	Name of the PhD: **Timothée BARBE** Title of the PhD thesis: **Development and modeling of a process for the synthesis of nanostructures based on two-dimensional materials under concentrated solar irradiation** Dates (start/end): 09.19 – 09.22
Supervisors	Françoise Bataille, Alexis Vossier, Elie Nadal, Gilles Flamant (PROMES) Jeffrey Gordon (Univ. Ben Gourion)

Context and objectives

Due to their electronic, mechanical, tribological properties, nanomaterials offer a wide range of possible applications in many fields. The development of these nanomaterials generally involves complex, energy-intensive and polluting processes. The use of concentrated solar energy could offer an advantageous alternative to conventional processes by promoting the development of « green », environmentally friendly and energy-efficient solutions: this project proposes to explore these promising processes.

This PhD thesis is set in a unique historical context: the PROMES laboratory was indeed at the forefront of these approaches to materials synthesis by solar means, during the 1990s. Today, with the recent discovery of new families of nanomaterials with high added value, the development of solar processes that allow the use of these materials in a "clean" way is undeniably arousing renewed interest. The laboratory, with its unique instrumentation combined with its extensive know-how, has strong assets to develop this research theme whose potential remains largely unexploited to date. The project is also part of a collaboration with the Ben Gurion University (Israel) which has initiated research work on this theme in recent years. This laboratory has developed processes for the synthesis of nanomaterials involving solar concentration at low power levels.

« In the motivational introduction, an important point is that solar ablation has succeeded in synthesizing singular nanostructures that no other methods did, for reasons that are only heuristically understood and are worthy of in-depth modeling and further detailed experimentation. »

Approach

This PhD aims to explore the nanomaterial synthesis through concentrated solar irradiation from 2D-materials solid precursors (MoS_2, WS_2). As this research area is still at its first steps of development, the envisaged strategy was therefore to first understand in depth the synthesis mechanisms (atomic interactions, inner reactor conditions) through the bibliography and the simulation work (Molecular Dynamic simulations, Computational Fluid Dynamic) in order to then be able to carry adapted and optimized experimental nanomaterial synthesis. Currently, the modelling work is completed and is effectively used to optimize and orientate the nanomaterial synthesis performed within the *Heliotron* reactor.

Main results

Three researches axis were defined in this PhD, each of them have been investigated with results to show for it

1. Model the fluid dynamics induced by solar ablation occurring during nanomaterial synthesis.

   The flows within the reactor were modeled, simulated and reproduced with a dedicated flow visualization experiment. Keys informations such as the residence time and the quenching temperature of vaporized species were extracted from the validated numerical simulations. Those information characterize directly the nucleation/growth process experienced by the vaporized species until its deposition on one given zone of the reactor. At the end this characterization will guide the experimental work towards the reactor operating conditions conducive to synthesize nanoparticles.

2. Understand the mechanisms of nucleation and growth of nanoparticles

Prior literature review and molecular dynamics simulation were done to identify first scenarios of nanoparticles synthesis. However, complete understanding of the synthesis mechanisms is yet not fully known.

Numerous attempts of MoS_2 nanoparticles synthesis with the *Heliotron* solar reactor and a tailored blackbody cavity proved to be unsuccessful by using solely MoS_2 as the solid precursors, mostly due to the incongruent behavior of the MoS_2 vaporization.

However the redundant obtention of MoS_2 nanoparticles (both in literature and in our work) with the use of MoO_3 as a catalyst points that a mechanism of nucleation in vapour phase with substitution of Oxygen atoms by Sulphur ones is seriously considered. Further experiments are planned to elucidate the respectives roles of the inner pressure, the temperature and the flushing Argon gas flowrate.

3. Carry experimental nanomaterial synthesis within the *Heliotron* solar reactor through solar concentrated irradiation.

Different experimental campaign were carried along the two first years of PhD. First ones were dedicated to identify whether homogeneous cooking of MoS_2 are favorable to obtaining nanoparticles. The unsuccessful results obtained at this time revealed that other parameters such as the use of catalysts and the transport of vaporized species in the reactor were key paths to investigate.

In response to that, the design of a tailored blackbody cavity enabling the transport of vaporized species and the design of a movable cold finger were made for future experiments.

Recently nanostructures obtained from a mixture of MoS_2 and MoO_3 solid precursors were observed with Scanning Electron Microscopy.

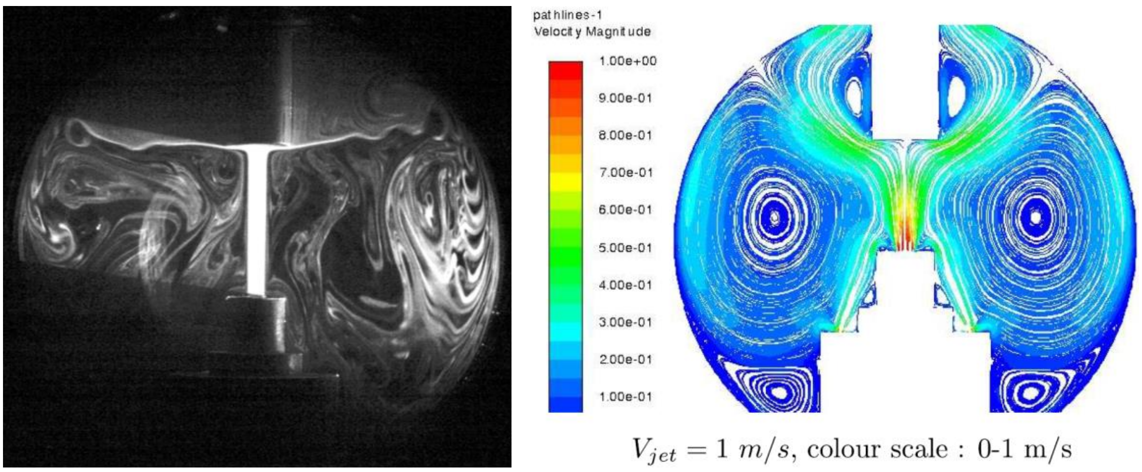

Fig 1. Smoke flow visualization (left) and corresponding simulated flow patterns (right), P_{in}=1 bar, V_{jet}=1 m/s.

Publications in scientific journals and international conferences

One poster was presented at the *Nanotech France 2021* conference.

One article was submitted to the *Chemical Engineering Journal,* under review