rate [1] and thus prevents accurate CSD control.

Industry circumvents the nucleation issue by seeding crystallizers with a specific amount of calibrated crystalline seeds at low supersaturation ratio in order to prevent undesired spontaneous nucleation event. Although this technique is satisfying, it can be constraining if crystallization is performed in a sterile environment, or if the seed material is not available in sufficient amount and quality.

Therefore, there is a need for *in situ*, on-demand and scalable seeding techniques allowing a high level of polymorph and crystal size distribution controls. Alternative techniques based on external fields are currently explored but their scalability is still an issue - e.g. sonocrystallization, laser-induced nucleation [2].

The INCRYS project (ANR PRC grant) aims to use cold plasma – a non-equilibrium ionized gas - for seeding crystallization reactors in a non-intrusive manner, in situ, and on-demand. Two main objectives will be addressed: (i) understanding the main nucleation mechanism using a plasma microfluidic reactor coupled with advanced diagnostics to capture plasma and nucleation dynamics, (ii) studying the scalability of plasma-induced nucleation in supersaturated flows typically encountered in batch stirred reactor.

Mission and objectives

We are looking for a post-doctoral associate highly motivated by interdisciplinary research in order to meet the first objective: understanding the main nucleation mechanism using a plasma microfluidic reactor coupled with advanced diagnostics to capture plasma and nucleation dynamics. To achieve this goal, we chose to use a microfluidic device equipped with fluorescence measurement. This allows us to observe the first moments of crystal formation. The chosen compound is a halogenated hybrid perovskite that does not give off a fluorescence signal until it is in crystalline.

First, the candidate will validate that the reactor is fully operational. The reactor is shared between the PPSM and LuMIn laboratories (ENS-Paris-Saclay).

Second, the candidate will define a protocol to generate and stabilize the supersaturated perovskite precursors in the microfluidic reactor. A verification of the structure of the crystals obtained will be done by X-ray diffraction at SPMS laboratory.

Third, he/she will use fluorescence lifetime microscopy (FLIM) technique available at PPSM and LuMIn laboratories (ENS-Paris-Saclay) to capture the nucleation of stable perovskite crystals in a define plasma condition [3].

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Fourth, he/she will find optimized plasma conditions in interactions with the work done at EM2C on the different plasma. Time-resolved data will be combined with plasma characterization at EM2C in order to have a complete view of the plasma and solution phases in order to identify the main plasma agents responsible for nucleation (e.g. ions, cavitation, shear)

These experiments and their understanding behind, will allow us to use a second characterization technique small-angle X-ray scattering (SAXS) at Synchrotron Soleil.

Therefore, the candidate will prepare an experimental project at Synchrotron Soleil, in order to use small-angle X-ray scattering (SAXS) to complete the characterization of the plasma-induced nucleation phenomenon.

Laboratory framework

The candidate will be formally attached to the laboratory SPMS located in CentraleSupélec on the campus of Paris Saclay university. The candidate will be involved in the INCRYS project and will thus work in close collaboration with the neighboring partners from CentraleSupélec (EM2C and LGPM laboratories) and ENS Paris-Saclay (LuMIn and PPSM laboratories). Most of the experimental work will be performed at the LuMIn and PPSM laboratories.

Profile required.

The candidate must hold a PhD and have a solid experimental background in Physical chemistry.

- Good laboratory skills (handling of chemicals, etc)

- Skills in programming (e.g. Python) for data treatment and acquisition
- Knowledge of main characterization techniques of solid materials (PXRD), knowledge on SC-XRD or SAXS will be an advantage
- Highly motivated by multidisciplinary research
- Fluency in scientific and technical English
- Autonomy
- Good interpersonal skills for a rapid integration into the laboratories

Contract duration and remuneration

The duration of the postdoc is 18 months, with remuneration based on experience and the statutory salary scale.

Constraints and risks

Work in a chemistry laboratory with health and safety constraints (wearing PPE, etc.) and handling of Chemicals including perovskite compound and organic solvent.

Application: CV and covering letter citing a reference and/or letter of recommendation.

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[1] C. Forsyth et al., Cryst. Growth Des., 2015, 15, 94–102. <u>https://doi.org/10.1021/cg5008878</u>

[2] B. Clair et al., J. App. Cryst., 2014, 47: 1252. <u>https://doi.org/10.1107/S160057671401098X</u>

[3] Z. Zhang et al. Methods in Microscopy, 2025, 2, 117-131. https://doi.org/10.1515/mim-2024-0030

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