

'Physique et Chimie des Matériaux' – ED 397 – année 2022

PhD project for funding, to send by 28/02/2022 to

nadine.witkowski@sorbonne-universite.fr under PDF form « acronyme labo_nom PI.pdf »

Research unit (full name + acronym) : Institut de Mineralogie, de Physique des Matériaux et de
Team if applicable : DEMARE + PHYSIX

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Nber of PhD under supervision 0.5

Participation to supervisor training? no Year

Co-supervisor : Sandra NINET

HDR? no Position : Lecturer SU

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Research unit : UMR7590

International co-supervision ? No

Keyword 1 : Synthesis

Keyword 2 : High pressure

Keyword 3 : nitrides

Keyword 4 : hydrides

Select co-funding programme if applicable : select

Project title : Synthesis and characterization of new nitrides and hydrides at extreme conditions

Project Description :

History shows that the successful synthesis of new materials has always been correlated to technological developments. Nowadays, the high pressure (HP) technology allows to generate static pressures of several million bars and the energy brought by such compressions becomes comparable to those of strong chemical bonds allowing the access to a whole new chemistry of elements. Emblematic examples include that of dihydrogen, an insulating solid at low T, which becomes a metallic solid when compressed to $P \approx 500$ GPa [1] and the ammonia and water ices which become superprotonic conductors at high P and high temperature [2,3]. The reactivity of the elements is also radically different from that under ambient P: for example, it has been shown that compounds considered as the most stable under ambient conditions (N_2 , Pt,...), become strongly reactive under extreme conditions and allowed the synthesis of new strategic nitrides.

The HP synthesized materials are strategic because they are frequently metastable at ambient conditions and can have useful mechanical, superconductive, energetic, magnetic, electronic, optical or thermo-electric properties that have great values for potential technological applications. For the large volume high-pressure synthesis under industrial P-T range (with Paris-Edinburgh or multi-anvil press), we can mention recent successful syntheses (in our laboratory IMPMC) of new patented ultrahard materials [4-6], some solar optoelectronic and infra-red photonics materials [7,8] or also (by other groups) high energy density materials [9], which are highly desired in various technological domains (especially aerospace).

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Up to now, high-pressure nitrides or hydrides have been generally synthesized by direct reaction of metals with N₂ or H₂. In this PhD thesis, we will exploit also new nitriding/hydriding agents with strong reactivity to induce the diffusion of elements within selected metals to synthesize new nitrides and/or hydrides at milder conditions in view of recovering them at ambient conditions. The synthesis will be performed at IMPMC on two types of high-pressure device: diamond anvil cell (DAC) coupled to laser heating and large-volume presses (Paris-Edinburgh press or multi-anvil press) coupled with resistive or inductive heating. The studies in DAC will allow to synthesize and characterize "rapidly" the products obtained. The discovery of new materials with strategic properties will then pave the way for synthesis in larger quantities, via original large-volume presses' devices, for which our laboratory has a large expertise. The properties of the synthesized material will be fully characterized with a large panoply of techniques available at IMPMC (spectroscopy, XRD, MEB, TEM, etc.). Finally, to follow in situ the chemical reaction at HPHT, experiments on large facilities will also be performed (synchrotron, neutrons sources, XFEL). Today, X-ray Free Electron Laser (XFEL) sources also open up new revolutionary perspectives for the HP synthesis as recently highlighted with the synthesis of sulfur hydride [10] and iron nitride [11].

The IMPMC with the two teams involved in this PhD project (DEMARE and PHYSIX) is the ideal laboratory for this study as it is recognized worldwide for its high-pressure expertise, both from a technical point of view, application and from fundamental physics at extreme conditions.

We are looking for highly motivated PhD candidate with a strong motivation for experiments and a solid background in material sciences.

References :

- [1] P. Loubeyre et al., Nature, 577, 631 (2020)
- [2] S. Ninet et al., Phys. Rev. Lett., 108,165702 (2012)
- [3] J.A. Queyroux et al., Phys. Rev. Lett., 125, 195501 (2020)
- [4] Y. Le Godec et al., European patent 08787929.2 (2011).
- [5] Y. Le Godec et al., US patent USPTO 20110230122 (2011)
- [6] Y. Le Godec et al., PCT patent WO2021/240074A1 (2021)
- [7] O. Kurakevych et al., Inorg. Chem. 55, 8943 (2016).
- [8] S. Pandolfi et al., Nano Letters 18, 5989 (2018).
- [9] MJ. Lipp et al., Nat Mat (2006)
- [10] E. J. Pace et al., J. Phys. Chem. Lett, 11, 1828 (2020)
- [11] H. Hwang et al., J. Phys. Chem. Lett., 12, 3246 (2021)