

TITLE:ASYMMETRIC MULTICOMPONENT REACTIONS IN CONTINUOUS-FLOW

Topic number : 2021_001

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team:

Research lab: C3M - Chimie Moléculaire, Macromoléculaire, et Matériaux

Lab location: Paris

Lab website:<https://www.cmc.espci.fr/Dr-Benjamin-Laroche>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Laroche Benjamin benjamin.laroche@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The main goal of this project is to develop environmentally benign flow reactions by means of heterogeneous catalysis and atom-economical transformations, two concept of green chemistry with extraordinary potential for sustainably preparing organic molecules. Capitalizing upon the recyclability and robustness of heterogeneous catalysts, we will develop conceptually new continuous procedures that can be easily telescoped to sequential flow systems. Specifically, we will explore asymmetric multicomponent reactions to generate chiral bioactive compounds in a continuous manner.

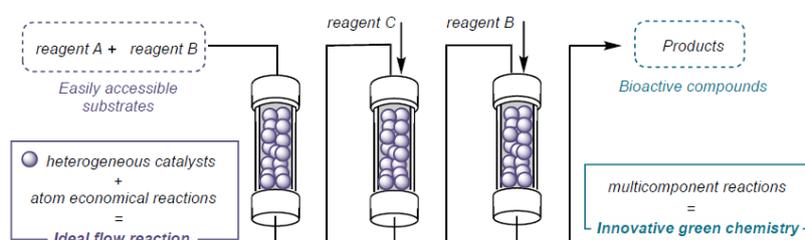
Required background of the student: The student will focus on the synthesis of new heterogeneous catalysts and study their reactivity in continuous-flow systems. In this sense, very good theoretical and working knowledge in organic synthesis are expected (Master level is required). The student should also be comfortable with classical analytical techniques in organic chemistry such as NMR, MS, IR spectroscopy. The research work will take place in an international environment including several research groups, so he/she will be expected to have very good communication skills (fluent english is mandatory) and a certain team spirit. In addition, we expect the student to be serious, motivated and

well-organized to allow him/her to progress smoothly in his research work. Experience in flow chemistry would be a plus but is not mandatory.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. B. Laroche, H. Ishitani, S. Kobayashi, *Adv. Synth. Catal.* 2018, 360, 4699–4704, DOI: 10.1002/adsc.201801457
2. B. Laroche, Y. Saito, H. Ishitani, S. Kobayashi, *Org. Process Res. Dev.* 2019, 23 (5), 961–967, DOI : 10.1021/acs.oprd.9b00048
3. W.-J. Yoo, H. Ishitani, Y. Saito, B. Laroche, S. Kobayashi, *J. Org. Chem.* 2020, 85 (8), 5132–5145, DOI :10.1021/acs.joc.9b03416
4. H. Ishitani, Y. Saito, B. Laroche, X. Rao, S. Kobayashi “Recent perspectives in catalysis under continuous flow”, in *Flow Chemistry - Integrated Approaches for Practical Applications*, No. 63 (2020), Ed. S. V. Luis, E. Garcia-Verdugo, Royal Society of Chemistry, Green Chemistry Series, ISBN: 978-1-78801-498-4.
- 5.

Illustrations :



Scheme 1. Continuous synthesis of bioactive compounds by means of heterogeneous catalysis and atom-economical transformations. Exploitation of multicomponent reactions.

TITLE: PRODUCTION OF NEW STRIKING VISUAL APPEARANCE WITH DISORDERED METASURFACES COMPOSED OF RANDOM ARRAYS OF RESONANT NANOPARTICLES.

Topic number : 2021_002

Field : Physics, Optics

Subfield:

ParisTech School: Institut d'Optique Graduate School

Research team: Light in complex nanostructures

<https://www.lp2n.institutoptique.fr/equipes-de-recherche-du-lp2n/light-complex-nanostructures>

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab website: <https://www.lp2n.institutoptique.fr>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: Lalanne Philippe Philippe.lalanne@institutoptique.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Optical metasurfaces are currently considered for a broad variety of applications, from quantum studies to imaging and holography. In relation with the present proposal, they are currently investigated to supply printings with vivid-colour palettes, using Mie or localized plasmon resonances have been shown. See Appl. Phys. Rev. 6, 041308 (2019) for a recent review.

The present project goes a step forward and proposes to control the appearance, rather than the colour. The latter is very important, but it is only one attribute of appearance. Haze, gloss, and the change of colour with viewing angle or illumination direction, considerably alter our perception and impact our aesthetic judgement. We have recently developed a numerical platform, which mixes nanoscale electrodynamics, mesoscale multiple scattering and macroscale rendering (as used in computer graphics). The platform allows us to model the scattering properties of random monolayers composed of resonant nanoparticles (a challenge) and to deliver true-to-life synthetic images of arbitrary objects

(cell phones, cars, rings) covered by random metasurfaces. This platform is as a new tool in nanophotonic. Results clearly indicate the high potential of random metasurfaces to produce unusual visual effects. We have also first experimental validations. Our first publication on the topic is under review.

Required background of the student: The PhD student needs to have a solid background in optics, electromagnetism, statistical optics as well as a strong interest in both numerical modelling and experimental physics. He/she will participate actively to the ongoing development of the numerical, design metasurfaces, interact with our partners specialized in nanofabrication, develop optical characterization setups to demonstrate new appearance.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Kevin Vynck, Romain Pacanowski, Adrian Agreda, Arthur Dufay, Xavier Granier, and Philippe Lalanne, "Stunning visual appearances of disordered optical metasurfaces", under review.
2. C. Gigli, Q. Li, P. Chavel, G. Leo, M. Brongersma, P. Lalanne, "Fundamental limitations of Huygens' metasurfaces for optical beam shaping", Laser Photonics Reviews 15, 2000448 (2021).
3. Q. Li, T. Wu, J. van de Groep, P. Lalanne, and M. L. Brongersma, "Structural color from a coupled nanowire pair beyond the bonding and antibonding model", Optica 8, 464-470 (2021).
4. P. Lalanne and P. Chavel, "Metalenses at visible wavelengths: past, present, perspectives", Laser Photonics Rev. 11, 1600295 (2017).
- 5.

Illustrations :



TITLE: DEVELOPMENT OF SELECTIVE ANTIBACTERIAL ORGANOMETALLIC DRUG CANDIDATES

Topic number : 2021_003

Field : Biology, Biophysics and Biochemistry, Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology

Subfield: Synthetic Chemistry, Medicinal Chemistry

ParisTech School: Chimie ParisTech - PSL

Research team: Laboratory for Inorganic Chemical Biology

<http://www.gassergroup.com>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website: <http://www.gassergroup.com>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Gasser Gilles gilles.gasser@chimieparistech.psl.eu

Advisor 2: Cariou Kevin kevin.cariou@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The discovery of penicillin was the start of a golden age for antibiotherapy that is now threatened by exponentially increasing antibioresistance phenomena. The World Health Organisation (WHO), in a report entitled « Antibacterial resistance: Global report on surveillance » painted an alarming picture, predicting a march toward a « post-antibiotic era » if no significant measures are taken by all the major health experts. Besides huge economic burden resistant bacteria would become the major cause of death by 2050 with 10 million yearly deaths, overpassing cancer (8.2 millions).

Surprisingly, despite a pressing need for novel antibacterial agents research and drug development, there is an apparent downturn in such activities, especially in comparison to the vibrant activities in areas such as cancer research. With the intention to grasp this unique opportunity, in this PhD thesis proposal, we wish to investigate the clinical potential of novel and promising organometallic complexes as chemotherapeutic agents, focusing not only on an improved biological effectiveness under different clinically relevant conditions, but also on the reduction of side-

effects compared to existing drugs. The results of this project may constitute the basis for a new generation of powerful and selective antibacterial chemotherapeutics.

Required background of the student: The applicant should have a strong knowledge (theoretical and practical) in both organic and inorganic chemistry and be proficient with analytical techniques such as NMR and MS. The applicant must be fluent in English since it is the language spoken in the group. Practical knowledge in biology would be an asset.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Y. Lin, H. Betts, S. Keller, K. Cariou, and G. Gasser, *Chem. Soc. Rev.*, 2021, 50, 10346-10402.
2. R. Rubbiani, T. Weil, N. Tocci, L. Mastrobuoni, S. Jeger, M. Moretto, J. Ng, Y. Lin, J. Hess, S. Ferrari, A. Kaech, L. Young, J. Spencer, A. L. Moore, K. Cariou, R. Giorgia, L. Romani, M. Pariano and G. Gasser, *RSC Chem. Biol.*, 2021, 2, 1263-1273.
3. Y. Lin, Y.C. Ong, S. Keller, J. Karges, R. Bouchene, E. Manoury, O. Blacque, J. Müller, N. Anghel, A. Hemphill, C. Häberli, A.C. Taki, R.B. Gasser, K. Cariou, J. Keiser, and G. Gasser, *Dalton Trans.*, 2020, 49, 6616-6626.
4. E. Romero, S. Oueslati, M. Benchekroun, A.C.A. D'Hollander, S. Ventre, K. Vijayakumar, C. Minard, C. Exilie, L. Tlili, P. Retailleau, A. Zavala, E. Elisée, E. Selwa, L. Nguyen, A. Pruvost, T. Naas, B.I. Iorga, R.H. Dodd, K. Cariou, *Eur. J. Med. Chem.* 2021, 219, 113418.
5. V. Buchter, Y.C. Ong, F. Mouvet, A. Ladacycia, E. Lepeltier, U. Rothlisberger,* J. Keiser,* and G. Gasser,* *Chem. Eur. J.* 2020, 26, 15232-15241.

Illustrations :

TITLE:PHOTOCATALYSIS IN LIVING CELLS WITH EARTH ABUNDANT METALS FOR CANCER THERAPY

Topic number : 2021_004

Field : Biology, Biophysics and Biochemistry, Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology

Subfield: Photochemistry, Medicinal Chemistry.

ParisTech School: Chimie ParisTech - PSL

Research team:Laboratory for Inorganic Chemical Biology

<http://www.gassergroup.com>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website:<http://www.gassergroup.com>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Gasser Gilles gilles.gasser@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Photodynamic Therapy (PDT) is an approved medical technique to treat certain types of cancer. However, cancer cells have a lower amount of oxygen than healthy ones, limiting the success of PDT treatments since oxygen is one of the three required components with the presence of a photosensitizer and light. Recently, it was demonstrated that Ir(III) complexes could kill cancer cells upon light irradiation without the presence of oxygen.¹ In this project, we aim at developing novel complexes based on biocompatible, earth-abundant metal complexes to kill cancer cells.

Required background of the student: The applicant should have a strong knowledge (theoretical and practical) in both organic and inorganic chemistry, be proficient with analytical (e.g., NMR and MS) and biological techniques (e.g., cell culture). The applicant must be fluent in English since it is the language spoken in the group.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. H. Huang, S. Banerjee, K. Qiu, P. Zhang, O. Blacque, T. Malcomson, M.J. Paterson, G.J. Clarkson, M. Staniforth, V.G. Stavros, G. Gasser, H. Chao, and P.J. Sadler, *Nature Chem.*, 2019, 11, 1041-1048.
2. J. Karges, S. Kuang, F. Maschietto, O. Blacque, I. Ciofini, H. Chao, and G. Gasser, *Nature Commun.*, 2020, 11, 3262.
3. J. Karges, F. Heinemann, M. Jakubaszek, F. Maschietto, C. Subecz, M. Dotou, R. Vinck, O. Blacque, M. Tharaud, B. Goud, E. Viñuelas Zahínos, B. Spingler, I. Ciofini, and G. Gasser, *J. Am. Chem. Soc.*, 2020, 142, 6578-6587.
4. S. McFarland, A. Mandel, R. Dumoulin-White and G. Gasser, *Curr. Op. Chem. Biol.*, 2020, 46, 5771-5804.
5. J. Karges, S. Kuang, Y.C. Ong, H. Chao, and G. Gasser, *Chem. Eur. J.*, 2021, 27, 362-367.

Illustrations :

TITLE: IODOARENE CATALYSIS THROUGH AEROBIC PHOTOCATALYTIC AND ELECTROCATALYTIC ACTIVATIONS.

Topic number : 2021_005

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team: Laboratory for Inorganic Chemical Biology

<http://www.gassergroup.com/>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website: <http://www.gassergroup.com/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Cariou Kevin kevin.cariou@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Hypervalent iodine(III) compounds have been known for 130 years, yet interest in their reactivity was very modest until the eighties, before witnessing a dramatic surge in the 2000's. Concomitantly, this renewed interest led to the investigation of iodoarenes as a particular subclass of organocatalysts. Yet, iodoarene catalysis requires the use of, often hazardous, stoichiometric oxidants, thus generating an equimolar quantity of inorganic or organic waste. In an effort to circumvent these drawbacks, we recently developed an aerobic photocatalytic system to promote iodoarene catalysis for the spiro-cyclization of N-Oxy-amides, where the only stoichiometric reagents are photons and oxygen. This project aims at pursuing these studies in photocatalysis and at complementing and expanding their scope by using electrosynthetic techniques.

Required background of the student: He/she will be expected to possess excellent theoretical and experimental skills in organic synthesis and in purification (chromatography, HPLC...) and characterization (NMR, IR, MS...) techniques. Previous experience in catalysis, photocatalysis and/or electrosynthesis will be strongly appreciated. The

candidate should also be fluent in English as it is the main language spoken in the group.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Habert, L.; Cariou, K.* *Angew. Chem. Int. Ed.*, 2021, 60, 171-175
2. Peilleron, L.; Retailleau, P.; Cariou, K.* *Adv. Synth. Cat.* 2019; 361, 1753-1769
3. Grayfer, T. D.; Retailleau, P.; Dodd, R. H.; Dubois, J.; Cariou, K.* *Org. Lett.* 2017, 19, 4766-4769.
- 4.
- 5.

Illustrations :

TITLE: DISSIPATIVE STRONG COUPLING WITH NON-HERMITIAN NANORESONATORS.

Topic number : 2021_006

Field : Physics, Optics

Subfield:

ParisTech School: Institut d'Optique Graduate School

Research team: Light in complex nanostructures

<https://www.lp2n.institutoptique.fr/equipes-de-recherche-du-lp2n/light-complex-nanostructures>

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab website: <https://www.lp2n.institutoptique.fr>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: Lalanne Philippe Philippe.lalanne@institutoptique.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Nanoresonators play an essential role in current fundamental and applied developments in nanophotonics and are the subject of considerable developments since two decades, from photonic-crystal cavities in the 2000's, plasmonic nanocavities in the 2010's to the last born, the picocavities that provide field confinements in volume below 1 nanometer cube, see ACS Photonics 8, 1522 (2021) for a review of the evolution. The theory of electromagnetic resonators has been initially developed in an Hermitian context for radiofrequency high-Q cavities and cavity quantum electrodynamics. With the development of low-Q plasmonic cavities, the Hermitian approach has become indefensible, and nowadays work is intensified to develop a general non-Hermitian framework, see ACS Photonics 8, 1522 (2021).

The thesis will elaborate a theoretical framework, in a non-Hermitian context, for modeling strong coupling between several nanoresonator modes and/or two-level systems. We will particularly focus on time-varying couplings introduced by a time-modulation of the material permittivity. Time-varying strong coupling phenomena rise fundamental

perspectives and have profound implications in many modern areas, such as topologically protected edge modes in time-varying coupled resonator arrays .

Required background of the student: The candidate is also expected to have a solid background in nanophotonics theory, such as Electrodynamics, Quantum Mechanics, plasmonic, non-Hermitian systems, light-matter interaction, computational physics. He/she will participate actively to the ongoing development of the research made in the group on quasinormal-mode theory and benefit from numerous interactions with experimentalists.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. P. Lalanne, W. Yan, K. Vynck, C. Sauvan and J.-P. Hugonin, "Light interaction with photonic and plasmonic resonances", *Laser Photonics Rev.* 12, 1700113 (2018).
2. Y. Yang, D. Zhu, W. Yan, A. Agarwal, M. Zheng, J. D. Joannopoulos, P. Lalanne, T. Christensen, K. K. Berggren, and M. Soljačić, "A General Theoretical and Experimental Framework for Nanoscale Electromagnetism", *Nature* 576, 248-252 (2019).
3. W. Yan, P. Lalanne, M. Qiu, "Shape deformation of nanoresonator: a quasinormal modes perturbation theory", *Phys. Rev. Lett.* 125, 013901 (2020).
4. T. Wu, M. Gurioli, and P. Lalanne, "Nanoscale light confinement: the Q's and V's", *ACS Photonics* 8, 1522-38 (2021).
5. D. Pellegrino, et al., "Non-Lorentzian Local Density of States in Coupled Photonic Crystal Cavities Probed by Near- and Far-Field Emission", *Phys. Rev. Lett.* 124, 123902 (2020).

Illustrations :

TITLE: NOVEL TWO DIMENSIONAL RASHBA MATERIALS FOR SPINTRONICS.

Topic number : 2021_007

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield: condensed matter physics, spintronic

ParisTech School: ESPCI Paris - PSL

Research team: QuantumSpecs/Phasme <https://qs.lpem.espci.fr/home>
and <https://phasme.lpem.espci.fr/spip.php?rubrique1>

Research lab: LPEM - Laboratoire Physique et d'études des matériaux

Lab location: Paris

Lab website: <https://www.lpem.espci.fr/spip.php?rubrique45&lang=fr>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Bergeal Nicolas nicolas.bergeal@espci.fr

Advisor 2: Vlaic Sergio sergio.vlaic@espci.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Spintronics, which aims to exploit the electrons spin for the development of novel information storage or logic devices, is nowadays a major and competitive research field in physics. Currently, one of the most promising way to achieve the desired control of the electrons spin is by the application of external electric field in presence of the so called Rashba spin-orbit coupling (SOC). The development of novel materials with strong and controllable Rashba SOC is indeed at the frontier of the contemporary research in spintronics.

We have recently developed a novel method which allows us to prepare ultrathin film with strong and controllable Rashba-SOC. By growing a surface alloy between a well-chosen heavy element and a semiconductor (such as Ge or Si) in ultra-high vacuum (UHV) environment by molecular beam epitaxy (MBE), we are able to prepare an ultrathin metallic film (alloy) with thicknesses of the order of 1 nm, which possess high spin-orbit interaction on top of a non-metallic substrate (see Figure)

This research project focuses on the study of the electronic properties of PtGe ultrathin films by means of ARPES and STM. After the identification of the role of the growth parameters on the development of Rashba-SOC we will proceed to transport measurements under high magnetic field going toward the fabrication of spintronic devices.

Required background of the student: The successful candidate should possess a good background in solid state physics and quantum mechanics. He/She should be at ease in the experimental work, be able to work in team and driven by natural curiosity for science. Experience in experimental research in physics will be a plus.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. K. Wang et al., Carbon 183, 251 (2021).
2. T. Vincent et al., J. Phys. Chem. Lett. 11, 1594 (2020).
3. L.M. Vicente-Arche et al., Adv. Mater. 2102102 (2021).
4. D.C. Vaz et al., Nat. Mater. 18, 1187 (2019).
- 5.

Illustrations :

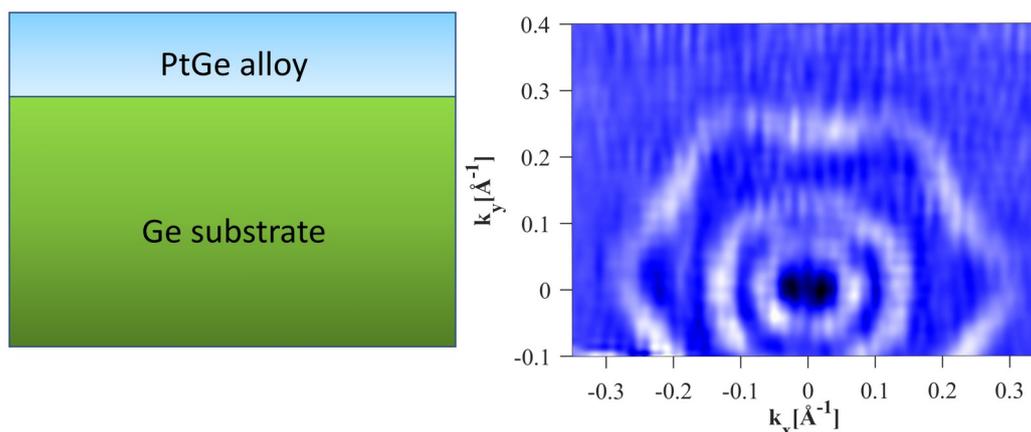


Figure: Left, schematic representation of the sample. Right, constant energy map (100 meV below Fermi level) measured by ARPES. Two circularly iso-energetic contours can be easily distinguished at the center of the Brillouin zone (0,0) demonstrating the presence of high Rashba effect.

TITLE:EFFICIENT AND STABLE SEMI-TRANSPARENT PEROVSKITE SOLAR CELLS

Topic number : 2021_008

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes, Material science, Mechanics and Fluids

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team:Micro & Nano Characterization Group

<https://www.espci.psl.eu/recherche/labos/lpem/mnc/index.html>

Research lab: LP EM - Laboratoire Physique et d'études des matériaux

Lab location: Paris

Lab website:<https://www.lpem.espci.fr>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Chen Zhuoying zhuoying.chen@espci.fr

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Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Solar cells, or photovoltaic devices, are one of the most promising solutions for replacing conventional fossil fuels in the fight against global warming. Among the various emerging “third-generation” solar cells, photovoltaic devices based on metal halide perovskites have attracted the attention of both the scientific and industry communities due to the remarkable rise in their power conversion efficiencies (PCE), reaching a certified 25.5% after only a decade of research. Metal halide perovskites follow the crystallographic structure ABX_3 , where A is either an organic (methylammonium, MA or formamidinium, FA) or inorganic (Cs) cation, B is typically either Pb or Sn, and X is a halide anion (I, Br, Cl). While perovskite based solar cells can be applied in a standard configuration for integration into solar panels in solar farms or rooftops, there is a rising interest to develop a semitransparent version of these devices, which are highly desirable for building integrated photovoltaic systems (BIPV). Semitransparent solar cells can function as windows providing shading as well as electricity for the building. The average transparency (AVT) of semitransparent perovskite solar cells, defined as the integration of the area under the transmittance curve between 370

and 740 nm, can be tuned by changing their composition, layer thickness, or other processing conditions. To date, semitransparent perovskite solar cells show however only a very limited efficiency. So far, the maximum PCE achieved by semitransparent perovskite solar cells varies from a few to 16 % PCE depending on the achieved AVT (e.g. a PCE of 10% was achieved with an AVT of 38%, a PCE of 13.6% with an AVT of 24.7%, or a PCE of 16.7% with an AVT of 10%). The development of routes to increase PCE and stability without reducing their transparency is currently an international hot topic.

In this PhD thesis, we propose to apply innovative material and optical approaches to boost the performance of semitransparent perovskite solar cells. In particular, on optical absorption-limited semitransparent perovskite solar cells, methods applying bottom-up -synthesized colloidal nanoparticles, and top-down-defined nanostructures, micro/nano-scale patterning will be investigated. Through this PhD thesis, the candidate will have a unique opportunity to learn and apply combined knowledge in colloidal plasmonic nanomaterials, nano-patterning, metal halide perovskite materials, photovoltaic devices, solar cell macroscopic and microscopic characterizations, together with various optical and spectroscopic techniques to investigate the fundamental roles of different optical absorption and device performance enhancement methods.

Required background of the student: Solid academic background and a Master Degree on chemistry, material science, physics or applied physics. Good speaking & writing skills in English. Passionate in scientific experiments.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Enhancing the Efficiency and Stability of Triple-Cation Perovskite Solar Cells by Eliminating Excess PbI₂ from the Perovskite/Hole Transport Layer Interface, Z. Hu et al., ACS Applied Materials & Interfaces, 12 (49), 54824-54832 (2020)
2. Thermal conductivity and diffusivity of triple-cation perovskite halide materials for solar cells, Z. Hu et al., Journal of Applied Physics, 127 (12), 125113 (2020)
3. TiO₂ Nanocolumn Arrays for More Efficient and Stable Perovskite Solar Cells, Z. Hu et al., ACS Applied Materials & Interfaces, 12 (5), 5979-5989 (2020)
4. Microscopic evidence of upconversion-induced near-infrared light harvest in hybrid perovskite solar cells, M. S. Sebag et al., ACS Applied Energy Materials, 1 (8), 3537-3543 (2018)

5. Compact layer free mixed-cation lead mixed-halide perovskite solar cells, Z. Hu et al., Chemical Communications, 54 (21), 2623-2626 (2018)

Illustrations :

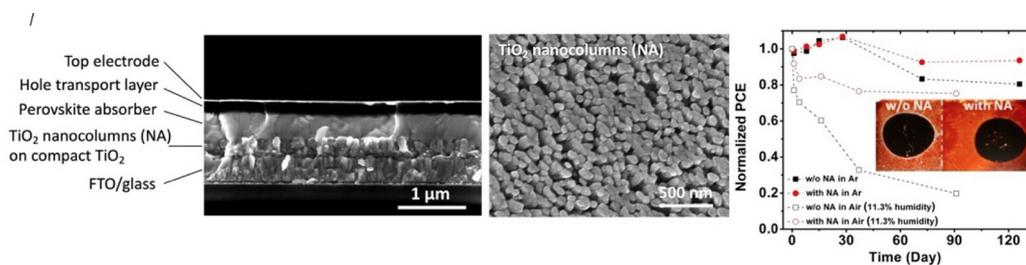


Figure: (Left) Cross-sectional SEM image of a typical triple-cation $\text{Cs}_{0.05}(\text{FA}_{0.83}\text{MA}_{0.17})_{0.95}\text{Pb}(\text{I}_{0.83}\text{Br}_{0.17})_3$ perovskite solar cell fabricated in our lab with a TiO_2 nanocolumn (NA) electron transport layer (ETL); (Center) Top-view SEM image of the TiO_2 NA electron transport layer; (Right) The evolution of power conversion efficiency (PCE) of the perovskite solar cells with and without TiO_2 NA ETL. Insets exhibit the optical images of the area around the top electrode of the two solar cells built on the same FTO substrate, with and without TiO_2 NA, after 91 days of degradation in air.

TITLE:CONTROLLING HYGROTHERMICS OF BIOBASED CONSTRUCTION MATERIAL

Topic number : 2021_009

Field : Environment Science and Technology, Sustainable Development, Geosciences, Material science, Mechanics and Fluids

Subfield: Civil Engineering - Construction

ParisTech School: Ecole des Ponts ParisTech

Research team:Rheophysics and Porous Media

<https://navier-lab.fr/en/research/rheophysique-et-milieux-poreux/>

Research lab: Laboratoire NAVIER (mécanique, physique des matériaux et des structures, géotechnique)

Lab location: Champs-sur-Marne

Lab website:<https://navier-lab.fr/en/>

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: COUSSOT Philippe philippe.coussot@univ-eiffel.fr

Advisor 2: HUBER Patrick patrick.huber@tuhh.de

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Reducing energy expenses and greenhouse gas emissions associated with heating or cooling down the housing depends largely on the use of good thermal insulator materials in construction. The use of various alternative bio-based materials is currently growing, such the dispersion of vegetal elements in a cementitious matrix for walls. The value of these materials is that in addition to their finely divided porous structure with a large porosity, they are hygroscopic, i.e. they can absorb a significant fraction of water in the solid structure, which is transported or released (evaporation) depending on external conditions. In that case, the walls ensure a further comfort to people, as they tend to regulate the ambient humidity. Thus it is crucial that the design of new buildings and renovation projects could rely on a proper evaluation of the “hygrothermics” of the used materials.

The moisture transfer process in the building envelopes is generally not taken into account in the current conventional thermal calculation and energy consumption analysis. The major problem hindering progress is the lack of information and proper description of water transport and

phase changes inside the porous structure. Measurements remain challenging, in particular considering that the materials are non-transparent and different states of water (free liquid water, bound water, vapor) can coexist. The Navier Laboratory has a Magnetic Resonance Imager (MRI) and several NMR Spectrometers for applications in civil engineering. We recently achieved a world first by demonstrating the possibility to measure the evolution of the distribution of free and bound water in wood, with the help of such techniques. The PhD work will apply such techniques to porous fiber packings representing the two main classes of insulating systems, subjected to various boundary conditions (temperature, relative humidity). Complementary in-situ X-ray imaging and X-ray wide- and small-angle X-ray scattering (SAXS/WAXS) are planned in a collaboration with P. Huber (Univ. Technol. Hambourg) to correlate the NMR data with spatio-temporally resolved water distributions in pore space. In addition an experimental set-up to measure the temperature along the sample axis and/or the heat exchanges during the process will be developed to get the thermal information. Finally a full hygrothermal modelling in agreement with these unique local data will be developed.

Required background of the student: Fluid mechanics - Possibly soft matter physics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. H. Penvern, M. Zhou, B. Maillet, D. Courtier-Murias, M. Scheel, J. Perrin, T. Weitkamp, S. Bardet, S. Caré, P. Coussot, How bound water regulates wood drying, *Physical Review Applied*, 14, 054051 (2020)
2. M. Zhou, S. Caré, A. King, D. Courtier-Murias, S. Rodts, G. Gerber, P. Aimedieu, M. Bonnet, M. Bornert, P. Coussot, Liquid uptake governed by water adsorption in hygroscopic plant-like materials, *Physical Review Research*, 1, 033190 (2019)
3. N. Ben Abdelouahab, A. Gossard, X. Ma, H. Dialla, B. Maillet, S. Rodts, P. Coussot, Understanding mechanisms of drying of a cellulose slurry by magnetic resonance imaging, *Cellulose*, 28, 5321-5334 (2021)
4. L.G. Cenchá, G. Dittrich, P. Huber, CLA Berli, R. Urteaga, Precursor Film Spreading during Liquid Imbibition in Nanoporous Photonic Crystals, *Phys. Rev. Lett.*, 125, 234502 (2020)
5. A. Jani, M. Butsch, J.B. Mietner, J. Ollivier, M. Appel, B. Frick, J.M. Zanotti, A. Ghoufi, P. Huber, M. Fröba, D. Morineau, Dynamics of water

confined in mesopores with variable surface interaction, *The Journal of Chemical Physics*, 154, 094505 (2021)

Illustrations :

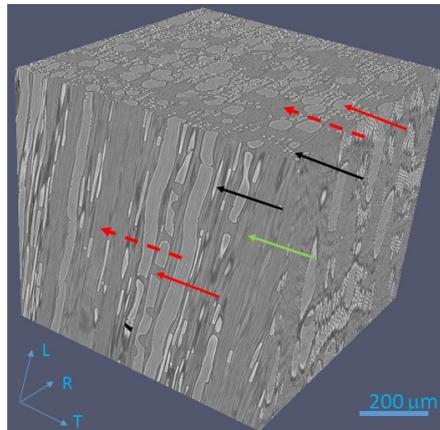


Figure 1: 3D XRCT view of the wood structure at 151% MC. Light gray correspond to air regions, darker gray areas correspond to liquid water or cell walls. Red arrows show the vessels, black arrows the fibers and green arrow the rays. Dashed arrows show vessels containing water. The wood samples are taken in a region as homogeneous as possible, and are tested either green, or re-soaked after drying. Although the resulting values of initial water content in vessels and fibers differed from one sample to another the trends observed by the different techniques and the mechanisms discussed below were qualitatively similar. Under these conditions we can consider that we are dealing with a single given material and focus on its physical properties.

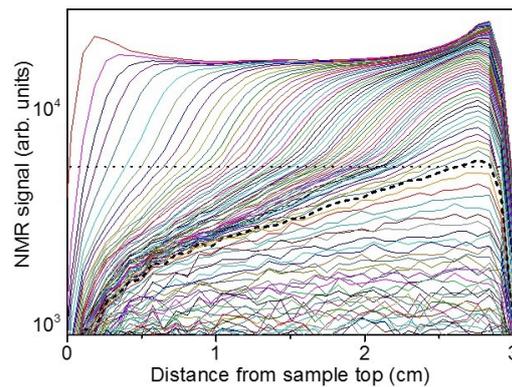


Figure 2: Total water 1D distribution from the SPI sequence in time during drying of a 3 cm long wood sample in the form of successive profiles in time (from top to bottom). First 5 profiles every 1h21, then every 2h42 up to the dashed profile, and afterwards every 5h24. The horizontal dotted line marks the region of apparent transition between two regimes of transport in the sample: bound + free water, then bound water only. The dashed profile is the last one which can be considered as partly in the upper range of water content. The process can be described by a two-step diffusion process.

TITLE: GAS TRANSFER IN THE COMPACTED BENTONITE-BASED MATERIALS

Topic number : 2021_010

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Ecole des Ponts ParisTech

Research team: Géotechnique

Research lab: Laboratoire NAVIER (mécanique, physique des matériaux et des structures, géotechnique)

Lab location: Champs-sur-Marne

Lab website: <https://navier-lab.fr/>

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: Cui Yujun yu-jun.cui@enpc.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Compacted bentonite-based materials have been planned to be used as filling/sealing materials in the geological storage of radioactive waste. In the long term, gas accumulation (hydrogen, oxygen, and CO₂...) would occur due to the corrosion of canisters and organic matter degradation, etc. To ensure the safety of the storage system, it is essential to well understand the mechanisms of gas transfer through compacted bentonite-based materials. In the proposed PhD study, laboratory tests will be performed on two selected bentonite-based materials. The water retention capacity, gas permeability and gas breakthrough phenomenon will be investigated. Emphasis will be put on the effects of bentonite content, dry density and microstructure.

Required background of the student: Good knowledge of soil mechanics; high capacity of data analysis; ability in laboratory testing; motivation for research

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. BIAN X., CUI Y.J., LI X.Z. 2019. Voids effect on the swelling behaviour of compacted bentonite. *Géotechnique* 69(7), 593-605.
2. ZHANG F., CUI Y.J., CONIL N., TALANDIER J. 2020. Assessment of Swelling Pressure Determination Methods with Intact Callovo Oxfordian Claystone. *Rock Mechanics and Rock Engineering* 53(4), 1879-1888.
3. CUI L.Y., YE W.M., WANG Q., CHEN Y.G., CHEN B., CUI Y.J. 2020. Insights into Determination of Gas Breakthrough in Saturated Compacted Gaomiaozi Bentonite. *Journal of Materials in Civil Engineering* 32(7), 04020190.
4. ZENG Z.X., CUI Y.J., CONIL N., TALANDIER J. 2020. Experimental study on the aeolotropic swelling behaviour of compacted bentonite/claystone mixture with axial/radial technological voids. *Engineering Geology* 278, 105846.
5. ZENG Z.X., CUI Y.J., CONIL N., TALANDIER J. 2021. Effects of technological voids and hydration time on the hydro-mechanical behaviour of compacted bentonite/claystone mixture. *Géotechnique*, online.

Illustrations :

TITLE: DESIGN OF NEW PHOTOACTIVABLE SYSTEMS USING THEORETICAL APPROACHES

Topic number : 2021_011

Field : Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology

Subfield: Theoretical Chemistry

ParisTech School: Chimie ParisTech - PSL

Research team: Chemical Theory and Modelling group

<https://www.quantich.fr/>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website: <https://iclehs.fr/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Ciofini Ilaria ilaria.ciofini@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Although computational approaches have reached a mature stage allowing the rationalization and even the prediction of several molecular properties, the accurate description of excited states and thus of phenomena depending on them is still difficult to be achieved. This is especially for photoactivated molecular systems of interest for application in the health domain. In this thesis we will focus on the development of accurate yet computationally affordable theoretical approaches allowing the description of the photophysical and the photochemical properties of dyes (both metal complexes and purely organic) of potential use for photodynamic therapy.

In particular, after having validated a computational protocol enabling to quantitatively describe the properties of existing photosensitizers (PS), we will particularly focus on the development of theoretical approaches, enabling the ab-initio design of new PS with enhanced penetration depth.

Required background of the student: The student should have a solid background in physical chemistry. Expertise in theoretical chemistry and programming will be considered as a plus.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. J. Karges, S. Kuang, F. Maschietto, O. Blacque, I. Ciofini, H. Chao and G. Gasser Ruthenium Complexes for 1- and 2-Photon Photodynamic Therapy: From In Silico Prediction to In Vivo Applications Nature Comm 11 (2020) 3262.
2. F. Maschietto, M. Campetella, J. Sanz-García, C. Adamo, I. Ciofini Chasing unphysical TD-DFT excited states in transition metal complexes with a simple diagnostic tool J Chem Phys. 154 (2021) 204102.
3. J. Sanz García, F. Maschietto, M. Campetella, I. Ciofini Using Density Based Indexes and Wavefunction Methods for the Description of Excited States: Excited State Proton Transfer Reactions as Test Case J Phys Chem A 122 (2018) 375-382.
- 4.
- 5.

Illustrations :

**TITLE: MACHINE LEARNING BASED ADAPTIVE MULTIVARIATE STATISTICAL
PROCESS CONTROL**

Topic number : 2021_012

Field : Design, Industrialization

Subfield: Industrial Eng., Artificial Intelligence

ParisTech School: Arts et Métiers

Research team:

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location:

Lab website: <http://lcfc.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: DANTAN Jean-Yves jean-yves.dantan@ensam.eu

Advisor 2: HOMRI Lazhar lazhar.homri@ensam.eu

Advisor 3: ZOUHRI Wahb wahb.zouhri@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: The product development decision should benefit from the feedback and information provided by the users. Today, companies are adopting “data-driven” approaches to improve the product design based on artificial intelligence tools. This enables to ensure the quality and the reliability of the product that better serve the customer in terms of availability and that basically by analysing data from the process, which are generally defined as time series.

Dynamic process control constantly drives process improvement by focusing on extracting knowledge from stored data for immediate actions, ensuring therefore more efficiency and schedule adherence. It could automatically analyse the process and send alerts for immediate improvement. By continually leading improvements, systems performance and quality are thus maximized. In fact, undefined anomalies usually result into a breakdown of the equipment or a fault in the working of the equipment. Thereby, adopting a new anomaly detection approach will lead to test’s cost reduction and allow a quick identification of anomalies and unexpected patterns. Moreover, the derived knowledge can be used to improve the product design specifications and defining its verification and validation plans to build functional and reliable models

Required background of the student: Industrial Engineering or Applied Mathematics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Ciancio V., Homri L., Dantan J.-Y., Siadat A., 2020. Towards prediction of machine failures: overview and first attempt on specific automotive industry application. IFAC-PapersOnLine 53, 289-294. 2020
2. Bassetto S., Siadat A., Martin P., Advanced Process Control Application Modelling. CIRP Intelligent Computation Manufacturing Engineering, Jul 2002, ischia, Italy
3. Zouhri, W., Homri, L., & Dantan, J. Y. (2020). Handling the impact of feature uncertainties on SVM: A robust approach based on Sobol sensitivity analysis. To appear in Expert Systems with Applications, 2021.
4. Zouhri, W., Dantan, J. Y., Häfner, B., Eschner, N., Homri, L., Lanza, G., Theile, O. & Schäfer, M. (2020). Optical process monitoring for Laser-Powder Bed Fusion (L-PBF). CIRP Journal of Manufacturing Science and Technology, 31, 607-617
5. Himeur Y., Ghanem K., Alsalemi A., Bensaali F., Artificial intelligence-based anomaly detection of energy consumption in buildings: A review, current trends and new perspectives, Applied Energy 287, 2021.

Illustrations :

TITLE: SUPERVISED MACHINE LEARNING FOR TOLERANCE ALLOCATION

Topic number : 2021_013

Field : Design, Industrialization, Mathematics and their applications

Subfield:

ParisTech School: Arts et Métiers

Research team:

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://www.lcfc.fr>

Contact point for this topic: Arts et Métiers

Advisor 1: DANTAN Jean-Yves jean-yves.dantan@ensam.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: It is well-established that all product design activities are performed under uncertainty. Accordingly, and in light of the ever-increasing demand for high quality products and components, the topic of uncertainty has also impacted the development of tolerancing approaches. In fact, tolerancing has become the key concept for bridging the gap between design and manufacturing, not only ensuring assemblability, suitable capabilities of the required manufacturing processes and minimised costs, but also essential to ensure high and consistent behaviour of multi-physical products.

Hereby, Tolerance allocation is understood as the assignment of tolerance values according to the impact of uncertainties on product performance, and the engineering cost of uncertainty reduction vs the accuracy increase.

This proposal aims to push the frontiers of the tolerance synthesis by setting up a new methodology based on supervised learning (classification techniques) to infer the tolerance allocation model. In fact, the factor “respect of functional requirements” or “compliant product(T)” is integrated into all mathematical formulations. But the data generated to evaluate this probability “compliant product(T)” is not analyzed by machine learning techniques.

Several machine learning techniques could allow to determine a

surrogate model of the conformity product hull based on the data generated by statistical tolerance analysis. We defined the mathematical formulation of the conformity product hull: the necessary and optimal constraints on deviations of each product component, and we developed several statistical techniques to estimate the conformity product probability. The next step is to develop or to adapt several machine learning techniques to predict the product conformity hull, not for tolerance analysis, for tolerance allocation.

Required background of the student: Mech. Eng. or Artificial Intelligence

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Goka, E., Beaurepaire, P., Homri, L., Dantan, J.-Y., 2019, Probabilistic-based approach using Kernel Density Estimation for gap modeling in a statistical tolerance analysis, *Mechanism and Machine Theory*, 139, pp. 294-309.
2. Goka, E., Homri, L., Beaurepaire, P., Dantan, J.-Y., 2019, Statistical tolerance analysis of over-constrained mechanical assemblies with form defects considering contact types, *Journal of Computing and Information Science in Engineering*, 19 (2), art. no. 021010-1.
3. Morse, E., Dantan, J.-Y., Anwer, N., Söderberg, R., Moroni, G., Qureshi, A., Jiang, X., Mathieu, L., 2018, Tolerancing: Managing uncertainty from conceptual design to final product, *CIRP Annals*, 67 (2), pp. 695-717.
4. Dantan, J.-Y., 2015, Comparison of Skin Model Representations and Tooth Contact Analysis Techniques for Gear Tolerance Analysis, *Journal of Computing and Information Science in Engineering*, 15 (2), art. no. 021010.
5. Dumas, A., Gayton, N., Dantan, J.-Y., Sudret, B., 2015, A new system formulation for the tolerance analysis of overconstrained mechanisms, *Probabilistic Engineering Mechanics*, 40, pp. 66-74.

Illustrations :

**TITLE: CONTRIBUTION TO THE INTEGRATION OF ADDITIVE MANUFACTURING
AND AUGMENTED REALITY IN EARLY DESIGN PHASES TO FOSTER
CREATIVITY**

Topic number : 2021_014

Field : Design, Industrialization, Information and Communication
Science and Technology

Subfield: Additive Manufacturing, Augmented Reality, Design
Methodology, Creativity, Computer Graphics.

ParisTech School: Arts et Métiers

Research team:

Research lab: LCPI - Laboratoire conception de produits et innovation

Lab location: Paris

Lab website: <http://lcpi.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: Segonds Frédéric frederic.segonds@ensam.eu

Advisor 2: LOU Ruding ruding.lou@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: In the product design process, early stages are crucial as 80% of the design costs are engaged during these phases. Creativity is among one of the most important early activity as it allows to create breakthrough innovative products. Ideas are usually produced from inspirational sources such as images, 3D representations etc. These ideas are then retranscribed in ideas sheets to allow to select one (or more) concept to develop and industrialize.

As part of Industry 4.0, the idea generation phase can be enriched by the manipulation of physical objects made in Additive Manufacturing (AM). These objects can be produced on the fly to faithfully represent a concept to develop. In order to make this manipulation even more realistic, Augmented Reality (AR) technologies make it possible to apply a color and texture to a low-fidelity model. It allows users to see different appearances of a physical prototypes through the AR device and, at the same time, users can touch physically the object. Furthermore, with AR users can even change the shape and do some intuitive shape design activities. AR usually allows people to interact with virtual 3D mock-up integrated in the real world. The coupling of the two technologies (AM&AR) will thus favor the innovation of the design teams.

The aim of this PhD is to device and experiment AM&AR applications in the product design creativity activities in order answer the following research question : can experiencing AM&AR technologies foster creativity and innovation?

Required background of the student: Product design, creativity, innovation, additive manufacturing. Computer science, computer graphics, geometric modeling, computer-aided design.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Rias, A. L., Segonds, F., Bouchard, C., & Abed, S. (2017). Towards additive manufacturing of intermediate objects (AMIO) for concepts generation. *IJIDeM*, 11(2), 301-315.
2. B. Li, F. Segonds, C. Mateev, R. Lou, F. Merienne (2018), Design in context of use: An experiment with a multi-view and multi-representation system for collaborative design, *Computers in Industry*, 103, pp. 28-37.
3. B. Faliu, A. Siarheyeva, R. Lou, F. Merienne (2019), Design and Prototyping of an Interactive Virtual Environment to Foster Citizen Participation and Creativity in Urban Design", *LNISO* (34), pp. 55 - 78.
- 4.
- 5.

Illustrations :



TITLE: DEVELOPMENT OF GUIDELINES TOOL TO PREVENT THE OCCURRENCE OF PLASTIC BUCKLING IN THIN STRUCTURES

Topic number : 2021_015

Field : Material science, Mechanics and Fluids

Subfield: Mechanical Engineering, Computational Mechanics

ParisTech School: Arts et Métiers

Research team: Méthodes Numériques, Instabilités et Vibrations
(Numerical Methods, Instabilities and Vibrations)

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website: <http://www.lem3.univ-lorraine.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: ABED-MERAIM Farid Farid.Abed-Meraim@ensam.eu

Advisor 2: BEN BETTAIEB Mohamed Mohamed.BenBettaieb@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Plastic buckling is one of the most common structural instability phenomena that a thin structure may undergo during plastic loading. This phenomenon involves a sudden loss in strength for a structure due to the resulting post-buckling shape. Hence, to ensure structural integrity of thin structures, it is vital to carefully study this phenomenon and to develop the appropriate numerical tools and techniques capable of accurately preventing its occurrence. Despite the significant progress achieved in this area, the existing numerical tools and software packages suffer from several limitations and shortcomings, such as the poor description of the mechanical behavior of the studied structures. The current project aims to overcome these limitations by developing several reliable numerical tools and techniques in standalone codes or within the Abaqus Finite Element (FE) software. In these tools, advanced constitutive models, allowing for an accurate description of the mechanical behavior (based on macroscopic approaches or micro-macro frameworks involving relevant multiscale schemes), will be implemented and assessed. For validation purposes, the results obtained by the developed tools will be compared to benchmarks available in the literature as well as to some theoretical and

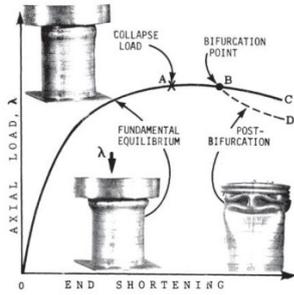
experimental results. Once fully developed and validated, these tools will be used as design guidelines by the industry of thin structures.

Required background of the student: - Solid background in non-linear solid mechanics and numerical methods;
- Good analytical and programming skills (e.g., Matlab, Mathematica, C/C++, Fortran);
- Experience with Finite Element modeling would be an asset.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. M. Ben Bettaieb, F. Abed-Meraim (2015), "Investigation of localized necking in substrate-supported metal layers: Comparison of bifurcation and imperfection analyses", *International Journal of Plasticity*, Vol. 65, pp. 168-190.
2. H.K. Akpama, M. Ben Bettaieb, F. Abed-Meraim (2017), "Localized necking predictions based on rate-independent self-consistent polycrystal plasticity: Bifurcation analysis versus imperfection approach", *International Journal of Plasticity*, Vol. 91, pp. 205-237.
3. M.Y. Jedidi, M. Ben Bettaieb, F. Abed-Meraim, A. Bouguecha, M.T. Khabou, M. Haddar (2020), "Prediction of necking in HCP sheet metals using a two-surface plasticity model", *International Journal of Plasticity*, Vol. 128, 102641.
4. J.C. Zhu, M. Ben Bettaieb, F. Abed-Meraim (2020), "Numerical investigation of necking in perforated sheets using the periodic homogenization approach", *International Journal of Mechanical Sciences*, Vol. 166, 105209.
5. J.C. Zhu, M. Ben Bettaieb, F. Abed-Meraim (2020), "Investigation of the competition between void coalescence and macroscopic strain localization using the periodic homogenization multiscale scheme", *Journal of the Mechanics and Physics of Solids*, Vol. 143, 104042.

Illustrations :



Plastic buckling of a cylindrical shell subjected to axial compression.



Buckled axially compressed axially stiffened cylindrical shell.



Railway tracks in the Netherlands affected by Sun kink (a kind of heat buckling).



Buckled skin panels on a B-52 aircraft.

TITLE: DEVELOPMENT OF AN ADVANCED CPFEM TOOL FOR THE PREDICTION OF FORMABILITY LIMITS OF POLYCRYSTALLINE THIN METAL SHEETS

Topic number : 2021_016

Field : Material science, Mechanics and Fluids

Subfield: Mechanical Engineering, Computational Mechanics

ParisTech School: Arts et Métiers

Research team: Méthodes Numériques, Instabilités et Vibrations (Numerical Methods, Instabilities and Vibrations)

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website: <http://www.lem3.univ-lorraine.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: ABED-MERAIM Farid Farid.Abed-Meraim@ensam.eu

Advisor 2: BEN BETTAIEB Mohamed Mohamed.BenBettaieb@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: In contrast to macroscopic constitutive models, multiscale approaches allow naturally and explicitly linking physical microstructural parameters to some relevant in-use macroscopic properties. Consequently, multiscale constitutive approaches are nowadays widely used to predict the formability limits of thin metal sheets. Crystal plasticity finite element method (CPFEM) is considered to be one of the most reliable multiscale schemes for the accurate description of the mechanical behavior of polycrystalline aggregates exhibiting complex microstructures and/or mechanical behavior. In recent research projects, we have developed a robust and effective CPFEM tool to predict the mechanical behavior of heterogeneous materials and their formability limits. The first objective of the present project is to extend this tool to be able to capture more complex physical phenomena not considered in the former version (such as second-order effects due to grain size...). The second objective is to improve the description of the mechanical behavior at the microscale by considering physical mechanisms and phenomena not sufficiently investigated so far (such as an adequate description of dislocation density

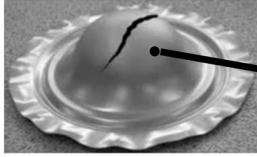
evolution, phase transformation present in TRIP and TWIP steels...). Once fully developed and validated, the resulting enhanced version of the CPFEM tool will be used, in academic and industrial contexts, to provide guidelines and assistance in the design of new generations of metallic alloys with improved ductility and in-use properties.

Required background of the student: - Solid background in non-linear solid mechanics and numerical methods;
- Good analytical and programming skills (e.g., Matlab, Mathematica, C/C++, Fortran);
- Experience with Finite Element modeling would be an asset.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

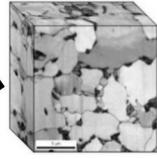
1. M. Ben Bettaieb, F. Abed-Meraim (2015), "Investigation of localized necking in substrate-supported metal layers: Comparison of bifurcation and imperfection analyses", *International Journal of Plasticity*, Vol. 65, pp. 168-190.
2. H.K. Akpama, M. Ben Bettaieb, F. Abed-Meraim (2017), "Localized necking predictions based on rate-independent self-consistent polycrystal plasticity: Bifurcation analysis versus imperfection approach", *International Journal of Plasticity*, Vol. 91, pp. 205-237.
3. M.Y. Jedidi, M. Ben Bettaieb, F. Abed-Meraim, A. Bouguecha, M.T. Khabou, M. Haddar (2020), "Prediction of necking in HCP sheet metals using a two-surface plasticity model", *International Journal of Plasticity*, Vol. 128, 102641.
4. J. Paux, M. Ben Bettaieb, F. Abed-Meraim, H. Badreddine, C. Labergere, K. Saanouni (2020), "An elasto-plastic self-consistent model for damaged polycrystalline materials: Theoretical formulation and numerical implementation", *Computer Methods in Applied Mechanics and Engineering*, Vol. 368, 113138.
5. J.C. Zhu, M. Ben Bettaieb, F. Abed-Meraim (2020), "Investigation of the competition between void coalescence and macroscopic strain localization using the periodic homogenization multiscale scheme", *Journal of the Mechanics and Physics of Solids*, Vol. 143, 104042.

Illustrations :

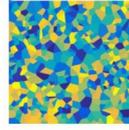


Deep drawing of steel sheet.

zoom



*Microstructure of
a TRIP steel.*



*Multiphase polycrystalline
aggregate.*



Metal part for automotive application.

TITLE: DEVELOPMENT OF AN ADVANCED NUMERICAL TOOL TO PREDICT THE BENDABILITY LIMITS DURING SHEET METAL FORMING PROCESSES

Topic number : 2021_017

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: Méthodes Numériques, Instabilités et Vibrations
(Numerical Methods, Instabilities and Vibrations)

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website: <http://www.lem3.univ-lorraine.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: ABED-MERAIM Farid Farid.Abed-Meraim@ensam.eu

Advisor 2: BEN BETTAIEB Mohamed Mohamed.BenBettaieb@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The vast majority of theoretical and numerical criteria developed to predict the occurrence of diffuse and/or localized necking are based on the simplifying modeling assumption that the studied metal sheets remain plane during forming processes. Hence, this conventional and widely-used assumption does not take into consideration the effect of sheet bending, and seems to be inadequate for analyzing the draw-type operations where sheet metal bends, slides and unbends over a draw radius. The main objective of the current PhD project is to extend the set of numerical tools, that we have developed within our research team for the prediction of diffuse necking (maximum force criterion, general bifurcation theory...) and localized necking (bifurcation theory, initial imperfection approach, ...), in order to include the bending effects. The effect of the heterogeneity of the strain through the sheet thickness on the onset of necking will be especially investigated. The mechanical behavior of the bent sheets will be also carefully analyzed by implementing advanced and elaborate constitutive models (phenomenological and multiscale constitutive models) in our numerical tools. Finite element simulations will be performed to assess the accuracy

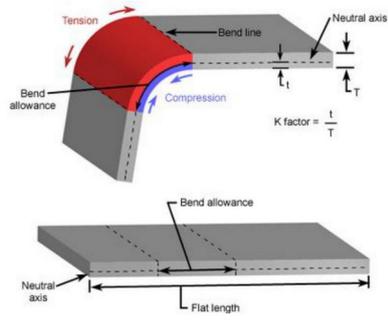
of the developed tools. Once fully developed and validated, these advanced numerical tools will be used to improve the prediction of the bendability in several industrial and academic applications.

Required background of the student: - Solid background in non-linear solid mechanics and numerical methods;
- Good analytical and programming skills (e.g., Matlab, Mathematica, C/C++, Fortran);
- Experience with Finite Element modeling would be an asset.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. M. Ben Bettaieb, F. Abed-Meraim (2015), "Investigation of localized necking in substrate-supported metal layers: Comparison of bifurcation and imperfection analyses", *International Journal of Plasticity*, Vol. 65, pp. 168-190.
2. M. Ben Bettaieb, F. Abed-Meraim, X. Lemoine (2019), "Numerical investigation of the combined effects of curvature and normal stress on sheet metal formability", *International Journal of Material Forming*, Vol. 12, Issue 2, pp. 211-221.
3. M.Y. Jedidi, M. Ben Bettaieb, F. Abed-Meraim, A. Bouguecha, M.T. Khabou, M. Haddar (2020), "Prediction of necking in HCP sheet metals using a two-surface plasticity model", *International Journal of Plasticity*, Vol. 128, 102641.
4. J. Paux, M. Ben Bettaieb, F. Abed-Meraim, H. Badreddine, C. Labergere, K. Saanouni (2020), "An elasto-plastic self-consistent model for damaged polycrystalline materials: Theoretical formulation and numerical implementation", *Computer Methods in Applied Mechanics and Engineering*, Vol. 368, 113138.
5. J.C. Zhu, M. Ben Bettaieb, F. Abed-Meraim (2020), "Investigation of the competition between void coalescence and macroscopic strain localization using the periodic homogenization multiscale scheme", *Journal of the Mechanics and Physics of Solids*, Vol. 143, 104042.

Illustrations :



Bending of a flat thin sheet.



Shearing and bending process.



Design information for bending.

**TITLE:IMPROVEMENT OF SURFACE PROPERTIES BY PVD-
THERMOCHEMISTRY HYBRID TREATMENT ON METAL SUBSTRATES OBTAINED
BY CONVENTIONAL MANUFACTURING PROCESSES AND BY POWDER
METALLURGY**

Topic number : 2021_018

Field : Material science, Mechanics and Fluids

Subfield: Material science and engineering, Surface treatment, PVD coatings, thermochemical treatment, powder metallurgy, diffusion

ParisTech School: Arts et Métiers

Research team:MSE Materials and Surfaces Engineering
<http://labomap.ensam.eu/materials-and-surfaces-engineering-100828.kjsp?RH=1415278881726&RF=1415870833775>

Research lab: LABOMAP - Laboratoire Bourguignon des matériaux et procédés

Lab location: Cluny

Lab website:labomap.ensam.eu

Contact point for this topic: Arts et Métiers

Advisor 1: Nouveau Corinne corinne.nouveau@ensam.eu

Advisor 2: Cotton Dominique dominique.cotton@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The LaBoMaP has a recognized expertise in vacuum treatment products, which are commonly used in numerous domains (transport, health, energy, etc.). The purpose is to improve the surface properties of the devices, in particular to protect them from severe solicitations (corrosion, abrasion, etc.). Both processes studied in the laboratory are Physical Vapor Deposition (PVD) and thermochemical treatments under vacuum, as well as their combination or "hybrid treatments". The aim is to thermochemically treat PVD metallic coatings (such as Cr, Ti..) to convert them in binary compounds (CrN, TiC etc). The objective of this PhD will be to master the numerous parameters that can influence both processes, to obtain the hard surface layer and the adequate gradient of hardness for its mechanical strength. First, substrates obtained by conventional manufacturing processes (forging, rolling) will be used. Then, the same substrates will be elaborated by metal powders in ICB laboratory

(University of Burgundy, Dijon), having a reputed expertise in this field, by Spark Plasma Sintering (SPS) and the Hot Isostatic Pressing (HIP). The project will be organized in 5 axes according to figure 1.

Required background of the student: 1. A master's degree in materials science (knowledge in metallurgy, surface treatments, diffusion, characterizations techniques such as SEM, XRD, EBSD etc).
2. Ability to work independently, to plan and carry out tasks, and to be a part of a large, dynamical group.
3. Good communication skills in English and/or French, both written and spoken.
4. Experience with powder metallurgy is an advantage but not an exclusion criterion

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Influence of Substrate Bias Voltage on Corrosion and Wear Behavior of Physical Vapor Deposition CrN Coatings, Aouadi, K., Tlili, B., Nouveau, C., ...Chafra, M., Souli, R., Journal of Materials Engineering and Performance, 2019, 28(5), pp. 2881-2891
2. Low-temperature plasma nitriding of martensitic stainless steel, Rao, K.R.M., Nouveau, C., Trinadh, K., Transactions of the Indian Institute of Metals, 2020, 73(6), pp. 1695-1699
3. Thermal treatment effect on structural and mechanical properties of Cr-C coatings, Fellah, M., Aissani, L., Zairi, A., ...Montagne, A., Iost, A., Transactions of the Institute of Metal Finishing, 2018, 96(2), pp. 79-85
4. A study of the tribological behavior of duplex treatment, Siad A., Nouveau C., Besnard A., Jacquet P, Annales de Chimie - Science Des Matériaux, 2015, 39(3-4), pp. 201-208
5. Influence of the process parameters on the microstructure of a hardfacing coating elaborated by hot isostatic pressing, Tellier, A., Ardigo-Besnard, M.R., Chateau-Cornu, J.-P., Archives of Metallurgy and Materials, 2019, 64(1), pp. 33-38

Illustrations :

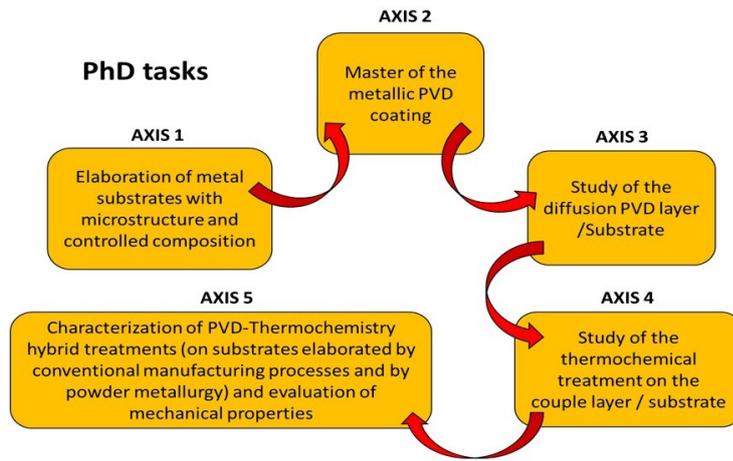


Figure 1. PhD tasks

TITLE: MEASUREMENT OF RESIDUAL STRESSES IN MATERIALS: FEM-BASED SIMULATION OF X-RAY DIFFRACTION

Topic number : 2021_019

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: MMS

Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés

Lab location: Aix-en-Provence

Lab website: <https://www.msmp.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: Depriester Dorian dorian.depriester@ensam.eu

Advisor 2: barrallier laurent laurent.barrallier@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: It is well known that, in many cases, residual stresses can improve lifespan of mechanical parts. In order to estimate those stresses, one of the most widely used techniques is based on X-ray diffraction (XRD). In crystalline materials, such as metals or ceramics, this techniques consists in measuring the reticular distances (distance between atomic plane of the crystals) thanks to the Bragg's law, thus providing information about the strain applied on the grains. Since the strain due to residual stresses is necessarily elastic, the residual stresses can be inferred from the reticular distances.

The aim of this project is to develop an innovative direct way to correlate XRD measurements with residual stresses. It will consists in simulating the XRD experiment on a strained polycrystal, generated with the aid of numerical tools dedicated to synthetic aggregate generation (e.g. NEPER software). Thanks to the results from Finite Element Analysis (FEA) performed at grain scale on polycrystalline aggregates, the local strain within each grain will be used to simulate the XRD experiment through implementation of the Bragg's law and ray-tracing techniques. Thus, the objective is to simulate the XRD experiment, taking into account the local

heterogeneities (phases, crystalline orientations...). This approach will also model the artefacts inherent to XRD (polychromatism, divergence of the X-ray beam etc.).

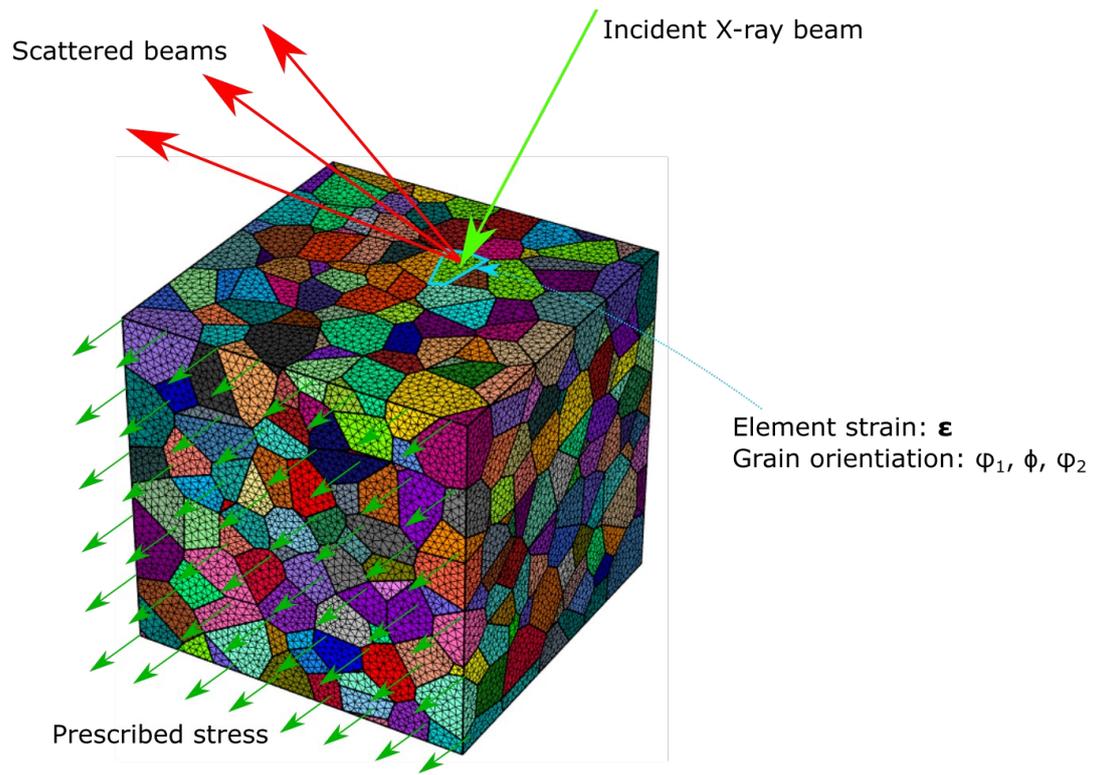
XRD experiments will be performed in order to assess the model. When the model is checked, numerical simulations will be performed in various conditions (in terms of microstructures, experimental conditions and residual stress distributions) so that sensitivity analysis will be performed. In terms, an Artificial Intelligence (AI) algorithm will be trained from these datasets, allowing to provide a new tool for analyzing XRD diagrams.

Required background of the student: Continuum mechanics, crystallography, Finite Element Methods, python programming

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Depriester D., Kubler R. (2019). Radical Voronoï tessellation from random pack of polydisperse spheres: Prediction of the cells' size distribution, Computer-Aided Design, Volume 107, 37-49, <https://doi.org/10.1016/j.cad.2018.09.001>
2. Depriester, D., Kubler, R. (2019). Resolution of the Wicksell's equation by Minimum Distance Estimation. Image Analysis & Stereology, Volume 38(3), 213-226 <https://doi.org/10.5566/ias.2133>
3. Depriester D., Kubler R. (2021). Grain size estimation in polycrystals: Solving the corpuscle problem using Maximum Likelihood Estimation, Journal of Structural Geology, Volume 151 <https://doi.org/10.1016/j.jsg.2021.104418>.
- 4.
- 5.

Illustrations :



TITLE: HIGH-POWER VERSATILE GHz FREQUENCY COMBS FOR SPECTRAL AND TEMPORAL DOMAINS APPLICATIONS

Topic number : 2021_020

Field : Physics, Optics

Subfield:

ParisTech School: Institut d'Optique Graduate School

Research team: Photonic Systems

<https://www.lp2n.institutoptique.fr/en/teams/photonics-systems>

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab website: <https://www.lp2n.institutoptique.fr/en>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: Cormier Eric eric.cormier@u-bordeaux.fr

Advisor 2: Santarelli Giorgio giorgio.santarelli@institutoptique.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Frequency combs with very high repetition rate in the GHz range have applications in optical telecommunications, photonic signal processing, spectroscopy, optical sampling, radio-frequency, metrology and many more. Such combs, mainly used for their spectral properties, have also shown fantastic potential in the time domain for the generation of arbitrary optical waveforms and shaped pulses with femtosecond to picosecond temporal resolution.

By coupling electro-optical modulation techniques derived from telecommunication and high-power fiber laser technologies based on Yb-doped fibers, we have developed in our group during the past years, an extended and unique knowledge on high-power highly tunable electro-optical comb generation. Various systems have been realized that deliver picosecond pulses with repetition rates adjustable from 1 to 20 GHz and used in various experiments such as laser processing or picosecond acoustics for instance. The Ph.D will focus on the study of a new generation of electro-optical combs featuring record breaking tens to hundreds of GHz repetition rates, with the ultimate goal targeting 1 THz.

The research will require to investigate physical processes and phenomena as diverse as laser amplification, ultrafast microwave signal manipulation, non-linear propagation in engineered waveguides, advanced dispersion management, ultrafast metrology, spectro-temporal shaping and more. The advances will be associated with application experiments either internally in the group or in collaboration with international laboratories and private companies. To cite a few, it is foreseen to use these synthetic combs for temporal shaping of intense laser pulse, as drivers for photo-injectors of a new generation of electron accelerators, to study ultrafast phenomena in solids and molecules, in the context of ultra-fast laser ablation and processing, and to study spintronics processes.

Required background of the student: Optics, optoelectronics, lasers, signal processing concepts, fibers

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. A. Aubourg, J. Lhermite, S. Hocquet, E. Cormier, and G. Santarelli, "Generation of picosecond laser pulses at 1030 nm with gigahertz range continuously tunable repetition rate," *Opt. Lett.* 40, 5610-5613 (2015).
2. H. Ye, L. Pontagnier, C. Dixneuf, G. Santarelli, and E. Cormier, "Multi-GHz repetition rate, femtosecond deep ultraviolet source in burst mode derived from an electro-optic comb," *Opt. Express* 28, 37209-37217
3. H. Ye, V. Freysz, R. Bello-Doua, L. Pontagnier, G. Santarelli, E. Cormier and E. Freysz "Electro-optic comb pumped optical parametric oscillator with flexible repetition rate at GHz level," *Opt. Lett.* 46, 1652-1655 (2021).
- 4.
- 5.

Illustrations :

TITLE: SURFACE INTEGRITY OF Ti-6Al-4V ALLOY COMPONENTS PRODUCED BY SLM AND MACHINING PROCESSES: MULTIPHYSICS SIMULATIONS AND EXPERIMENTAL VALIDATION

Topic number : 2021_021

Field : Material science, Mechanics and Fluids

Subfield: Mechanical Engineering, Manufacturing processes, Additive Manufacturing, Machining

ParisTech School: Arts et Métiers

Research team: High Speed Machining

Research lab: LABOMAP - Laboratoire Bourguignon des matériaux et procédés

Lab location: Cluny

Lab website: <http://labomap.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: OUTEIRO Jose jose.outeiro@ensam.eu

Advisor 2: Moufki Abdelhadi abdelhadi.moufki@univ-lorraine.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Selective Laser Melting (SLM) is an additive manufacturing (AM) process used to produce functional prototypes and small series of Titanium alloys components with high mechanical properties and high geometrical complexity. Additionally, to obtain a functional product with geometrical/dimensional and surface integrity requirements, the components produced by SLM need to be finished using a machining process. The rapid cooling of the material during SLM leads to thermally induced residual stresses distributions in the components. These stresses can affect the machining process, causing part distortion and poor surface integrity. This will affect the functional performance and life of the titanium components, such as fatigue life and corrosion resistance. In this work, the physical phenomena and the surface integrity of Ti-6Al-4V alloy generated by both SLM and machining processes will be investigated using Multiphysics Simulations, carefully validated by experimental tests. The aim of Multiphysics Simulations is to determine the SLM and machining processes conditions that will enhance the surface integrity of SLM-produced components.

Required background of the student: We are looking for a highly motivated candidate with a Master's degree in Mechanical Engineering or Materials Science. A knowledge of the finite element method and continuum mechanics will be considered a strong merit. Other desirable experience but not essential includes the MATLAB programming language.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. K.S.Djaka, A.Moufki, M.Nouari, P.Laheurte, A.Tidu. A semi-analytical modelling of cutting using crystal plasticity theory and flow line approach. *Int. J. of Mechanical Sciences*, 146-147, 49-59, 2018.
2. A. Moufki, D. Dudzinski, G. Le Coz, Prediction of cutting forces from an analytical model of oblique cutting, application to peripheral milling of Ti-6Al-4V alloy, *International Journal of Advanced Manufacturing Technology*, 81 (1-4), 615-626, 2015.
3. X. Xu, Jun Zhang, J.C. Outeiro, B. Xu, W. Zhao. Multiscale simulation of grain refinement induced by dynamic recrystallization of Ti6Al4V alloy during high speed machining. *Journal of Materials Processing Technology*, 286, 116834, 2020.
4. F. Careri, S. Imbrogno, D. Umbrello, M. M. Attallah, J.C. Outeiro, A. C. Batista, Machining and Heat Treatment as Post-Processing Strategies for Ni-Superalloys Structures Fabricated using Direct Energy Deposition, *Journal of Manufacturing Processes*, Vol. 61, pp. 236-244, 2021
5. I.S. Jawahir, E. Brinksmeier, R. M'Saoubi, D.K. Aspinwall, J.C. Outeiro, D. Meyer, D. Umbrello, A.D. Jayal. Surface Integrity in Material Removal Processes: Recent Advances. *CIRP Annals - Manufacturing Technology*, keynote paper, 60 (2), 603-626, 2011.

Illustrations :

TITLE: ACTIVE COLLOIDAL GELS

Topic number : 2021_022

Field : Chemistry, Physical chemistry and Chemical Engineering, Material science, Mechanics and Fluids, Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team: Olivier Dauchot

Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle

Lab location: Paris

Lab website: <https://www.gulliver.espci.fr>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Dauchot Olivier olivier.dauchot@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Colloidal Gels are obtained from the aggregation of attractive colloids. Tuning the density of particles, and the attraction strength and range allow us to control the gel morphology. Embedding colloids, that can be activated by light, inside the gel, we can form an active material, the response of which is controlled by light.

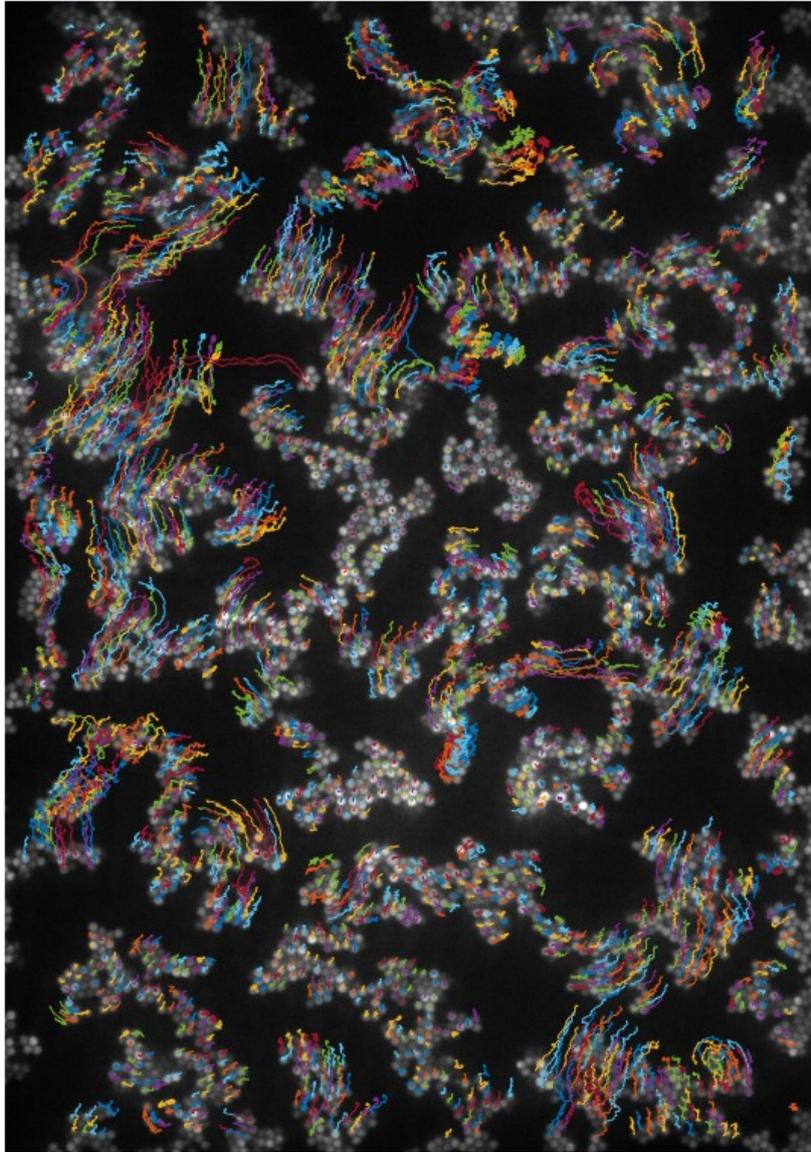
The main goal of this project is to study experimentally the coupling between the activity level and the mechanical properties of the gel. In particular, one expects the strain field induced by the active forces to induce a feedback on the active units, eventually leading to some form of collective actuation. Unveiling such a process would be a major breakthrough both in our understanding of living bodies and I towards the design of new functional materials.

Required background of the student: Colloidal Science, Physico-Chemistry

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Chemical Physics of Active Matter O. Dauchot, H. Löwen J. Chem. Phys. 151, 114901 (2019)
2. Interrupted Motility Induced Phase Separation in Aligning Active Colloids. Marjolein N. van der Linden, Lachlan C. Alexander, Dirk G. A. L. Aarts, Olivier Dauchot
Phys. Rev. Lett. 123, 098001 (2019)
3. The flow field around a confined active droplet. C. de Blois, M. Reyssat, S. Michelin and O. Dauchot Physical Review Fluids 4, 054001 (2019).
4. Active versus Passive Hard Disks against a Membrane: Mechanical Pressure and Instability, G. Junot, G. Briand, R. Ledesma-Alonso, and O. Dauchot, Phys. Rev. Lett. 119, 028002, (2017).
5. Elastic interactions between topological defects in chiral nematic shells, Alexandre Darmon, Olivier Dauchot, Teresa Lopez-Leon, Michael Benzaquem, Phys. Rev. E 94, (2016)

Illustrations :



TITLE: SURFACE TREATMENTS OF ALUMINIUM ALLOYS AND CORRESPONDING CORROSION BEHAVIOR. FOCUS ON THE ROLE OF INTERMETALLIC PARTICLES.

Topic number : 2021_023

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Surface Science, Material Science, Corrosion

ParisTech School: Chimie ParisTech - PSL

Research team: PCS Physico-Chimie des Surfaces

<https://www.ircp.cnrs.fr/la-recherche/equipe-pcs/>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <https://www.ircp.cnrs.fr/le-laboratoire/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Swiatowska Jolanta

jolanta.swiatowska@chimieparistech.psl.eu

Advisor 2: Wiame Frédéric frederic.wiame@chimieparistech.psl.eu

Advisor 3: Marcus Philippe philippe.marcus@chimieparistech.psl.eu

Advisor 4:

Short description of possible research topics for a PhD: This PhD thesis will be focused on surface treatments of aluminium alloys, their characterisation by surface sensitive techniques and corrosion tests. The objective of thermal or chemical treatments is to improve the mechanical or corrosion properties of the alloy. These treatments lead to significant morphological, structural and surface modifications, which are highly dependent on the presence of alloying elements such as Cu, Fe or Mg forming intermetallic particles. Depending on the alloy modifications induced by treatments, the corrosion resistance can be significantly influenced. The principal objective of this PhD thesis will be to evaluate the chemical surface modifications of Al alloys (e.g. AA2024, AA2050), induced by thermal or chemical treatments (in different gases or solutions, respectively, and for various exposure times) at the nanometric level and their influence on the corrosion behaviour. To do so, in situ XPS and ex situ techniques such as ToF-SIMS, nano-Auger or TEM will be applied.

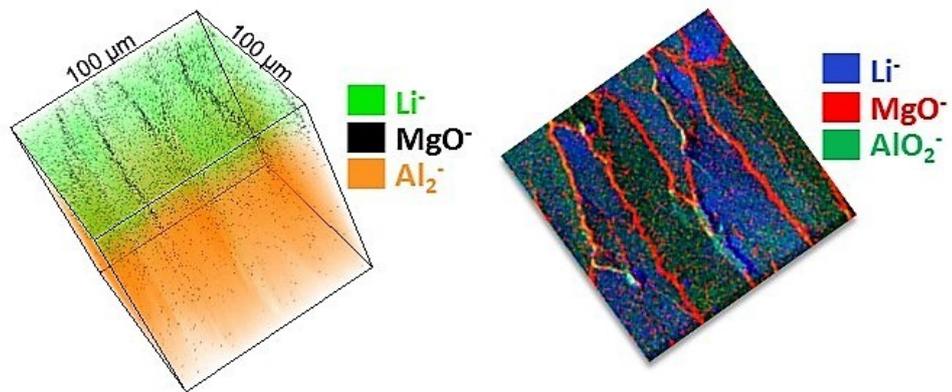
Required background of the student: The candidate should have a good background in chemistry, physical chemistry, electrochemistry and material science (e.g., metals, alloys, metallic oxides). The former experience in corrosion, corrosion protection and corrosion mechanisms, electrochemical characterization by cyclic voltammetry, impedance spectroscopy and materials characterization (by scanning electron microscopy, transmission electron microscopy, X-ray diffraction or surface sensitive techniques such as X-ray photoelectron spectroscopy) is a plus.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. M. Li, F. Wiame, A. Seyeux, P. Marcus, J. Światowska, Effect of thermal oxidation on surface chemistry and elemental segregation of Al-Cu-Li alloy, *Applied Surface Science*, 534 (2020) 147633. Doi: 10.1016/j.apsusc.2020.147633.
2. M. Li, A. Seyeux, F. Wiame, P. Marcus and J. Światowska, Insights on the Al-Cu-Fe-Mn intermetallic particles induced pitting corrosion of Al-Cu-Li alloy, *Corrosion Science*, 176 (2020) 176, 109040. Doi: 10.1016/j.corsci.2020.109040
3. M. Li, A. Seyeux, F. Wiame, P. Marcus, J. Światowska, Localized corrosion induced surface modifications of Al-Cu-Li alloy studied by ToF-SIMS 3D imaging, *NPJ Mat. Deg.* 5 (2021) 23. DOI: 10.1038/s41529-021-00170-9.
4. T. Sanchez, S. Zanna, A. Seyeux, M. Vaudescal, P. Marcus, P. Volovitch, J. Światowska, Conversion coating distribution on rough surfaces analyzed by combining surface analytical techniques, *Appl. Surf. Sci.* 556 (2021) 149734. DOI: 10.1016/j.apsusc.2021.149734.
5. A.-I. Stoica, J. Światowska, A. Romaine, F. Di Franco, J.-T. Qi, D. Mercier, A. Seyeux, S. Zanna and P. Marcus, Influence of post-treatment time of Trivalent Chromium Protection coating on Aluminium Alloy 2024-T3 on improved corrosion resistance, *Surface and Coatings Technology*, 369 (2019), 186-197. Doi: 10.1016/j.surfcoat.2019.04.051.

Illustrations :

3D chemical mapping by ToF-SIMS of Al-Cu-Li alloy after thermal treatment



Results published in Appl.Surf. Sci. 534 (2020) 147633. Doi: 10.1016/j.apsusc.2020.147633

TITLE:MORPHOLOGICAL SWARM ROBOTICS

Topic number : 2021_024

Field : Physics, Optics

Subfield: Mechanical and Electronic Engineering

ParisTech School: ESPCI Paris - PSL

Research team:Olivier Dauchot

Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle

Lab location: Paris

Lab website:<https://www.gulliver.espci.fr>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Dauchot Olivier olivier.dauchot@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: In this project, we are interested in swarm robotics, where a large number of robots with limited computation and communication power are considered. Our goal is to propose new design methods, with a particular focus on collective decision making using both morphological and logical computation.

To do so, we aim at new kind of swarm bots, where the shape factor guarantees the group dynamics, while each robot embeds a lightweight system-on-chip, sensors and actuators that can be used to modulate the robot behaviors on-the-fly.

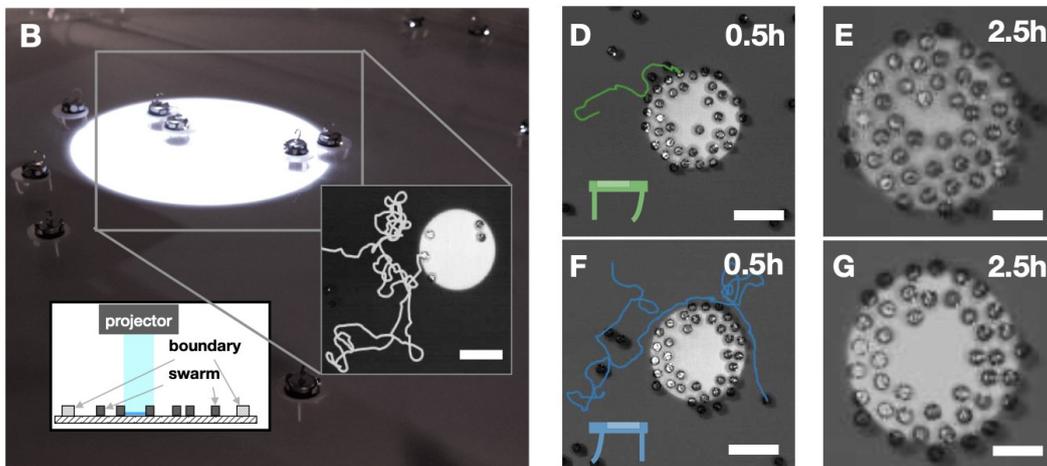
We will then look for specific educated collective behaviors: starting from the spontaneous phase obtained from the purely physical interactions of our robots we aim at applying minimal control from embodied capabilities on each bot, to induce specific collective behavior, which we will refer to as operational phases. Optimizing such behavior, we will aim at the realization of complex collective tasks.

Required background of the student: Physics, Mechanical Engineering

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Distributed On-line Learning in Swarm Robotics with Limited Communication Bandwidth. Nicolas Fontbonne, Olivier Dauchot and Nicolas Bredeche. Proceedings of the IEEE Congress on Evolutionary Computation (CEC), 2020
2. Dynamics of a Self-Propelled Particle in a Harmonic Trap. O. Dauchot, and V. Démery. Phys. Rev. Lett. 122, 068002 (2019).
3. Spontaneously Flowing Crystal of Self-Propelled Particles. G. Briand, M. Schindler and O. Dauchot. Phys. Rev. Lett 120, 208001 (2018).
4. Active versus Passive Hard Disks against a Membrane: Mechanical Pressure and Instability, G. Junot, G. Briand, R. Ledesma-Alonso, and O. Dauchot, Phys. Rev. Lett. 119, 028002, (2017).
5. Self-propelled hard disks: implicit alignment and transition to collective motion Khanh- Dang Nguyen Thu Lam, Michael Schindler, Olivier Dauchot New Journal of Physics (2015)

Illustrations :



TITLE: ENTRANCE EFFECTS IN OSMOTIC NANOFLUIDICS FOR BLUE ENERGY

Topic number : 2021_025

Field : Energy, Processes, Material science, Mechanics and Fluids

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team: MIE (Innovative Materials for Energy)

<http://mie.spip.espci.fr/>

Research lab: CBI - Chimie, Biologie et Innovation

Lab location: Paris

Lab website: <http://www.cbi.espci.fr/accueil-22/>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Trégouët Corentin corentin.tregouet@espci.fr

Advisor 2: Colin Annie annie.colin@espci.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Osmosis is the phenomenon responsible for spontaneous liquid transfers through porous membranes separating water reservoirs with different salinities. In specific conditions, these phenomena enable the generation of electrical currents between two reservoirs of brine and fresh water. Based on this principle, the production of electricity where sea water meets fresh water from the river: this is called the Blue Energy. The available blue energy to be harvested worldwide is estimated to be 1 TW, which represents not less than 10 times the total solar-energy consumption. Therefore, Blue Energy has the potential to be a game changer for the energy transition. However, there is a huge and yet unexplained discrepancy between the promising results based on single nanopores, and the maximum power that can actually be harvested with nanoporous membranes.

Consequently, before being able to harvest efficiently this energy, it is necessary to finely understand the flows occurring in the membrane nanopores. More specifically, complex effects at the entrance and the exit of nanopores result from couplings between ion concentrations, electric fields, electrostatic forces, pressure and flow, described by the advection-diffusion equation, Navier-Stokes, Boltzmann, and Poisson equations.

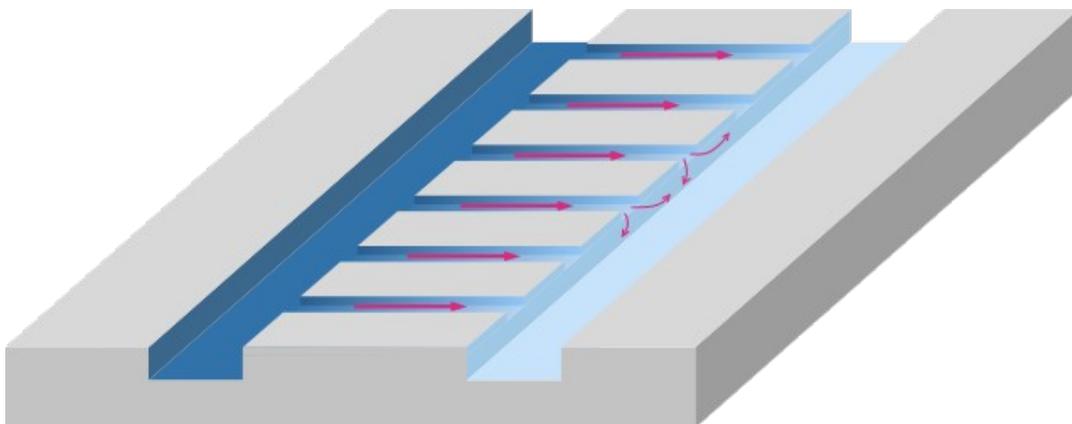
The aim of the PhD is to use nanofluidic chips which model nanoporous membranes to study experimentally these phenomena in well-controlled conditions. More specifically, we will first focus on the effect of the surface treatment (and hence surface charges) on diffusio-osmosis, and based on this, on the effect of the density of nanopores. This second part, the core of the project, is experimental and possibly numerical, and will be focused on the coupling between neighboring nanopores. Experimentally, the concentration field of an ionic dye will be measured using confocal microscopy to measure and understand this coupling.

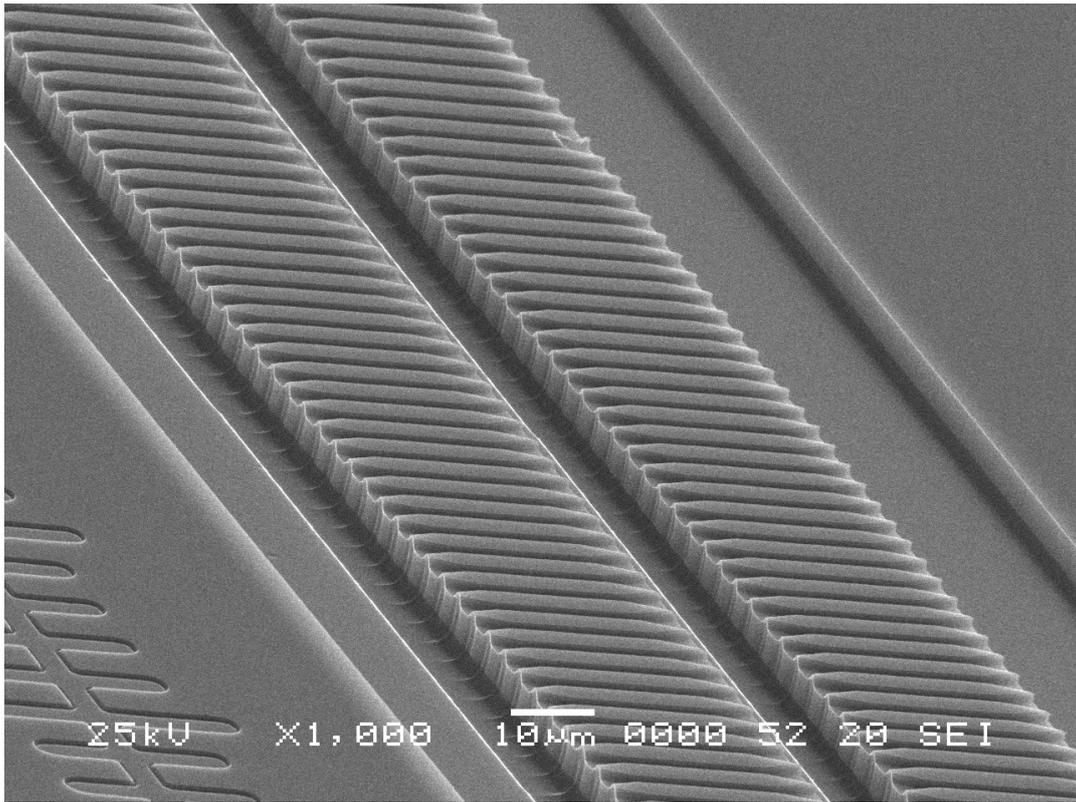
Required background of the student: Fluid mechanics and chemical physics.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Siria, A., Bocquet, M. & Bocquet, L. New avenues for the large-scale harvesting of blue energy. *Nat. Rev. Chem.* 1, (2016).
2. Marbach, S., Yoshida, H. & Bocquet, L. Osmotic and diffusio-osmotic flow generation at high solute concentration. I. Mechanical approaches. *J. Chem. Phys.* 146, (2017).
3. Gao, J. et al. Understanding the Giant Gap between Single-Pore- and Membrane-Based Nanofluidic Osmotic Power Generators. *Small* 15, 1-8 (2019).
- 4.
- 5.

Illustrations :





TITLE:SIMULTANEOUS OPTIMIZATION OF ANISOTROPY AND TOPOLOGY OF COMPOSITES FROM ADDITIVE MANUFACTURING PROCESS BY CONSIDERING STRENGTH CRITERIA BASED ON INVARIANTS

Topic number : 2021_026

Field : Design, Industrialization, Material science, Mechanics and Fluids, Mathematics and their applications

Subfield: Mechanics of materials and structures, additive manufacturing, topology optimisation, material optimisation, multi-scale analysis

ParisTech School: Arts et Métiers

Research team:IMC departement

<https://www.i2m.u-bordeaux.fr/Recherche/IMC-Ingenierie-Mecanique-et-Conception>

Research lab: I2M - Institut de Mécanique et d'ingénierie

Lab location: Bordeaux

Lab website:<https://www.i2m.u-bordeaux.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: Montemurro Marco marco.montemurro@ensam.eu

Advisor 2: Catapano Anita anita.catapano@bordeaux-inp.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The development of a general multi-scale modelling strategy coupled with a general optimization methodology and a dedicated mathematical formalism to represent both the topology and the anisotropy of the continuum (at each scale) is of paramount importance to carry out the concurrent optimization of the topology and of the fibres-path for variable stiffness composites (VSCs) fabricated through the Fused Filament Fabrication (FFF) + Continuous Filament Fabrication (CFF) technology. Moreover, the design strategy must take into account the specificities of the FFF+CFF process since the preliminary design phase to get optimized and manufacturable products.

The heterogeneity at the microscale (the scale of the constituents) and the anisotropy involved at the mesoscale (the scale of the ply) as well as at the macroscale (the scale of the structure), represent the main difficulties in the design process of these structures.

The following three main challenges will be addressed in this Thesis:

1. The simultaneous optimization of the anisotropy and the topology descriptors at the macroscopic scale through a suitable mathematical description of the anisotropy based on invariants related to the elastic symmetries
2. The formulation of the manufacturing constraints involved at the mesoscopic scale (i.e. fibres-path within each lamina) as equivalent constraints on the elastic invariants at the macroscopic scale. Typical manufacturing constraints are on the minimum steering radius, resin-rich areas, fiber tape width, etc.
3. The development of suitable criteria to take into account local damage mechanisms to be translated into equivalent mechanical constraints on the elastic invariants at the macroscopic scale.

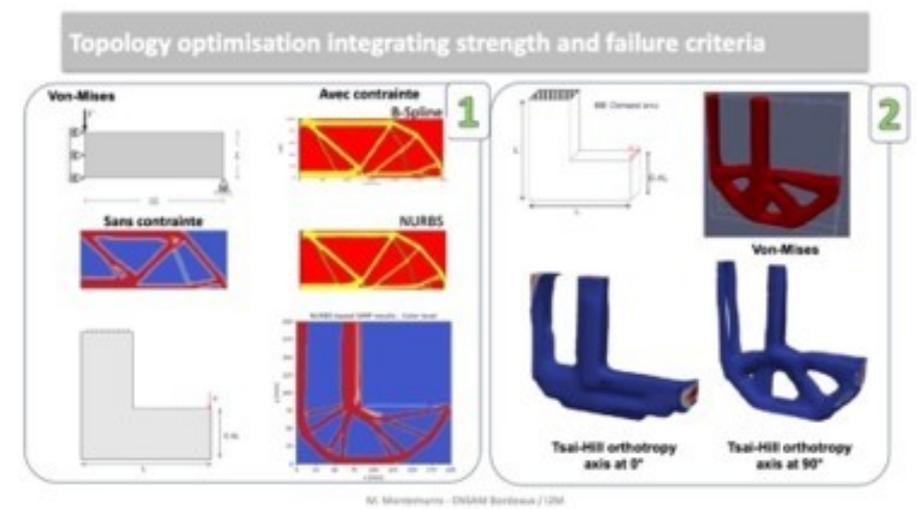
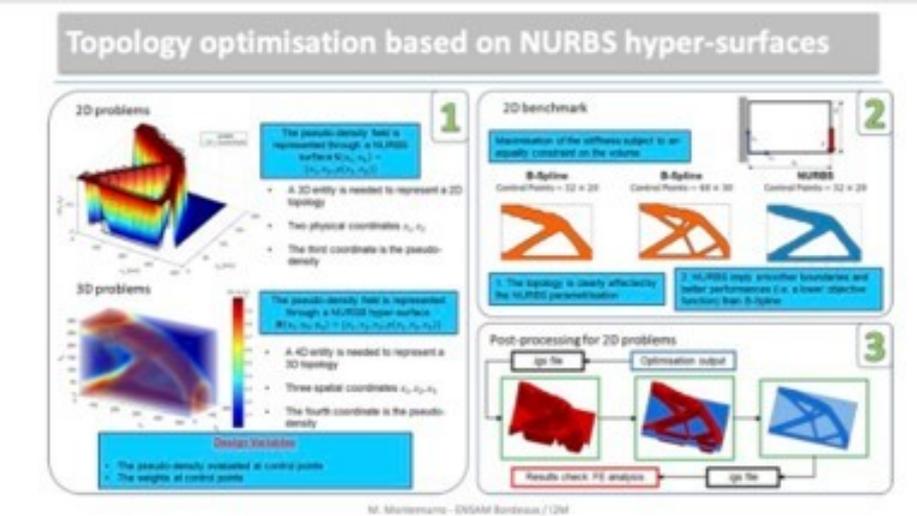
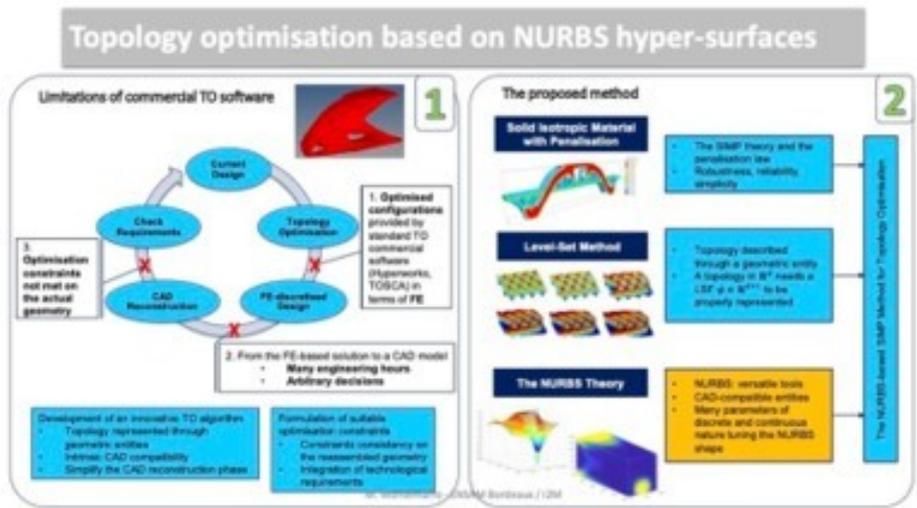
Required background of the student: Theoretical and applied mechanics, applied mathematics, programming skills, good knowledge of the finite element method

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. M. Montemurro, A. Catapano. A general B-Spline surfaces theoretical framework for optimisation of variable angle-tow laminates. *Composite Structures* 209: 561-578, 2019. URL: <https://doi.org/10.1016/j.compstruct.2018.10.094>
2. G. A. Fiordilino, M. I. Izzi, M. Montemurro. A general isogeometric polar approach for the optimisation of variable stiffness composites : application to eigenvalue buckling problems. *Mechanics of Materials* 153: 103574, 2021. URL : <https://doi.org/10.1016/j.mechmat.2020.103574>
3. M. I. Izzi, A. Catapano, M. Montemurro. Strength and mass optimisation of variable-stiffness composites in the polar parameters space. *Structural and Multidisciplinary Optimization* volume 64: 2045-2073, 2021. URL: <https://doi.org/10.1007/s00158-021-02963-7>
4. G. Costa, M. Montemurro, J. Pailhès. A 2D topology optimisation algorithm in NURBS framework with geometric constraints. *International Journal of Mechanics and Materials in Design*, v. 14 (4), pp. 669-696, 2018. URL: <https://doi.org/10.1007/s10999-017-9396-z>
5. T. Roiné, M. Montemurro, J. Pailhès. Stress-Based Topology Optimisation through Non-Uniform Rational Basis Spline Hyper-Surfaces.

Mechanics of Advanced Materials and Structures, URL:
<https://doi.org/10.1080/15376494.2021.1896822>, 2021 (in press).

Illustrations :



Multi-material topology optimisation

Single-scale Problems

The problem
Minimize the compliance subject to constraint on each material phase volume fraction

Two-material solution

Optimal solution: $\rho_1 = 0.1, \rho_2 = 0.9 \Rightarrow V_1 = 20 \Rightarrow V_2 = 480$

Optimal solution: $\rho_1 = 0.1, \rho_2 = 0.9 \Rightarrow V_1 = 20 \Rightarrow V_2 = 480$

Optimal solution: $\rho_1 = 0.1, \rho_2 = 0.9 \Rightarrow V_1 = 20 \Rightarrow V_2 = 480$

Three-material solution

Optimal solution: $\rho_1 = 0.1, \rho_2 = 0.1, \rho_3 = 0.8 \Rightarrow V_1 = 20 \Rightarrow V_2 = 20 \Rightarrow V_3 = 460$

Multi-scale Problems

Multi-scale problem:

Minimize the compliance subject to constraint on each material phase volume fraction

Formulation du problème:

$$\min_{\rho} C(\rho)$$

$$\text{subject to } \int_{\Omega} \rho \, d\Omega = V$$

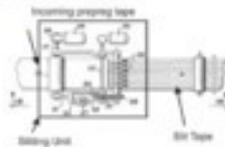
$$\rho \in \{0, 1\}$$

Optimised RVE of the material at the microscopic scale

M. Montemurro - ENSAM Bordeaux / ICM

Additive manufacturing of composites

Automated Fibre Placement (AFP)



- AVANTAGES:**
- Matériaux à haute performance
- INCONVENIENTS:**
- Solutions 2D (plaque, coque)

Continuous filament fabrication (CFF) + Fused filament fabrication (FFF)



- AVANTAGES**
- fabrication pièces composites 3D de géométrie complexe et rigidité variable
 - réparer/renforcer pièces existantes
 - ajout de fonctionnalités (capteurs, actuateurs)
 - solutions multi-matériaux
- INCONVENIENTS**
- polymères peu performants

M. Montemurro - ENSAM Bordeaux / ICM

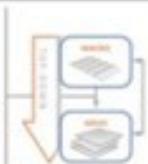
TOPIC 1: Development of *ad-hoc* design strategies

MULTI-SCALE TWO-LEVEL OPTIMISATION STRATEGY (MSZLOS)

Direct design of the macroscopic properties of the laminates without imposing simplifying rules on the stacks

PROPER FORMULATION OF THE OPTIMISATION PROBLEM

- MAIN FEATURE:**
- Polar formalism
- MAIN ADVANTAGES:**
- Great reduction of variables count (1st level)
 - Requirement on the elastic symmetries of the laminates are properly formulated at the macro scale
 - The full set of variables is considered and no simplifying rules are employed
 - Mechanical response of the structure evaluated by FE analyses



B-SPLINE FRAMEWORK

Description of complex continuous fields through a limited number of parameters

VARIABLES COUNT REDUCTION and CONTINUITY OF THE FIELDS

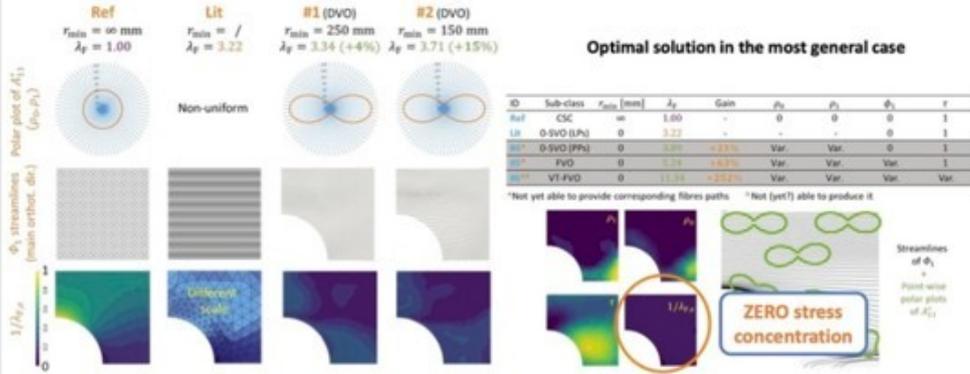


- Feasibility conditions in the 1st level to ensure the existence of the solution of the 2nd level problem
- The effect of the laminate transverse shear stiffness is taken into account

M. Montemurro - ENSAM Bordeaux / ICM

Strength optimisation of variable stiffness composites

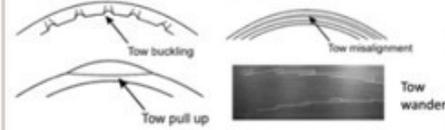
Effect of the max tow curvature constraint



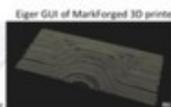
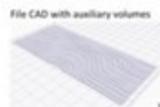
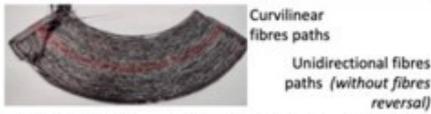
M. Montemurro - ENSAM Bordeaux / I2M

Analysis of process induced singularities → integration into the design strategy

Automated Fibre Placement (AFP)



CFF+FFF



M. Montemurro - ENSAM Bordeaux / I2M

TITLE:SYNTHESIS OF BIODEGRADABLE POLYMERS FROM RENEWABLE RESOURCES

Topic number : 2021_027

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Chemistry and Materials Science

ParisTech School: Chimie ParisTech - PSL

Research team:COCP - Organometallic Chemistry and Polymerization Catalysis <https://www.ircp.cnrs.fr/la-recherche/equipe-cocp/>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website:<https://www.ircp.cnrs.fr/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Gauvin Regis regis.gauvin@chimieparistech.psl.eu

Advisor 2: Thomas Christophe
christophe.thomas@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The ring opening polymerization (ROP) of N-carboxyanhydrides (NCA) can yield homopolymers and block-copolymers with well-controlled structures where the repeat units are natural amino acids.(publication 1) Similarly to proteins, these synthetic polypeptides possess well-defined secondary structures (alpha-helix and beta-sheets), whereas synthetic polymers generally present a disordered coil structure. Therefore, these biomimetic polymers produce sophisticated superstructures with new material properties. Our aim will be to develop an efficient route from readily available reactants to synthesize new polypeptide analogues with a conserved ability to form well-defined secondary structures.

In this regard, there is growing evidence that magnesium or zinc derivatives can be effective catalysts for homogeneous polymerization. Their low toxicity, low cost, and accessibility make them attractive candidates for the development of affordable, sustainable and green catalysts, potentially offering a biocompatible route to diverse materials. Bimetallic reagents are ideal candidates for this purpose since the polar organometallic moiety will act as a strong nucleophile with a concomitant electrophilic assistance created through the coordination of carbonyl

oxygen of urea by the lithium cation (See attached Figure). Therefore we want to use these bimetallic systems to synthesize aliphatic polyureas and polyurethanes via an auto-tandem catalytic transformation (publication 2) where cyclic urethanes or ureas are synthesized from respectively epoxides or aziridines and subsequently polymerized by ROP. (publication 3)

Required background of the student: Organic Chemistry, Polymer Chemistry, Catalysis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. S. K. Raman, E. Brulé, M. J.-L. Tschan, C. M. Thomas, Chem. Commun., 2014, 50, 13773-13776
2. C. Robert, F. de Montigny, C. M. Thomas, Nature Communications, 2011, DOI: 10.1038/ncomms1596
3. C. Robert, C. M. Thomas, Chem. Soc. Rev., 2013, 42, 9392-9402
4. L. Guillaume, A. Marshall, N. Niessen, P. Ni, R. M. Gauvin, C. M. Thomas, Green Chem., 2021, 23, 6931-6935.
- 5.

Illustrations :

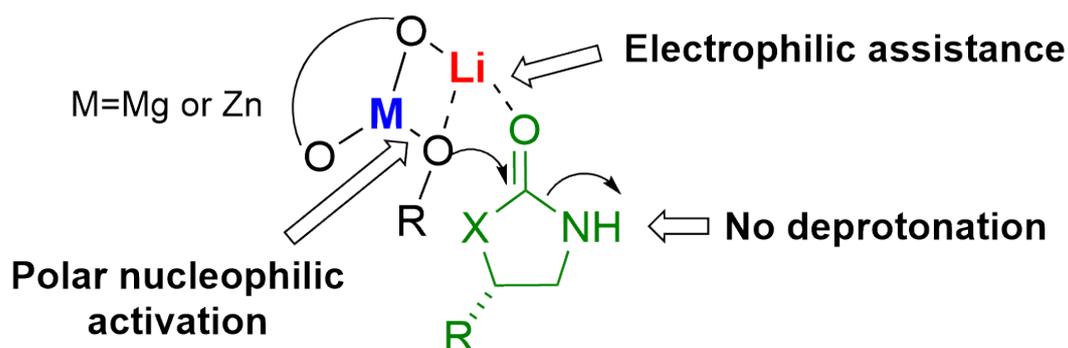


Figure 1. Foreseen catalytic systems

TITLE: USING GOOD VIBRATIONS TO DECREASE THE VISCOSITY OF NON BROWNIAN SUSPENSIONS.

Topic number : 2021_028

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team: MIE <https://mie.spip.espci.fr/spip.php?rubrique2>

Research lab: CBI - Chimie, Biologie et Innovation

Lab location: Paris

Lab website: <https://www.cbi.espci.fr/accueil-22/>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Colin Annie annie.colin@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Suspensions, which are dispersion of solid particles in a liquid are everyday objects: cement, particle suspensions for printing houses, polymer suspensions for 3D printing, polymer suspensions for forming coatings, carbon suspensions for preparing electrodes, mascara. The viscosity of the suspension increases until it becomes infinite when the concentration increases. To facilitate the flow of suspensions, it is possible to use formulations with surfactants or to use mechanical vibrations. Vibration has been used empirically in the industry for many years: vibrating conveyor belts for transporting dry granular materials, vibrating rulers or needles for evacuating air bubbles and leveling fresh concrete. Vibrations can also induce involuntary liquefaction of soils, as it was the case during the Nigata earthquake in Japan (see figure 1). However, the reasons for the action of vibrations are still poorly understood. In this thesis we will perform rheology measurements under ultrasound (frequency range 100 Khertz-600 Khertz) of model dispersions. These measurements will be completed by shear-reversal measurements to know if the contacts are broken or not in the flow, by measurements of friction coefficient under vibration to know if it is modified by the vibrations, last but not the least avalanche effects will be studied. This will allow us to understand the action of ultrasound on

dispersions. In the last year of the thesis, ultrasound will be added on a printing nozzle to facilitate the printing of suspensions.

Required background of the student: Soft matter, fluid mechanics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Ovarlez, G., Le, A. V. N., Smit, W. J., Fall, A., Mari, R., Chatté, G., & Colin, A. (2020). Density waves in shear-thickening suspensions. *Science advances*, 6(16), eaay5589.
2. Comtet, J., Chatté, G., Nigues, A., Bocquet, L., Siria, A., & Colin, A. (2017). Pairwise frictional profile between particles determines discontinuous shear thickening transition in non-colloidal suspensions. *Nature communications*, 8(1), 1-7.
3. Madraki, Y., Oakley, A., Nguyen Le, A., Colin, A., Ovarlez, G., & Hormozi, S. (2020). Shear thickening in dense non-Brownian suspensions: Viscous to inertial transition. *Journal of Rheology*, 64(2), 227-238.
4. Goyon, Julie, Annie Colin, G. Ovarlez, A. Ajdari, and L. Bocquet. "Spatial cooperativity in soft glassy flows." *Nature* 454, no. 7200 (2008): 84-87.
- 5.

Illustrations :



a Concrete, b Mascara, c earthquake in Japan

TITLE: VECTORIZING NANOPARTICLES USING BIOCOMPATIBLE AND BIODEGRADABLE POLYMER COATING MEDIATED BY SURFACE ORGANOMETALLIC CHEMISTRY

Topic number : 2021_029

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Chemistry and Materials Science

ParisTech School: Chimie ParisTech - PSL

Research team: COCP - Organometallic Chemistry and Polymerization Catalysis <https://www.ircp.cnrs.fr/la-recherche/equipe-cocp/>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <https://www.ircp.cnrs.fr/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Gauvin Regis regis.gauvin@chimieparistech.psl.eu

Advisor 2: Thomas Christophe
christophe.thomas@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The design of efficient vectorizing agents is at the cornerstone of modern pharmaceutical agents. In this view, the tailoring of specific (molecular) objects by covalent bonding with polymer chains is of major interest, to confer them significant compatibility with physiological environments. (Publication 1)

In this view, biocompatible and biodegradable polymers are ideal candidates as components within such advanced formulations. These can be most efficiently prepared using ring opening polymerization (ROP) of lactones or lactides into polyesters or polylactic acid mediated by organometallic initiators. (Publications 2 and 3) On the top of that, immobilization of organometallics on inorganic surfaces via surface was demonstrated to boost stereoselectivity of these considered polymerization processes. (Publication 4) In this project, we propose to combine surface organometallic chemistry and ROP of polar monomers to design specific nano-objects by “growing from” or “growing on” approaches, where chain growth is mediated by specifically designed supported organometallic entities (See attached Figure). The ultimate

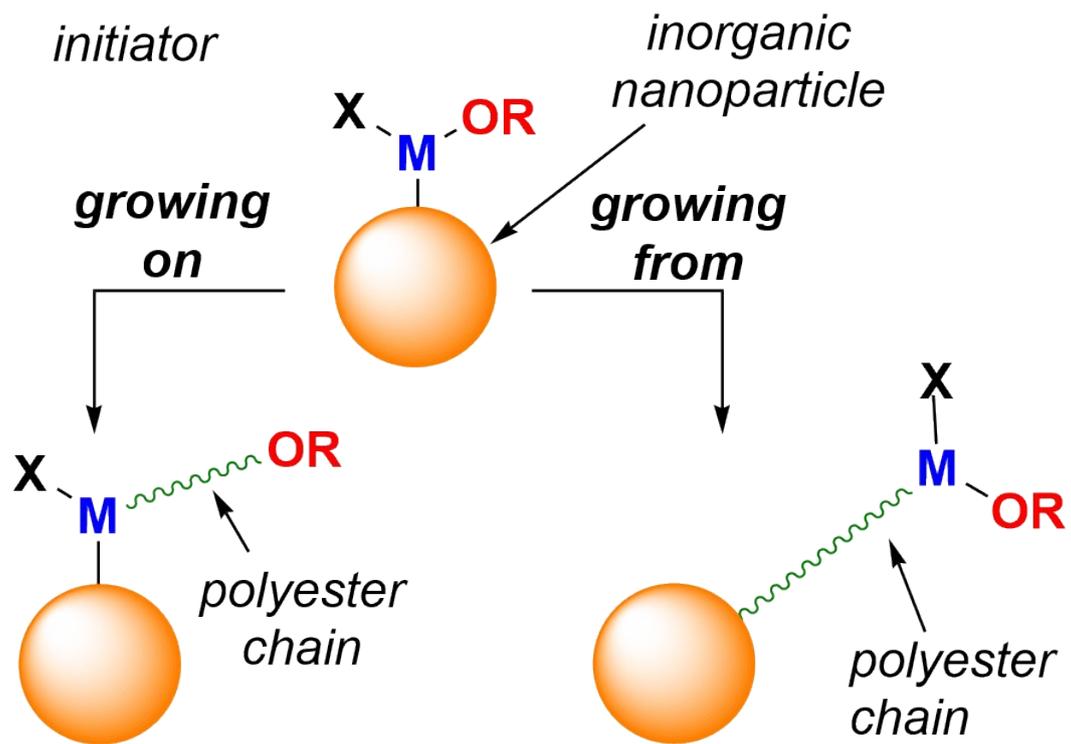
goal will be the development of biopolymer-coated nanoparticles for future implementation into delivery systems.

Required background of the student: Organic Chemistry, Polymer Chemistry, Catalysis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. N. Soliman, L. K. McKenzie, J. Karges, E. Bertrand, M. Tharaud, M. Jakubaszek, V. Guérineau, B. Goud, M. Hollenstein, G. Gasser, C. M. Thomas, *Chem. Sci.*, 2020, 11, 2657-2663.
2. P. Marin, M. J.-L. Tschan, F. Isnard, C. Robert, P. Haquette, X. Trivelli, L.-M. Chamoreau, V. Guérineau, I. del Rosal, L. Maron, V. Venditto, C. M. Thomas, *Angew. Chem. Int. Ed.* 2019, 58, 12585.
3. C. Robert, T. E. Schmid, V. Richard, P. Haquette, S. K. Raman, M.-N. Rager, R. M. Gauvin, Y. Morin, X. Trivelli, I. del Rosal, L. Maron, C. M. Thomas, *J. Am. Chem. Soc.*, 2017, 139, 6217.
4. N. Ajellal, G. Durieux, L. Delevoye, G. Tricot, C. Dujardin, C. M. Thomas, R. M. Gauvin, *Chem. Commun.* 2010, 46, 1032-1034.
- 5.

Illustrations :



TITLE: 2D/3D PEROVSKITES FOR STABLE AND HIGH-EFFICIENCY SOLAR CELLS

Topic number : 2021_030

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes, Environment Science and Technology, Sustainable Development, Geosciences

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team: Opto-electronics, Photovoltaics and Nanostructures
<http://www.pauportegroup.com>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <https://www.chimieparistech.psl.eu/recherche/les-laboratoires/ircp/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Pauporté Thierry thierry.pauporte@chimie-paristech.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Recently, hybrid halogen perovskites (PVKs) have emerged as fascinating materials and highly versatile semiconductors. These compounds can be prepared as 2D (two-) and 3D (three-dimensional) materials, and their composition can be varied over a quite large extend. This ensures the possible fine tuning of their optoelectronic properties. Their superior properties make them especially attractive for an application in photovoltaic (PV) solar cells. If their PV power conversion efficiency is now reaching impressive values, these devices still suffer from a problem of stability.

The host group, which is leader in France on perovskite solar cells (PSCs) research, has discovered recently precursor solution chemistries that allow the preparation of highly stable of quasi-2D and 2D/3D perovskite layers. Moreover the power conversion efficiency achieved with these perovskites is very promising.

The aim of the PhD will be to get further insights into the preparation of these layers with special stoichiometry and additive. The student will investigate the role of the additives and the effect of the composition on

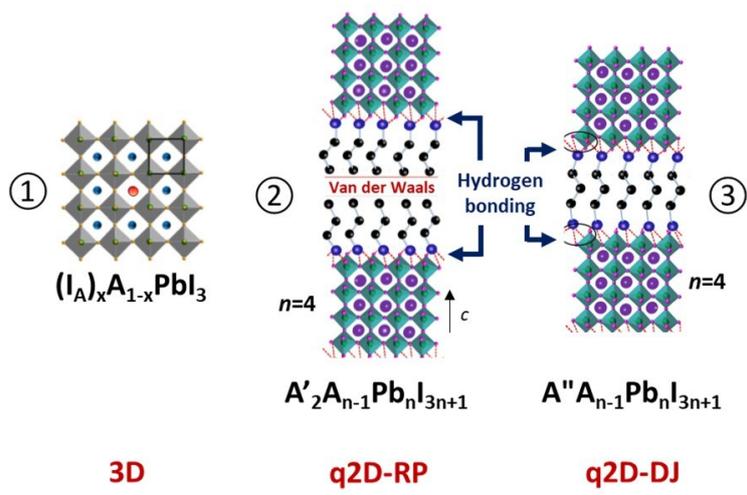
the layers morphological, structural, optical and electronic properties. PV cells based on these new materials will be prepared and characterized by various techniques (J-V curves, impedance spectroscopy, spectral response, GD-OES...). The objective will be to better understand the effect of chemistry and composition on the devices stability and high performances.

Required background of the student: Material science, Chemistry, if possible: Physics of semiconductors, Photovoltaics.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. D. Zheng, T. Pauporté, Control by Mixed-Chloride Additives of the Quality and Homogeneity of Bulk Halide Perovskite upon Film Formation Process. *J. Mater Chem. A* 9 (2021) 17801-17811. DOI: 10.1039/D1TA04651A
2. F. Cheng, J. Zhu, Th. Pauporté, Chlorides, other Halides and Pseudohalides as Additives for the Fabrication of Efficient and Stable Perovskite Solar Cells. *ChemSusChem* 14 (2021) 3665–3692. DOI: 10.1002/cssc.202101089
3. D. Zheng, T. Zhu, T. Pauporté, A Co-Additives Strategy for Blocking Ionic Mobility in Methylammonium-Free Perovskite Solar Cells and High Stability Achievement. *Solar RRL.*, 5 (2021) 2100010.
4. T. Zhu, D. Zheng, J. Liu, L. Coolen, Th. Pauporté, Electrical Response of High Efficiency and Stable Solar Cells Based on MA_{0.94}MA_{0.06}PbI₃ Perovskite. *ACS Appl. Mater. Interfaces* 12 (2020) 37197–37207.
5. D. Pitarch-Tena, T.T. Ngo, M. Vallés-Pelarda, Th. Pauporté, I. Mora-Seró, Impedance Spectroscopy Measurements in Perovskite Solar Cells. Device Stability During the Measurement and Noise Reduction. *ACS Energy Lett.*, 3 (2018) 1044–1048.

Illustrations :



**TITLE: SYNTHESIS OF BIOBASED POLYMERS FROM RENEWABLE RESOURCES:
A NEW TANDEM APPROACH**

Topic number : 2021_031

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Chemistry and Materials Science

ParisTech School: Chimie ParisTech - PSL

Research team: Organometallic Chemistry and Polymerization Catalysis
<https://www.ircp.cnrs.fr/la-recherche/equipe-cocp/research-topics/>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <https://www.ircp.cnrs.fr/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Thomas Christophe
christophe.thomas@chimieparistech.psl.eu

Advisor 2: Gauvin Regis regis.gauvin@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

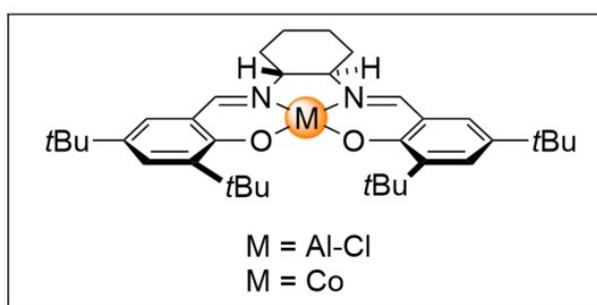
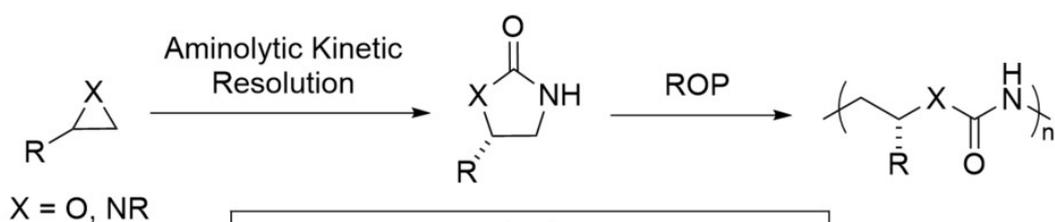
Short description of possible research topics for a PhD: Tandem catalysis is one of the strategies used by Nature for building macromolecules. However, these biological processes rely on highly complex biocatalysts thus limiting their industrial applications. In the same biomimetic spirit, we want to initiate a research effort to synthesize biodegradable polymers via tandem catalytic transformations, where “activated” monomers are synthesized from raw materials (in one or more steps) and subsequently (co)polymerized. The objectives for this are clear: not only can a reduction in workload, waste and energy consumption be achieved, but also the synthesis of complex products that are otherwise difficult to obtain (e.g., because of thermodynamic hurdles) comes within reach. In other words, the combination of chemistries may allow the direct synthesis of macromolecules with high structural complexity. Therefore, we want to direct investigative efforts toward the synthesis of new renewable monomers and the subsequent catalytic conversion of these monomers into their corresponding polymers. The general idea is to use a tandem procedure of combining synthesis of new biomass derived monomers with subsequent polymerization by well-defined metal-based catalysts, aiming at novel polymeric materials.

Required background of the student: Polymer Chemistry, Catalysis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Nature Comm., 2011, 2, 586
2. J. Am. Chem. Soc. 2017, 139, 6217-6225
3. Angew. Chem. Int. Ed. 2019, 58, 12585-12589
4. J. Am. Chem. Soc. 2021, 143, 13401-13407
5. Angew. Chem. Int. Ed. 2021, 60, 19374-19382

Illustrations :



TITLE: THE MECHANICS OF EARTHQUAKES AND FAULTING: INFLUENCE OF FRICTION PROPERTIES AND FAULT MATERIAL ON RUPTURE TIP PROPAGATION

Topic number : 2021_032

Field : Environment Science and Technology, Sustainable Development, Geosciences, Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team:

Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation

Lab location: Angers

Lab website: lampa.ensam.eu

Contact point for this topic: Arts et Métiers

Advisor 1: AMMAR Amine amine.ammar@ensam.eu

Advisor 2: EL AREM Saber saber.elarem@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: In the last two decades, considerable observational and theoretical work has been devoted to all aspects of earthquake prediction research, for solving

fundamental questions concerning the mechanics of fault systems, as well as for

answering questions regarding earthquake hazard. The european natural

observatory of the Corinth Rift (<http://crlab.eu>), a very rapidly deforming area

(opening strain rate of $\sim 10^{-6}$ /yr) where one or more earthquakes with

magnitudes above 6 are expected in the coming decades provides a framework

in which the mechanics of faults can be studied in details. It is densely

instrumented and provides an exceptional data base (seismological, GPS and

strain data). All the prediction approaches in the literature rely on some probabilistic description of earthquake generation and timing, through empirical laws guided, or structured, by some simplification of the underlying physical process. This requires that relevant physical models and observational constraints are put at the core of any probabilistic law seismic-hazard assessment. Based on advanced numerical modeling, our objective is to examine the fault zones material behavior and its relation to earthquake dynamics, the description friction at slow rates (interseismic period) and earthquake nucleation, and the dynamics of fault weakening during rapid slip. Numerical results will be compared to in laboratory experiments and to field observation.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Christopher Scholz, The Mechanics of Earthquakes and Faulting, Cambridge University Press, 2019
2. James R. Rice, Nadia Lapusta, K. Ranjith, Rate and state dependent friction and the stability of sliding between elastically deformable solids, Journal of the Mechanics and Physics of Solids, September 2001
3. P. Bernarda, H. Lyon-Caen et al., Tectonophysics, Volume 426, Issues 1-2, 30 October 2006, Pages 7-30
4. S. El Arem, H. Lyon-Caen, P. Bernard, J-D Garaud, F. Rolandone, and P. Briole. In EGU General Assembly Conference , volume 15, page 14477, Vienna, Austria, 2013
- 5.

Illustrations :

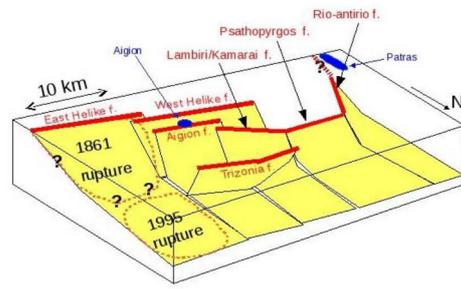


Figure 1: sketch of the major active faults of the CRL area. Surface scarps in red. Trizonia fault is the only south dipping fault. The 1995 may have occurred on the Helike fault (uncertain dip and connectivity)

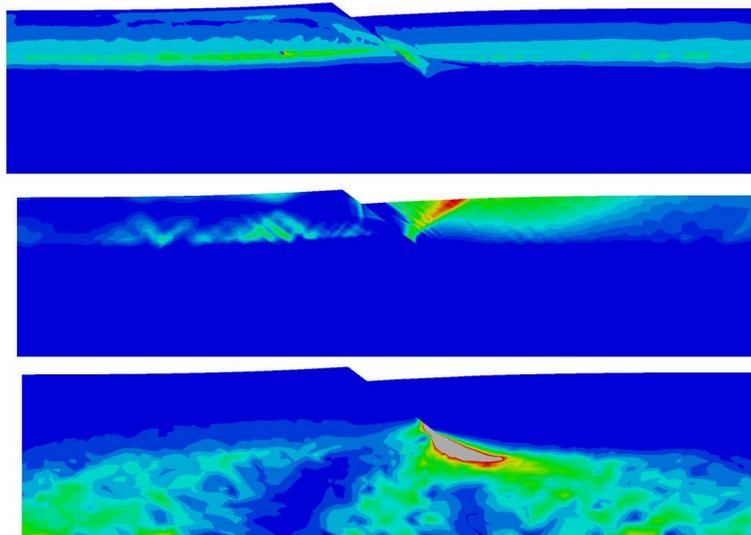
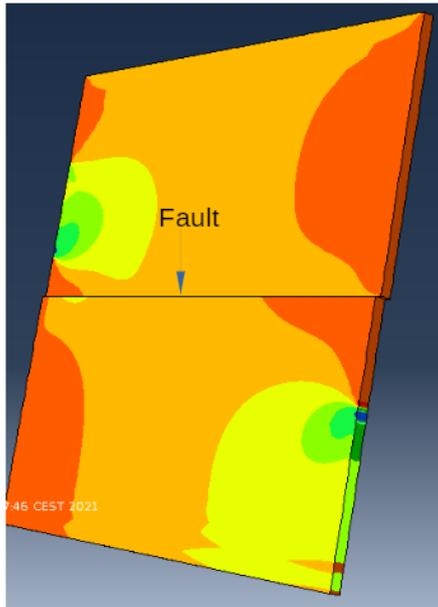


Figure 1: Stress and strain near fault zone. (a) Mises equivalent stress (b) Equivalent plastic strain (c) Equivalent creep strain.



Slipping (green) and sticking (red) zones during the fault interseismic rapid sliding

**TITLE: SMART MULTI-CATALYTIC SYSTEMS FOR THE PRODUCTION OF
BIOCOMPATIBLE POLYMERS**

Topic number : 2021_033

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Chemistry and Materials Science

ParisTech School: Chimie ParisTech - PSL

Research team: Organometallic Chemistry and Polymerization Catalysis
<https://www.ircp.cnrs.fr/la-recherche/equipe-cocp/research-topics/>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <http://www.ircp.cnrs.fr>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Thomas Christophe
christophe.thomas@chimieparistech.psl.eu

Advisor 2: Gauvin Regis regis.gauvin@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

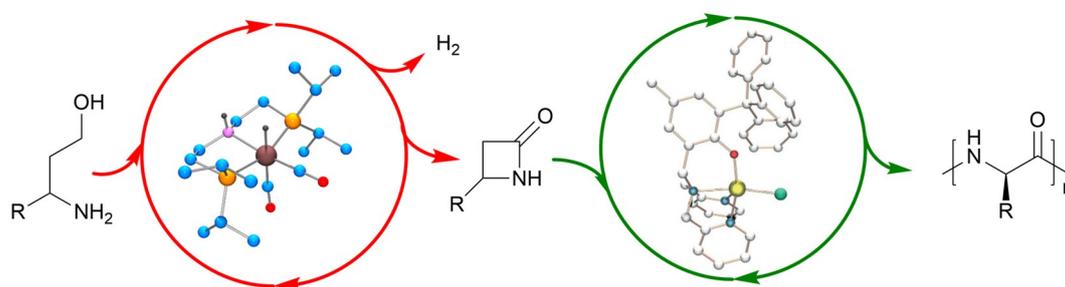
Biocompatible materials such as polyesters and polyamides hold a prominent position in the portfolio of specialty and commodity polymers. Controlling their structural features such as chain size and microstructure is key in establishing specific properties. In this context, organometallic catalysis is instrumental, thanks to its outstanding ability to achieve both high degree of stereoselectivity and mass control. Smart approaches such as tandem catalysis can be game changers: Combining several complementary systems is a unique opportunity to perform series of chemical reactions with higher efficiency. In this project, hydrogen borrowing, a clean, atom-economical technology, will be harnessed in a first step to synthesize lactones or lactames monomers from biosourced raw materials. These will then be polymerized via stereoselective ring opening polymerization, affording novel polyesters or polyamides. A strong emphasis will be put on the design of novel organometallic catalysts based on Earth-abundant metals, as well as on establishing catalysts structure and polymers' physicochemical properties relationships.

Required background of the student: Organic and polymer synthesis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Nature Comm., 2011, 2, 586
2. ACS Catal., 2014, 4, 3586-3589
3. ACS Catal., 2017, 7, 2022-2032
4. Angew. Chem. Int. Ed. 2021, 60,19374-19382
5. J. Am. Chem. Soc. 2021, 143, 13401-13407

Illustrations :



**TITLE: MULTISCALE STRESS/STRAIN ANALYSIS OF POLYCRYSTALLINE SILICON
FOR PHOTOVOLTAIC APPLICATIONS**

Topic number : 2021_034

Field : Material science, Mechanics and Fluids

Subfield: Photovoltaic

ParisTech School: Arts et Métiers

Research team: MMS <https://www.msmp.eu/equipes/mms/>

Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés

Lab location: Aix-en-Provence

Lab website: [msmp.eu](https://www.msmp.eu)

Contact point for this topic: Arts et Métiers

Advisor 1: barrallier laurent laurent.barrallier@ensam.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Polycrystalline silicon (PS) is a raw material used by the solar photovoltaic (PV) and electronics industry. The reduction of the cost of PV cells production is largely possible by using PS. Nevertheless, the limitation of PS use is directly linked to the microstructure of the material i.e. i) the active defects such as grain boundaries, dislocation arrangements, ... ii) but also the mechanical fields induced by these defects. The efficiency of PV cells is depending on the mastering of the defect generation, their repartition and the induced strain/stress fields during the fabrication of PS.

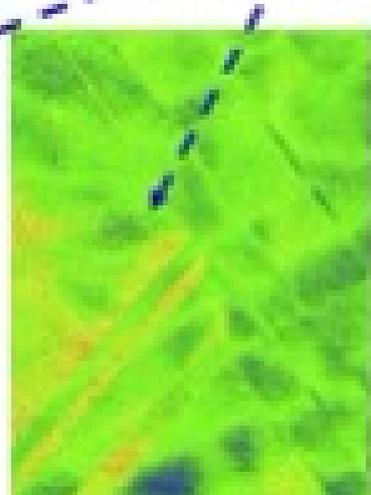
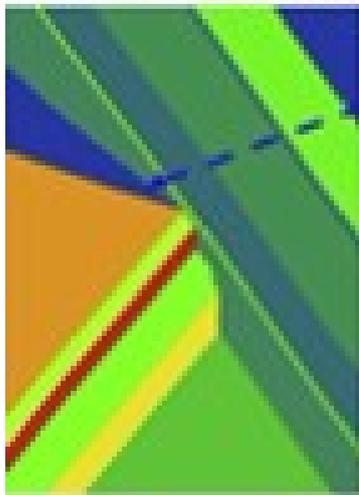
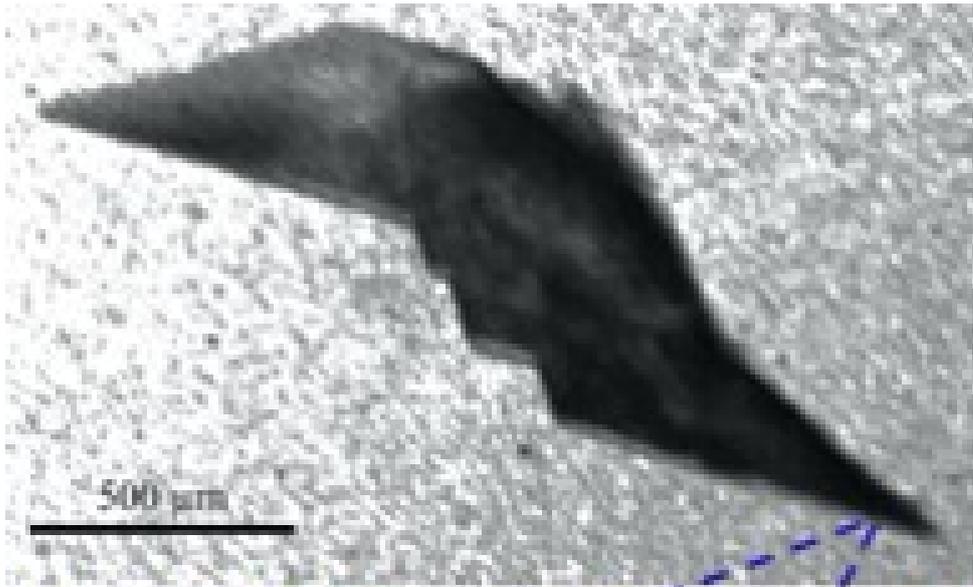
The aim of this project is to characterize the induced residual stress fields of PS in relation with their microstructure. Experimental methods used to determine residual stresses fields will be based on multiscale diffraction in-lab technics such as High-Resolution Electron Backscatter Diffraction (HR-EBSD), X-ray diffraction (XRD) of synchrotron facility. To understand the origin of residual stress fields in PS cells, the temperature HR-EBSD and XRD measurements will be coupled with polycrystalline thermo-elasto-plasticity simulation using finite element method (FEM).

Required background of the student: Materials Science and/or Mechanical Engineering

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. M. Becker, E. Pihan, F. Guittonneau, L. Barrallier, G. Regula, H. Ouaddah, G. Reinhart, and N. Mangelinck-Noël. Investigation of subgrains in directionally solidified cast mono-seeded silicon and their interactions with twin boundaries. *Solar Energy Materials & Solar Cells*, 218(110817):1-10, décembre 2020.
2. N. Mangelinck-Noel, H. Ouaddah, M. Becker, T. Ribéri-Beridot, M. Tsoutsouva, V. Stamelou, G. Regula, G. Reinhart, I. Péricaud, F. Guittonneau, L. Barrallier, J.-P. Valade, A. Rack, E. Boller, and J. Baruchel. X-ray based in situ investigation of silicon growth mechanism dynamics-application to grain and defect formation. *Crystals*, 10(7):1-25, july 2020.
3. T. Ribéri-Béridot, M.G. Tsoutsouva, G. Regula, G. Reinhart, F. Guittonneau, L. Barrallier, and N. Mangelinck-Noël. Strain building and correlation with grain nucleation during silicon growth. *Acta Materiala*, 177:141-150, 09 2019.
4. M.G Tsoutsouva, T. Ribéri-Béridot, G. Regula, G. Reinhart, J. Baruchel, F. Guittonneau, L. Barrallier, and N. Mangelinck-Noël. In situ investigation of the structural defect generation and evolution during the directional solidification of 110 seeded growth si. *Acta Materiala*, 115:210-223, August 2016.
5. T. Ribéri-Beridot, N. Mangelinck-Noel, A. Tandjouai, G. Reinhart, B. Billia, B. Lafford, J. Baruchel, and L. Barrallier. On the impact of twinning on the formation of the grain structure of multi-crystalline silicon for photovoltaic applications during directional solidification. *Journal of Crystal Growth*, (418):38-44, 2015.

Illustrations :



TITLE:LEARNING WITH IMMERSIVE TECHNOLOGIES

Topic number : 2021_035

Field : Design, Industrialization, Information and Communication
Science and Technology

Subfield: Virtual Reality

ParisTech School: Arts et Métiers

Research team: Presence & Innovation

Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation

Lab location:

Lab website:<http://lampa.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: RICHIR SIMON simon.richir@ensam.eu

Advisor 2: Gorisse Geoffrey geoffrey.gorisse@ensam.eu

Advisor 3: Fleury Sylvain sylvain.fleury@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: The proposed research project aims at investigating the potential of immersive technologies (virtual reality, augmented reality) to learn technical and/or scientific contents. Virtual and augmented reality have developed rapidly over the last twenty years, both in terms of hardware and software quality, which offers several potentialities and use cases. However, these technologies remain under-exploited in several fields. The digital learning transformation, particularly in higher education and professional training, requires further investigations in order to adapt to the cognitive characteristics of learners and to develop pedagogical approaches that integrate these technologies in a relevant way. Today, the main obstacles to the use of immersive technologies for learning are not only technical, but also ergonomics and pedagogical. It is necessary to identify the conditions of effectiveness of these devices by working on a better understanding of users' cognitive functioning in learning situations. More specifically, we want to study how virtual agents (autonomous characters controlled by the computer) can be used to facilitate learning. For instance, we could investigate how a virtual agent acting as a tutor could facilitate the learning of a technical procedure.

We could also study how to "capture" a teacher's lesson and how to reproduce it in a virtual environment, through a virtual agent (using the "CAPLAB" platform being installed in Laval).

In this context, experiments could be carried out to identify the optimal characteristics of this virtual tutor, in terms of realism, attractiveness and behavior, in order to enhance learners' motivation. Evaluations could focus on learning performance (memorization, understanding, ability to reproduce the task in realistic context), participant involvement, but also on learners' satisfaction in order to guarantee the acceptability of the technologies used in such contexts.

The use of artificial intelligence modules could be considered if this subject interests the selected candidate for the thesis.

This work will lead to high-level international publications that will shed light on relevant pedagogical tools and good practices for learning using immersive technologies.

Required background of the student: Master's degree in computer science with extended knowledge of virtual reality. We are looking for a candidate with an interest in multidisciplinary research, at the frontier of virtual reality and experimental psychology. A strong interest for experimental research is required: production of protocols, conducting experiments, data analysis and writing. Applicants are expected to read, speak and write academic english.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Buttussi, F., & Chittaro, L. (2017). Effects of different types of virtual reality display on presence and learning in a safety training scenario. *IEEE transactions on visualization and computer graphics*, 24(2), 1063-1076.
2. Hamilton, D., McKechnie, J., Edgerton, E., & Wilson, C. (2021). Immersive virtual reality as a pedagogical tool in education: a systematic literature review of quantitative learning outcomes and experimental design. *Journal of Computers in Education*, 8(1), 1-32.
3. Hew, K. F., & Cheung, W. S. (2010). Use of three-dimensional (3-D) immersive virtual worlds in K-12 and higher education settings: A review of the research. *British journal of educational technology*, 41(1), 33-55.
4. Makransky, G., Andreasen, N. K., Baceviciute, S., & Mayer, R. E. (2020). Immersive virtual reality increases liking but not learning with a science simulation and generative learning strategies promote learning in immersive virtual reality. *Journal of Educational Psychology*.

5. Parong, J., & Mayer, R. E. (2018). Learning science in immersive virtual reality. *Journal of Educational Psychology*, 110(6), 785.

Illustrations :

TITLE: THERMAL AND MECHANICAL FATIGUE BEHAVIOR OF SELECTIVE LASER MELTING MARAGING STEEL (H11 OR H13)

Topic number : 2021_036

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: I2MP Multiphysical and multiscale approach to manufacturing processes

Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés

Lab location: Châlons-en-Champagne

Lab website: <https://www.msmp.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: KANG Nan nan.kang@ensam.eu

Advisor 2: EL MANSORI Mohamed mohamed.elmansori@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Due to the high strength, high hardness and wear resistance, Maraging steel has been considered as one of popular candidates for die manufacturing. Recently, selective laser melting (SLM) process has been widely used to prepare the complex die with desirable conforming cooling system. However, the uniform equilibrium solidification condition induced heterogenous microstructure makes the SLM processed component presenting intrinsic different mechanical performance, especially, the dynamic fatigue behavior. In this project, the thermal and mechanical fatigue behavior of SLM processed maraging steel will be investigated with focus on the defects and multi-scale structure. The crack behavior at different stage will be characterized using the X-ray CT instrument for obtaining an effective fatigue prediction method.

Required background of the student:

1. Candidates should have a master degree in materials science or mechanical engineering;
2. A background in additive manufacturing, laser materials processing will be a clear advantage;
3. The Fatigue behavior investigation experience on SLM processed

component is preferred;

4. Candidates should be able to work in a multidisciplinary environment and be fluent in English (both oral and written)

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. (1) P. Kumar, R. Jayaraj, J. Suryawanshi, U.R. Satwik, J. McKinnell, U. Ramamurty, Fatigue strength of additively manufactured 316L austenitic stainless steel, Acta Mater. 199 (2020) 225-239.

2. (2) R.Branco, J.D. Costa, J.A. Martins Ferreira, C. Capela, F.V. Antunes, W. Macek, Multiaxial fatigue behaviour of maraging steel produced by selective laser melting, Mater. Design 201 (2021) 109469.

3. (3) S. Afkhami, M. Dabiri, S. Habib Alavi, T. Björk, A. Salminen, Fatigue characteristics of steels manufactured by selective laser melting, International Journal of Fatigue, 122 (2019) 72-83.

4.

5.

Illustrations :

**TITLE: MULTI-SCALED STRUCTURE DESIGN OF THERMAL CONTROLLABLE
COMPLEX CONFORMING COOLING CHANNEL SYSTEM IN SELECTIVE LASER
MELTING PROCESS**

Topic number : 2021_037

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: I2MP Multiphysical and multiscale approach to manufacturing processes

Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés

Lab location: Châlons-en-Champagne

Lab website: <https://www.msmp.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: EL MANSORI Mohamed mohamed.elmansori@ensam.eu

Advisor 2: KANG Nan nan.kang@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Selective laser melting (SLM), a laser assisted powder bed fusion technology, presents an outstanding forming ability in the component with extremely high complex morphology. Design for Additive Manufacturing (DfAM) is the art, science and skill to design for manufacturability using AM technology. Until now several works have been done in this field and realized the real component with focus on the 3D geometrical conception. But, the coupled thermal-stress field during manufacturing procedure is materials-guided and dynamic, which should be considered for the extremely complex component, such as conforming cooling system. The objective of this work is the investigation of the effect of in-situ and ex-situ heat, stress and strain on structure-material design with emphasis on thermal-stress coupling simulation. The outcomes include design guidelines for geometric conception and experimentally realization to meet the SLM processed component.

Required background of the student: 1. Candidates should have a master degree in materials science or mechanical engineering;

2. A background in additive manufacturing, laser materials processing, and topology optimization and solidification will be a clear advantage;
3. The Computer Aided Design (CAD) and Finite Elemental Analysis (FEA) experience on the thermal-coupled simulation is preferred;
4. Candidates should be able to work in a multidisciplinary environment and be fluent in English (both oral and written)

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Cao Y., Lin X., Kang N., Ma L., Wei. L, Zheng M., Yu J., Peng D.J., Huang W.D., A novel high-efficient finite element analysis method of powder bed fusion additive manufacturing Addi Manuf 46 (2021) 102187
2. Kang N., Coddet P., Ammar M.R., Liao H.L., Coddet C. Characterization of the microstructure of a selective laser melting processed Al-50Si alloy: Effect of heat treatments, Mater. Character., 130 (2017) 243-249.
3. R.Magana-Carranza, C.J.Sutcliffe, E.A. Patterson, The effect of processing parameters and material properties on residual forces induced in Laser Powder Bed Fusion (L-PBF) Addi Manuf 46 (2021) 102192.
- 4.
- 5.

Illustrations :

TITLE: MECHANICAL AND FUNCTIONAL FATIGUE BEHAVIOR OF SELECTIVE LASER MELTED NiTi SHAPE MEMORY ALLOY

Topic number : 2021_038

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: I2MP Multiphysical and multiscale approach to manufacturing processes

Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés

Lab location: Châlons-en-Champagne

Lab website: <https://www.msmp.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: EL MANSORI Mohamed mohamed.elmansori@ensam.eu

Advisor 2: El Hadrouz Mourad mourad.elhadrouz@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Shape memory alloys (SMAs) are one class of materials exhibiting functional properties, which can return to a predetermined shape when heated. To fully utilize these properties, NiTi needs to be processed into various geometries for different applications. However, conventional manufacturing methods have several limitations including the contamination of the crucible by oxygen. In addition, NiTi is a material that is difficult to process due to its compositional sensitivity and poor machinability. Recently, Selective Laser Melting (SLM) has been considered as one possible near net-shaped process to overcome these shortages. In this project, the mechanical and functional fatigue behavior of SLM processed NiTi will be investigated. The correlation analyses between fatigue life and the factors of surface roughness, porosity, and residual stress will be evaluated. The crack behavior at different stage will be characterized using the X-ray CT instrument for obtaining an effective fatigue prediction method. The synergistic effects of part densification, residual stress, and microstructure variable will be quantified to assess the fatigue performance.

Required background of the student: 1. Candidates should have a master degree in materials science or mechanical engineering;
2. A background in additive manufacturing, laser materials processing will be a clear advantage;
3. The Fatigue behavior investigation experience on SLM processed component is preferred;
4. Candidates should be able to work in a multidisciplinary environment and be fluent in English (both oral and written)

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Ayati, P., Safaei, K., Nematollahi, M., Jahadakbar, A., Yadollahi, A., Mahtabi, M., Elahinia, M. Toward understanding the effect of remelting on the additively manufactured NiTi (2021) International Journal of Advanced Manufacturing Technology, 112 (1-2), pp. 347-360.
2. Bayati, P., Jahadakbar, A., Barati, M., Nematollahi, M., Saint-Sulpice, L., Haghshenas, M., Chirani, S.A., Mahtabi, M.J., Elahinia, M. Toward low and high cycle fatigue behavior of SLM-fabricated NiTi: Considering the effect of build orientation and employing a self-heating approach (2020) International Journal of Mechanical Sciences, 185, art. no. 105878.
3. Speirs, M., Van Hooreweder, B., Van Humbeeck, J., Kruth, J.-P. Fatigue behaviour of NiTi shape memory alloy scaffolds produced by SLM, a unit cell design comparison (2017) Journal of the Mechanical Behavior of Biomedical Materials, 70, pp. 53-59
- 4.
- 5.

Illustrations :

**TITLE: RISK MANAGEMENT OF ENGINEERING PRODUCTS DRIVEN BY
ARTIFICIAL INTELLIGENCE**

Topic number : 2021_039

Field : Design, Industrialization

Subfield: Industrial Engineering

ParisTech School: Arts et Métiers

Research team:

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://lcfc.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: SIADAT Ali ali.siadat@ensam.eu

Advisor 2: PETRONIJEVIC Jelena jelena.petronijevic@ensam.eu

Advisor 3: ETIENNE Alain alain.etienne@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: With the pace of technological development, the complexity of industrial products is increasing. As a result, its risk management is becoming demanding and data-driven risk models are needed. However, the adoption of these approaches is still slow as risk management is highly dependent on experts whose knowledge is often captured in textual and descriptive form (e.g. FMEA and risk register) including at the same time the source of risk, interaction and effect. Building the model based on this form requires understanding of human perception and communication. The aim of this thesis is to bridge the gap between the conventional way in which risks are represented and the desired model-based risk management. More specifically, the research involves risk identification and analysis with the use of artificial intelligence conducted in two phases. Beginning with text-based risk knowledge, the objective is to apply deep learning techniques (e.g. natural language processing) to the identification of risk drivers. Based on this step, the risk model of the engineering product is to be developed. The thesis therefore leads towards automated risk management, which minimizes the costs and time required for this process.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Azarian, A., Siadat, A., & Martin, P. (2011). A new strategy for automotive off-board diagnosis based on a meta-heuristic engine. *Engineering Applications of Artificial Intelligence*, 24(5), 733-747.
2. Mili, A., Bassetto, S., Siadat, A., & Tollenaere, M. (2009). Dynamic risk management unveil productivity improvements. *Journal of Loss Prevention in the Process Industries*, 22(1), 25-34.
3. Petronijevic, J., Etienne, A., Siadat, A., & Bassetto, S. (2019, September). Operational Framework for Managing Risk Interactions in Product Development Projects. In 2019 International Conference on Industrial Engineering and Systems Management (IESM) (pp. 1-6). IEEE.
4. Petronijevic, J., Etienne, A., & Dantan, J. Y. (2019). Human factors under uncertainty: A manufacturing systems design using simulation-optimisation approach. *Computers & Industrial Engineering*, 127, 665-676.
5. Shah, L. A., Etienne, A., Siadat, A., & Vernadat, F. (2016). Decision-making in the manufacturing environment using a value-risk graph. *Journal of Intelligent Manufacturing*, 27(3), 617-630.

Illustrations :

**TITLE: OPTIMIZED SET-UP TO CHARACTERIZE THE CONTACT FATIGUE
DAMAGE OF MATERIAL WITH GRADIENT PROPERTIES**

Topic number : 2021_040

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: Mechanics, Materials and Surfaces

<https://www.msmp.eu/equipes/mms/>

Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés

Lab location: Aix-en-Provence

Lab website: <https://www.msmp.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: Goulmy Jean-Patrick jean-patrick.goulmy@ensam.eu

Advisor 2: barrallier laurent laurent.barrallier@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Surface treatments (coating, shot peening, sandblasting, nitriding) aim to modify the properties (chemical, mechanical, ...) on the surface or subsurface of a part in order to improve its initial characteristics by creating a microstructure gradient associated with a residual mechanical field (Fabre et al. 2013; Klotz et al. 2018). This type of process is used in many industrial fields (aeronautics, automotive, ...), on very diverse critical parts (turbine disks, gears, connecting rods...) (Gerin et al. 2017). A fine characterization of the impact of surface treatments on the improvement of part performance is paramount for safety issues, optimization of their shape and process parameters. This project aims to contribute to the understanding of damage mechanisms observed during contact fatigue. It will develop new experiments to characterize the integrity of surfaces with gradients in properties during repeated cycles between a sphere and the part. Damage monitoring will be performed using different characterization techniques (DIC, SEM, EBSD, XRD) (Stinville et al. 2016). Particular attention will be paid to define a representative volume of macroscopic damage with the different characterization techniques used. To the experimental tests, a modeling of the test will be coupled in

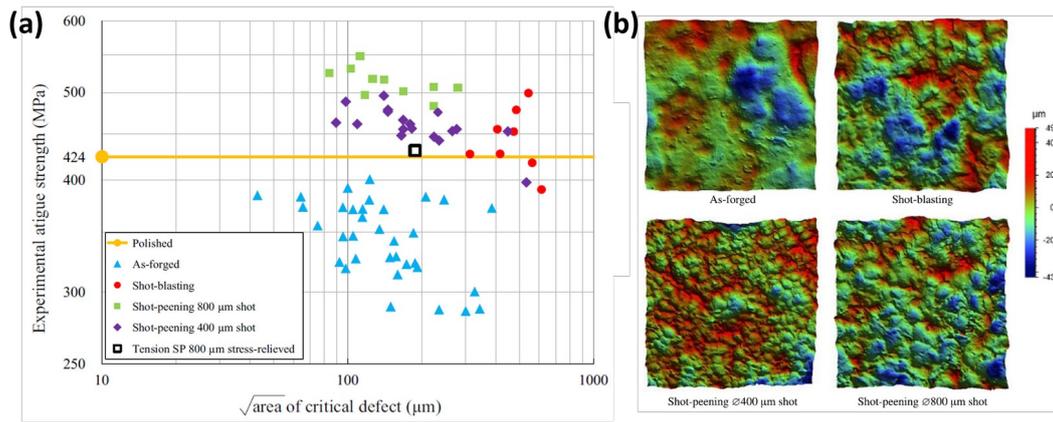
order to better understand the mechanisms at the origin of the damage of the studied parts.

Required background of the student: material and mechanics

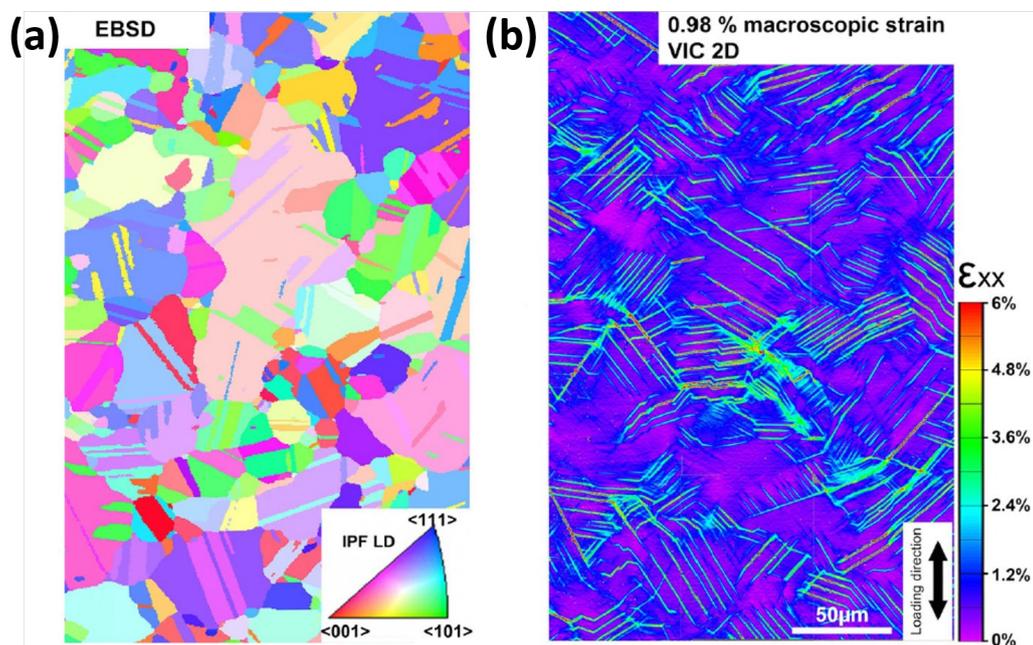
A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Fabre, A., H.P. Evans, L. Barrallier, K.J. Sharif, and M. Desvignes. 2013. "Prediction of Microgeometrical Influences on Micropitting Fatigue Damage on 32CrMoV13 Steel." *Tribology International* 59 (March): 129-40. <https://doi.org/10.1016/j.triboint.2012.07.018>.
2. Gerin, B., E. Pessard, F. Morel, and C. Verdu. 2017. "Influence of Surface Integrity on the Fatigue Behaviour of a Hot-Forged and Shot-Peened C70 Steel Component." *Materials Science and Engineering: A* 686: 121-33. <https://doi.org/10.1016/j.msea.2017.01.041>.
3. Klotz, T., D. Delbergue, P. Bocher, M. Lévesque, and M. Brochu. 2018. "Surface Characteristics and Fatigue Behavior of Shot Peened Inconel 718." *International Journal of Fatigue* 110 (May): 10-21. <https://doi.org/10.1016/j.ijfatigue.2018.01.005>.
4. Stinville, J.C., P. Echlin, Damien Texier, F. Bridier, P. Bocher, and T.M. Pollock. 2016. "Sub-Grain Scale Digital Image Correlation by Electron Microscopy for Polycrystalline Materials during Elastic and Plastic Deformation." *Experimental Mechanics* 56 (2): 197-216. <https://doi.org/10.1007/s11340-015-0083-4>.
- 5.

Illustrations :



Examples of surface treatments influence. a) Kitagawa diagram of the fatigue tests, b) Close-ups of surface scans of the specimens after different surface treatments (Gerin et al. 2017)



Examples of coupling of characterization techniques to characterize material behavior. a) EBSD measurements, b) strain field xx from DIC measurements (Stinville, 2016)

TITLE: HYDRODYNAMICS OF ELECTRONS AND PHONONS IN BULK SEMIMETALS

Topic number : 2021_041

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield: Condensed matter physics

ParisTech School: ESPCI Paris - PSL

Research team: Quantum matter group

Research lab: LPEM - Laboratoire Physique et d'études des matériaux

Lab location: Paris

Lab website: <https://www.lpem.espci.fr/spip.php?rubrique4>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Behnia Kamran kamran.behnia@gmail.com

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Heat travels in solids thanks to phonons and mobile electrons. The rate of collisions that they suffer along their trajectory sets the amplitude of this flow. These collisions often lead to a loss of momentum. This diffusive regime of heat transport is rather well understood. The so-called hydrodynamic regime emerges when most collisions conserve momentum. This exotic situation occurs in bulk semimetals like bismuth, graphite or antimony. Heat transport in this regime is poorly understood. The subject of this research is an experimental investigation of this regime. We intend to determine the diagonal and off-diagonal thermal and thermoelectric transport coefficients of bulk semi-metals in a wide range of temperature and magnetic field. The data will be scrutinized in order to detect new signature of quasi-particle hydrodynamic flow near the diffusive-ballistic crossover.

Required background of the student: Background in Condensed matter physics. Basic knowledge of the quantum theory of solids

A list of 5 (max.) representative publications of the group: (Related to the research topic)

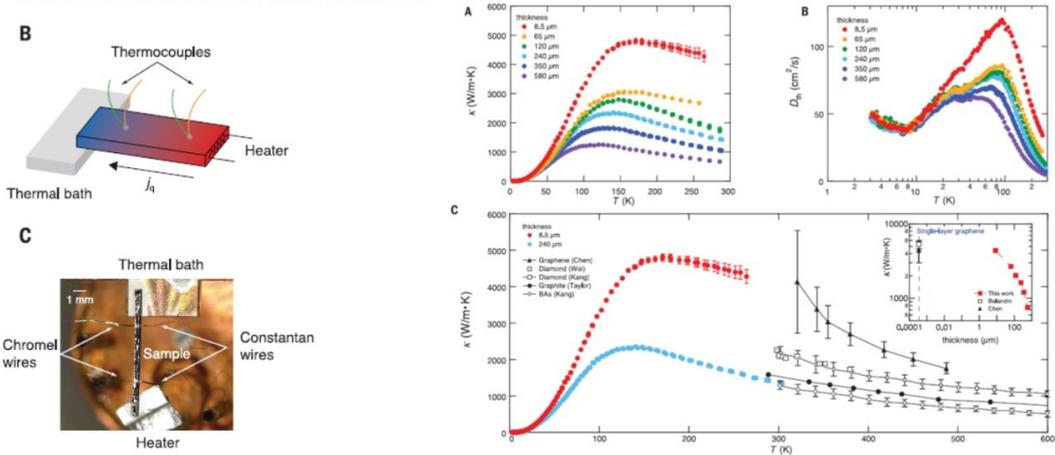
1. Y. Machida, N. Matsumoto, T. Isono, and K. Behnia, “Phonon hydrodynamics and ultrahigh-room-temperature thermal conductivity in thin graphite”, *Science* 367, 309 (2020)
2. A Jaoui, B Fauqué, K Behnia, “Thermal resistivity and hydrodynamics of the degenerate electron fluid in antimony”, *Nature Communications* 12: 195 (2021)
3. A. Jaoui, A. Gourgout, G.l Seyfarth, A. Subedi, T.Lorenz, B. Fauqué, K. Behnia, Formation of an electron-phonon bi-fluid in bulk antimony, arXiv:2105.08408 (2021)
4. L.Xu, X. Li, X. Lu, C. Collignon, H. Fu, B. Fauqué, B. Yan, Z. Zhu, K. Behnia, Finite-temperature violation of the anomalous transverse Wiedemann-Franz law, *Science Advances* 6 : eaaz3522 (2020)
5. X. Li, B. Fauqué, Z. Zhu, and K. Behnia, Phonon thermal Hall effect in strontium titanate, *Phys. Rev. Lett.* 124, 105901 (2020)

Illustrations :

THERMAL CONDUCTIVITY

Phonon hydrodynamics and ultrahigh-temperature thermal conductivity in thin graphite

Yo Machida^{1*}, Nayuta Matsumoto¹, Takayuki Isono¹, Kamran Behnia^{2*}



Formation of an electron-phonon bi-fluid in bulk antimony

Alexandre Jaoui,^{1,2,*} Adrien Gourgout,² Gabriel Seyfarth,³ Alaska Subedi,^{4,5} Thomas Lorenz,⁶ Benoît Fauqué,¹ and Kamran Behnia^{2,†}

¹JEIP, USR 3573 CNRS, Collège de France, PSL Research University, 11, Place Marcelin Berthelot, 75231 Paris Cedex 05, France.

²Laboratoire de Physique et d'Étude des Matériaux

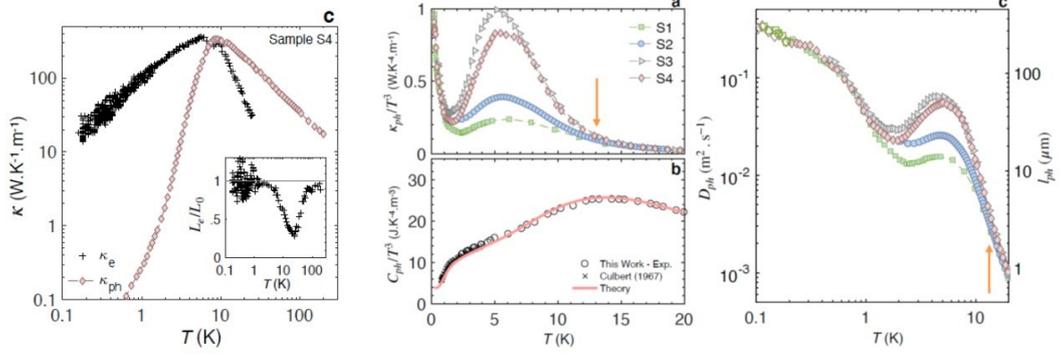
(ESPCI - CNRS - Sorbonne Université), PSL Research University, 75005 Paris, France.

³LNCMI-EMFL, CNRS, Univ. Grenoble Alpes, INSA-T, UPS, Grenoble, France.

⁴CPHT, CNRS, Ecole Polytechnique, IP Paris, F-91128 Palaiseau, France

⁵Collège de France, 11 Place Marcelin Berthelot, 75005 Paris, France

⁶II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany



**TITLE: NANOPARTICLES, NANOWIRE, AND NANOSHEETS OF HYBRID
PEROVSKITE HALIDES: FROM SYNTHESIS TO APPLICATIONS**

Topic number : 2021_042

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes, Material science, Mechanics and Fluids, Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team: Micro & Nano Characterization Group

<http://optoelec.lpem.espci.fr>

Research lab: LPEM - Laboratoire Physique et d'études des matériaux

Lab location: Paris

Lab website: <https://www.lpem.espci.fr>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Chen Zhuoying zhuoying.chen@espci.fr

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Advisor 3: Monteverde Miguel miguel.monteverde@u-psud.fr

Advisor 4:

Short description of possible research topics for a PhD: Hybrid organic-inorganic perovskite halides represent a class of emerging optoelectronic materials which shows a striking progress in terms of solar cell power conversion efficiency in the last few years. Indeed, while most of these established progresses are based on bulk or thin film perovskites, nanostructured hybrid perovskite systems, such as those in the form of nanoparticle (quantum dots), nanowire, and nanosheets, may offer new advantages in terms of material compositional (doping) design, structural (phase) and device stability, and flexibility to fine-tune device architectures. Nevertheless, many fundamental properties (e.g. spintronic properties) of nanostructured perovskites are still unexplored. In terms of optical properties, advanced microscopy techniques are required to investigate nanowires and nanosheets of perovskites, the maximal sample size of which is only a few micrometers. The spatial resolution requirements are even more demanding for nanoparticles. This thesis program will therefore focus on the development of nanostructured hybrid perovskites, such as quantum dots, nanowires and nanosheets. Three main aspects will be involved in this 48-month thesis:

(1) Besides the well-established lead-containing model systems (e.g. ACS Nano, 2016, 10, 3536-3542), this project aims to investigate new synthesis of lead-free perovskites (or double-perovskites) in terms of quantum dots, nanowires or nanosheets (examples see Energy Environ. Sci., 2020, 13, 2363); (2) The photovoltaic properties of the perovskite nanomaterials developed in (1) will be explored; (3) In-depth fundamental investigation on the (spin-dependent) optical properties of the developed nano-objects. The low temperature micro-fluorescence microscope (developed in LPS) will allow the application of a magnetic field of up to 1.5 Tesla to investigate for the first time the spin-dependent optical properties of these nanostructure perovskites. Such experiments will also allow to investigate the properties of triplet excitons in perovskite samples to understand how their properties are affected by confinement effects. The control of the properties of triplet excitons is important for multiple carrier generation through singlet fission sensitization and for spintronic applications of this class of materials.

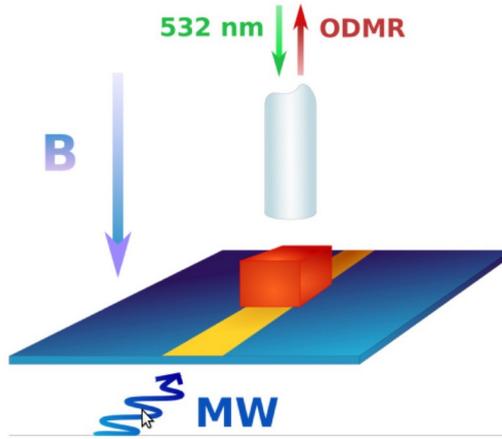
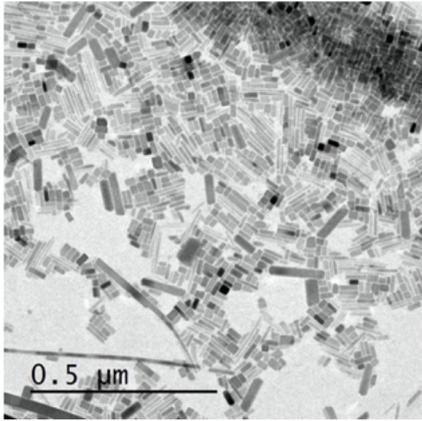
Figure caption: (Left) TEM image of the CsPbBr₃ nanosheets fabricated in our laboratory; (Right) Sketch of an optically detected magnetic resonance experiment using a broadband stripline from our recent work (ref. no in the list of representative publications) .

Required background of the student: Master Degree on physics, or material science, or applied physics. Good speaking & writing skills in English. Passionate in scientific experiments.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. "TiO₂ Nanocolumn Arrays for More Efficient and Stable Perovskite Solar Cells", ACS Applied Materials & Interfaces, 12, 5979-5989 (2020)
2. "Enhancing the Efficiency and Stability of Triple-Cation Perovskite Solar Cells by Eliminating Excess PbI₂ from the Perovskite/Hole Transport Layer Interface", Z. Hu et al., ACS Applied Materials & Interfaces 12 (49), 54824-54832 (2020)
3. "Spin Fine Structure Reveals Biexciton Geometry in an Organic Semiconductor", K.M. Yunusova et al. Phys. Rev. Lett. 125, 097402 (2020)
- 4.
- 5.

Illustrations :



**TITLE: INNOVATIVE DESIGN FOR ADDITIVE MANUFACTURING THROUGH
KNOWLEDGE MANAGEMENT AND TRIZ**

Topic number : 2021_043

Field : Design, Industrialization

Subfield:

ParisTech School: Arts et Métiers

Research team:

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://lcfc.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: SIADAT Ali ali.siadat@ensam.eu

Advisor 2: Hassan Alaa alaa.hassan@univ-lorraine.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Additive manufacturing (AM) offers significant opportunities for product innovation in many fields. The Design for Additive Manufacturing (DfAM) approach could be considered as a guideline for the design team in the early phase of the product development process. However, AM is becoming a data-intensive activity and the design of a new product can be facilitated by using previous knowledge from successful projects and the literature. This relevant knowledge is not easy to find or reuse. The theory of inventive problem solving methodology (TRIZ) is a well-established accelerator to support problem solving by linking specific engineering problems and solutions to general patterns and laws. TRIZ method can be coupled with a well-structured knowledge base (KB) in order to build a DfAM support system that helps the engineers in finding the most suitable rules and constraint-solving principles to fully exploit the potential of AM. The objectives of this PhD proposal are 1) To develop a KB in order to capture and structure the DfAM principles and knowledge Web Ontology Language (OWL) or System Modelling Language (SysML) could be used to develop this KB, and 2) To integrate the TRIZ inventive principles into the KB in order to build DfAM support system. Artificial Intelligence could be used to map the problem space to the solution space and to retrieve the relevant information.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. T. J. Hagedorn, S. Krishnamurty, and I. R. Grosse, "A Knowledge-Based Method for Innovative Design for Additive Manufacturing Supported by Modular Ontologies," *J. Comput. Inf. Sci. Eng.*, vol. 18, no. 2, pp. 1-12, 2018.
2. S. Kadkhoda-Ahmadi, A. Hassan, and E. Asadollahi-Yazdi, "Process and resource selection methodology in design for additive manufacturing," *Int. J. Adv. Manuf. Technol.*, vol. 104, no. 5-8, pp. 2013-2029, 2019.
3. U. K. uz Zaman, M. Rivette, A. Siadat, and S. M. Mousavi, "Integrated product-process design: Material and manufacturing process selection for additive manufacturing using multi-criteria decision making," *Robot. Comput. Integr. Manuf.*, vol. 51, no. December 2017, pp. 169-180, 2018.
4. N. Kretschmar and S. Chekurov, "The applicability of the 40 TRIZ principles in design for additive manufacturing," *Ann. DAAAM Proc. Int. DAAAM Symp.*, vol. 29, no. 1, pp. 888-893, 2018.
5. L. Liu, Y. Li, Y. Xiong, and D. Cavallucci, "A new function-based patent knowledge retrieval tool for conceptual design of innovative products," *Comput. Ind.*, vol. 115, p. 103154, 2020.

Illustrations :

TITLE: FLUID DYNAMIC UNSTEADINESS IN MULTIPHASE TURBOMACHINERY

Topic number : 2021_044

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: Rotating Flows <https://lmfl.cnrs.fr/en/research/th2-rotating-flows/>

Research lab: LMFL - Laboratoire de mécanique des fluides de Lille

Lab location: Lille

Lab website: <https://lmfl.cnrs.fr/en/home/>

Contact point for this topic: Arts et Métiers

Advisor 1: Dazin Antoine antoine.dazin@ensam.eu

Advisor 2: Romano Francesco francesco.romano@ensam.eu

Advisor 3:

Advisor 4:

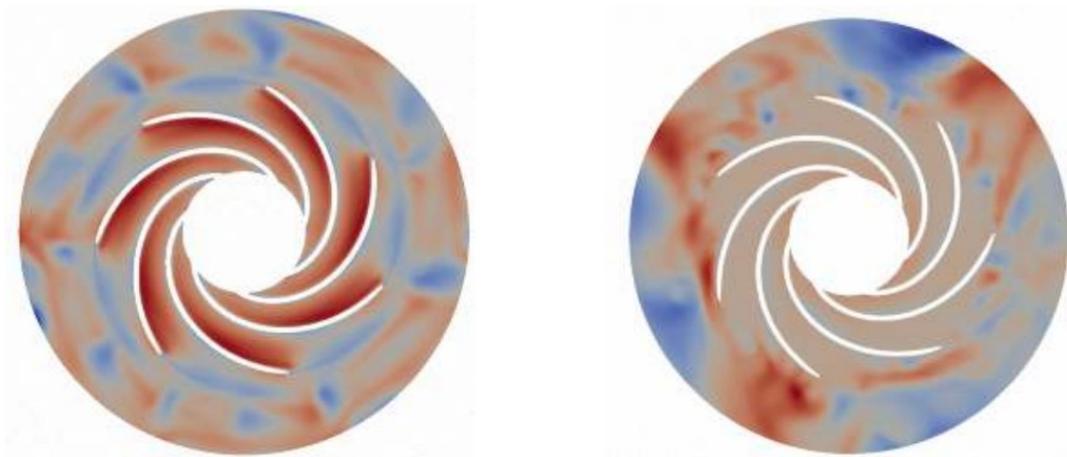
Short description of possible research topics for a PhD: Rotating flows in centrifugal pumps operating at partial flow rates could experience unsteady phenomena (boundary layer detachment, rotating stall ...) leading to a decay of their operational performance (see figures below). The presence of static and rotating parts, with a typically complex geometry, induces a complex base flow and makes difficult to predict and characterize these flow unsteadiness. Such phenomena become even more complex when a two-phase flow is considered. In this project an air-water multiphase flow is considered, with the aim to investigate how the interplay between the two phases participating in the turbomachinery flow changes the nature of the unsteadiness and affects the performances. Both, numerical simulations and experiments will be carried out in this project.

Required background of the student: Master of Science in Fluid Mechanics or equivalent

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Dazin, A., Cavazzini, G., Pavesi, G. et al. High-speed stereoscopic PIV study of rotating instabilities in a radial vaneless diffuser. *Exp Fluids* 51, 83–93 (2011). <https://doi.org/10.1007/s00348-010-1030-x>
2. Y. Heng, A. Dazin, M. N. Ouarzazi, and Q. Si. Experimental study and theoretical analysis of the rotating stall in a vaneless diffuser of radial flow pump. *IOP Conference Series : Earth and Environmental Science*, 49 :032006, 2016
3. Y. Heng, A. Dazin, M. N. Ouarzazi, and Q. Si. A study of rotating stall in a vaneless diffuser of radial flow pump. *J. Hyd. Res.*, 56 :494–504, 2018.
4. Liao, M.; Si, Q.; Fan, M.; Wang, P.; Liu, Z.; Yuan, S.; Cui, Q.; Bois, G. Experimental Study on Flow Behavior of Unshrouded Impeller Centrifugal Pumps under Inlet Air Entrainment Condition. *Int. J. Turbomach. Propuls. Power* 2021, 6, 31. <https://doi.org/10.3390/ijtp6030031>
- 5.

Illustrations :



TITLE: DEVELOPMENT AND OPTIMIZATION OF TOOL DESIGN/GEOMETRY FOR DRILLING AEROSPACE ALLOYS USING LCO₂ AND OTHER ENVIRONMENTALLY FRIENDLY METALWORKING FLUIDS

Topic number : 2021_045

Field : Energy, Processes, Material science, Mechanics and Fluids

Subfield: Mechanical Engineering, Manufacturing Processes, Fluid dynamics

ParisTech School: Arts et Métiers

Research team: High Speed Machining

Research lab: LABOMAP - Laboratoire Bourguignon des matériaux et procédés

Lab location: Cluny

Lab website: <http://labomap.ensam.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: OUTEIRO Jose jose.outeiro@ensam.eu

Advisor 2: Deligant Michael michael.deligant@ensam.eu

Advisor 3: Rossi Frédéric frederic.rossi@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: Because 36% of all the machine time is spent performing drilling operations, the use of high-performance drilling tools can reduce the drilling time and cost. Unfortunately, practically all drills used today in industry have problems with excessive wear/low tool life due to their suboptimal designs including the particularities of coolant supply. Recent drilling tests using a newly designed drill with peripheral coolant holes (located at the corners region), conducted at an automotive shop floor, have shown an increase of tool life up to 8 times when compared to the traditional drill. Further improvement of the performance of the proposed design are needed to achieve its full potential.

The main objective of this Ph.D proposal is to significantly increase tool life and quality of the drilled holes (both surface roughness and shape) in drilling difficult-to-cut aerospace alloys using liquid CO₂ (LCO₂) and other environmentally friendly metalworking fluids through the optimization of the drill design/geometry. To achieve this objective, drilling simulations using different numerical approaches (including Coupled Eulerian-Lagrangian) and considering fluid flow will be

developed. Experimental drilling tests of aerospace alloys will be conducted to validate such model. Both simulated and experimental data will be used in artificial intelligence and optimization algorithms to find the optimal tool geometry parameters.

Required background of the student: We are looking for a highly motivated candidate with a Master's degree in Mechanical Engineering. A knowledge of the finite element method, fluid mechanics and heat transfer will be considered a strong merit. Other desirable knowledge/experience but not essential includes manufacturing processes.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. X. Xu, J.C. Outeiro, J. Zhang, B. Xu, W. Zhao, "Machining simulation of Ti6Al4V using coupled Eulerian-Lagrangian approach and a constitutive model considering the state of stress", *Simulation Modelling Practice and Theory*, Vol. 110, pp. 102312, 2021.
2. A. Attanasio, E. Ceretti, J.C. Outeiro, G. Poulachon, Numerical Simulation of Tool Wear in Drilling Inconel 718 under Flood and Cryogenic Cooling Conditions, *Wear*, Vol. 458-459, pp. 203403, 2020.
3. J.C. Outeiro, P. Lenoir, A. Bosselut, "Thermo-Mechanical Effects in Drilling Using Metal Working Fluids and Cryogenic Cooling and their Impact in Tool Performance", *Production Engineering, Research and Development*, Springer, Vol. 9, pp 551-562, 2015.
4. M. Deligant, M. Specklin, and S. Khelladi. A naturally anti-diffusive compressible two phases kapila model with boundedness preservation coupled to a high order finite volume solver. *Computers and Fluids*, 114, 2015.
5. M. Specklin, M. Deligant, S. Porcheron, M. Wagner, F. Bakir Experimental study and modelling of a high-pressure ratio liquid piston compressor. HEFAT 2019, Wicklow, Ireland.

Illustrations :

**TITLE: INTEGRATED VIRTUAL SIMULATION AND VISUALIZATION OF
MANUFACTURING PROCESSES USING NUMERICAL SIMULATION AND
AUGMENTED REALITY**

Topic number : 2021_046

Field : Information and Communication Science and Technology,
Material science, Mechanics and Fluids

Subfield: Manufacturing Processes, Augmented Reality, Virtual Reality
and Mixed Reality

ParisTech School: Arts et Métiers

Research team: High Speed Machining

Research lab: LABOMAP - Laboratoire Bourguignon des matériaux et
procédés

Lab location: Cluny

Lab website: <http://labomap.ensam.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: OUTEIRO Jose jose.outeiro@ensam.eu

Advisor 2: Chardonnet Jean-Rémy jean-remy.chardonnet@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The 4th industrial revolution (Industry 4.0) is characterized by a fusion of technologies which erases the border between the real and virtual worlds. We are assisting to an exponential penetration of the digital technologies into the manufacturing industry. Nowadays, numerical simulation is often used for predicting manufacturing processes performance and part quality, aiming for optimizing and reducing their cost. To completely merging these two worlds and take advantage of both experimental data acquired by sensors connected to the process and simulation data from robust physical models, the simultaneous visualization of both data in an immersive environment is necessary. The objective of this Ph.D proposal is twofold. First, to develop robust physical models of real machining operations (turning, milling, and drilling) using recent advances on numerical simulation. Second, to develop augmented and virtual reality applications allowing simultaneous adaptive and intuitive real-time visualization of simulation and experimental data during a real machining operation.

Required background of the student: We are looking for a highly motivated candidate with a Master's degree in Mechanical Engineering or Computer Science. A knowledge of the finite element method and C++/C# programming languages will be considered a strong merit. Other desirable knowledge/experience but not essential includes manufacturing processes and real-time application development and mixed reality.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. X. Xu, J.C. Outeiro, J. Zhang, B. Xu, W. Zhao, "Machining simulation of Ti6Al4V using coupled Eulerian-Lagrangian approach and a constitutive model considering the state of stress", *Simulation Modelling Practice and Theory*, Vol. 110, pp. 102312, 2021.
2. A. Attanasio, E. Ceretti, J.C. Outeiro, G. Poulachon, Numerical Simulation of Tool Wear in Drilling Inconel 718 under Flood and Cryogenic Cooling Conditions, *Wear*, Vol. 458-459, pp. 203403, 2020.
3. M. Ghinea, D. Frunza, J.-R. Chardonnet, F. Merienne, and A. Kemeny, "Perception of Absolute Distances within Different Visualization Systems: HMD and CAVE," in 5th International Conference on Augmented Reality, Virtual Reality, and Computer Graphics, Otranto, Italy, Jun. 2018, vol. 10850, pp. 148-161.
4. J.-R. Chardonnet, G. Fromentin, and J. Outeiro, "Augmented reality as an aid for the use of machine tools," *Research and Science Today*, vol. Supplement No. 2, pp. 25-31, Oct. 2017.
5. F. Ababsa, J. He, and J.-R. Chardonnet, "Combining HoloLens and Leap-Motion for Free Hand-Based 3D Interaction in MR Environments," in 7th International Conference on Augmented Reality, Virtual Reality, and Computer Graphics, Online, Sep. 2020, vol. 12242, pp. 315-327.

Illustrations :

TITLE:ENVIRONMENTAL BEHAVIOR OF NOVEL MULTI-PRINCIPAL ELEMENT ALLOYS CONTAINING MOLYBDENUM

Topic number : 2021_047

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team:Physical Chemistry of Surfaces team

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website:<https://www.ircp.cnrs.fr/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: MERCIER Dimitri dimitri.mercier@chimieparistech.psl.eu

Advisor 2: Marcus Philippe philippe.marcus@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Multi principal element alloys (MPEA), also called high entropy alloys (HEA), is a new class of metallic alloys (first elaborated in 2004) having a great interest as engineering alloys. Their mechanical properties have been widely studied and currently a detailed approach of the design of these alloys (microstructure, composition) allows elaborating specific alloys with excellent mechanical properties, that may outperform those of conventional alloys. In contrast to the mechanical properties, the surface reactivity of these materials, and particularly their corrosion resistance, has only been slightly studied. Different studies have shown that the original "Cantor" alloy does not provide good corrosion resistance, due to its high (equimolar) Mn content. Combining what we know of the origin of the corrosion resistance of Ni and Fe-based stainless alloys, and applying a thermodynamic approach for the composition optimization, our research group was able to design and synthesize two new single phase HEA/MPEA alloys containing molybdenum, which show excellent corrosion resistance.

The purpose of this research program is to develop a deep understanding of the surface reactivity and corrosion behavior (passivity, passivity breakdown, localized corrosion resistance) of MPEA/HEA alloys with high Cr and Mo contents and explore a range of compositions that can be

maintained as single fcc phase after rapid cooling or contain Mo-rich secondary phases. The surface oxides (native and passive films), which are key factors for the corrosion resistance, will be characterized for the different alloy compositions by advanced surface analysis techniques, including X-ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Spectrometry (ToF-SIMS). A focus will be placed on the stability and the growth mechanisms of these layers using an original approach developed by our research group, using in situ isotopic labelling ($^{18}\text{O}_2$).

Required background of the student: Corrosion Science, Surface Science, Materials Science, Electrochemistry

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Study of the surface oxides and corrosion behaviour of an equiatomic CoCrFeMnNi high entropy alloy by XPS and ToF-SIMS, Luntao Wang, Dimitri Mercier, Sandrine Zanna, Antoine Seyeux, Mathilde Laurent-Brocq, Loïc Perrière, Ivan Guillot, Philippe Marcus, Corrosion Science, 167,2020, 108507
2. Insight on passivity of high entropy alloys: Thermal stability and ion transport mechanisms in the passive oxide film on CoCrFeMnNi surfaces, Luntao Wang, Antoine Seyeux, Loïc Perrière, Dimitri, Mercier, Vincent Maurice, Philippe Marcus, Corrosion Science, 188,2021, 109540
3. XPS and ToF-SIMS Investigation of Native Oxides and Passive Films Formed on Nickel Alloys Containing Chromium and Molybdenum, Zuo Cheng Wang, Charly Carrière, Antoine Seyeux, Sandrine Zanna, Dimitri Mercier, Philippe Marcus, Journal of the Electrochemical Society, 168, 2021, 041503
4. Design, processing and passivation behavior of new highly corrosion resistant Cr-Fe-Co-Ni-Mo multi component alloys, Xueying Wang, Dimitri Mercier, Yolaine Danard, Thomas Rieger, Loïc Perrière, Mathilde Laurent-Brocq, Ivan Guillot, Vincent Maurice, Philippe Marcus, Acta Materialia, submitted
- 5.

Illustrations :

TITLE: SINGLE AND MULTIPLE CAVITATING BUBBLES NEAR A WALL

Topic number : 2021_048

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: Rotating Flows <https://lmfl.cnrs.fr/en/research/th2-rotating-flows/>

Research lab: LMFL - Laboratoire de mécanique des fluides de Lille

Lab location: Lille

Lab website: <https://lmfl.cnrs.fr/en/home/>

Contact point for this topic: Arts et Métiers

Advisor 1: Romano Francesco francesco.romano@ensam.eu

Advisor 2: Coutier-Delgosha Olivier olivier.coutier-delgosha@ensam.eu

Advisor 3: Dazin Antoine antoine.dazin@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: Cavitation is among the most studied phenomena in classic and modern fluid mechanics. It strongly affects the performance of engineering designs such as hydraulic turbomachineries and pumps and it encompasses a complex physics that is best investigated studying the behaviour of a cavitating bubble near a wall. In this project aim at unravelling the role of temperature, pressure waves, microjets and bubble composition in cavitation erosion. Promising predictive tools are represented by modern CFD solvers, extensively tested against experiments for a relevant collapsing bubble configuration, see figures below. The experimental activity is carried out at VirginiaTech. The numerical simulations will be performed at Art et Metiers, Lille. Several regimes will be investigated to understand the impact of several parameters like the composition of the bubble, the temperature and pressure conditions at which the cavitation occurs, as well as the properties of the wall.

Required background of the student: Master of Science in Fluid Mechanics or equivalent

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Chebli, R., Audebert, B., Zhang, G., Coutier-Delgosha, O. Influence of the turbulence modeling on the simulation of unsteady cavitating flows.

Computers and Fluids, 2021, 221, 104898

2. Zhang, X.-L., Ge, M.-M., Zhang, G.-J., Coutier-Delgosha, O.

Compressible effects modeling for turbulent cavitating flow in a small venturi channel: An empirical turbulent eddy viscosity correction.

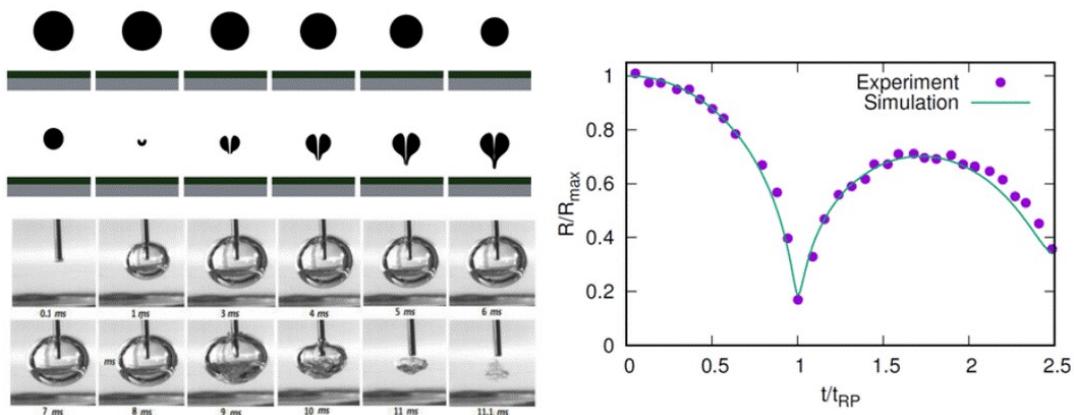
Physics of Fluids, 2021, 33(3), 035148

3. Hamdi, M., Coutier-Delgosha, O., & Baudoin, M. (2018). Measurements of the temperature variations during the growth and collapse of cavitation bubbles. Proceedings of the 10th International Symposium on Cavitation (CAV2018), ASME. <https://doi.org/10.1115/1.861851>

4.

5.

Illustrations :



TITLE: A MECHANO-CHEMICAL MODEL OF HYDRA MORPHOGENESIS

Topic number : 2021_049

Field : Biology, Biophysics and Biochemistry, Material science, Mechanics and Fluids, Physics, Optics

Subfield: Theoretical biophysics

ParisTech School: ESPCI Paris - PSL

Research team: Soft Matter, Microfluidics and Biology

Research lab: Physique et mécanique des Milieux Hétérogènes

Lab location: Paris

Lab website: <https://www.pmmh.espci.fr/>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Marcq Philippe philippe.marcq@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Biological pattern formation refers to the spontaneous emergence of order in an originally homogeneous organism. Following Alan Turing's seminal work, biological pattern formation has long been explained by the reaction and diffusion of morphogens. However, fully characterized examples of Turing patterns in biology remain scarce. It is becoming clear that many models of pattern formation need to be extended to include two major aspects of living organisms that have been largely overlooked until now: first their complex shape and dynamics; and perhaps more importantly the interactions between biochemistry and mechanical cues, the topic of the growing field of mechanobiology.

Hydra vulgaris is a freshwater polyp famous for its regenerative capacities. Virtually any tissue piece amputated from an adult Hydra or even re-aggregated cells can regenerate into a viable organism and do so through a de novo axis definition. We propose to use the regeneration of Hydra vulgaris as a model system for biological pattern formation. Hydra possesses a single organizing axis going from head to foot and the whole animal is made of two cellular monolayers. Furthermore, Hydra tissue pieces always start their regeneration by folding back into a sphere. Therefore, the problem studied in this project is that of the patterning of

an active spherical shell to define a single organizing axis.

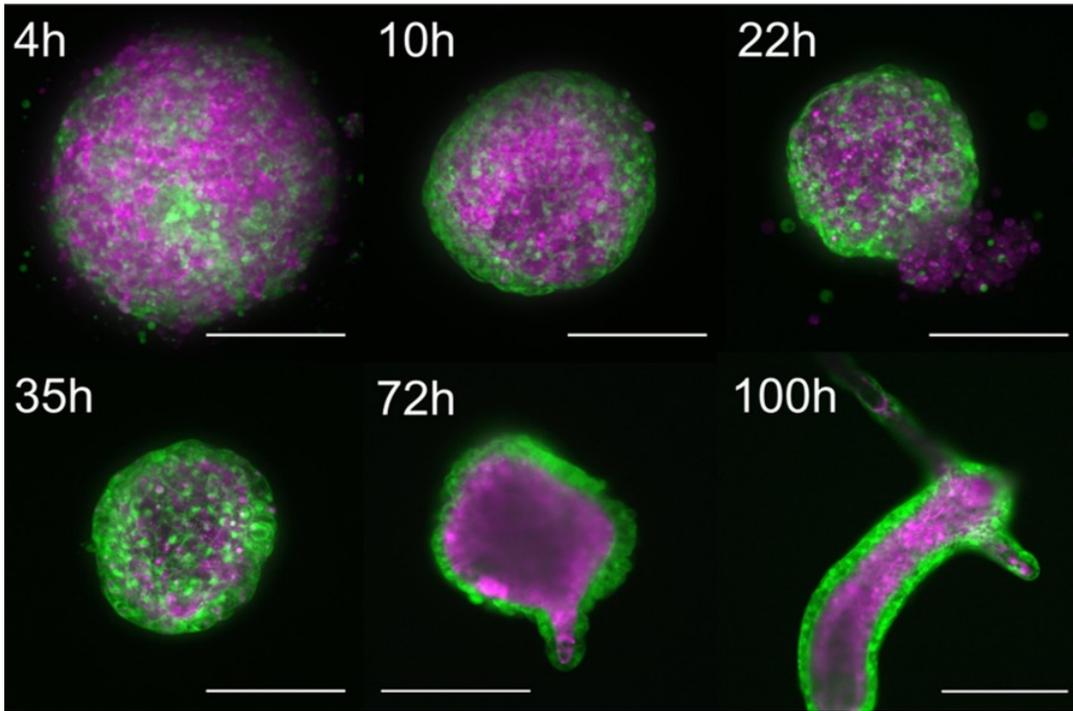
Concretely, the objective of this interdisciplinary project is to uncover how mechanical determinants interact with morphogen dynamics, and to inform a mechano-chemical model acting on an evolving shape. The techniques employed by the candidate will be both theoretical and numerical, including finite element simulations. The project will take place in close collaboration with Dr. Cochet-Escartin, an experimental biophysicist at Institut Lumière Matière in Lyon, France. Developments of the model will suggest original perturbation experiments, either biochemical or mechanical, for cross-validation; conversely experimental observations will directly inform these theoretical developments.

Required background of the student: Physics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Turing, A. M. The Chemical Basis of Morphogenesis. *Philos. Trans. R. Soc. B Biol. Sci.* 237, 37-72 (1952)
2. Howard, J., Grill, S. W. & Bois, J. S. Turing's next steps: The mechanochemical basis of morphogenesis. *Nature Reviews Molecular Cell Biology* 12, 400-406 (2011)
3. Chiou, K. & Collins, E.-M. S. Why we need mechanics to understand animal regeneration. *Dev. Biol.* 433, 155-165 (2018).
4. Cochet-Escartin, O., Locke, T. T., Shi, W. H., Steele, R. E. & Collins, E.-M. S. Physical Mechanisms Driving Cell Sorting in Hydra. *Biophys. J.* 113, 2827-2841 (2017)
5. Cochet-Escartin, O., Ranft, J., Silberzan, P. & Marcq, P. Border forces and friction control epithelial closure dynamics. *Biophys. J.* 106, (2014)

Illustrations :



TITLE:DECIPHERING THE PERIOFACTOME OF A PEST SPECIES

Topic number : 2021_050

Field : Biology, Biophysics and Biochemistry, Life Science and Engineering for Agriculture, Food and the Environment

Subfield:

ParisTech School: AgroParisTech

Research team:Équipe Chimioréception et Adaptation "CreA"
<https://iees-paris.fr/equipes/chimiorception-et-adaptation/>

Research lab: IEES Paris - Institut d'Ecologie et des Sciences de l'Environnement de Paris

Lab location: Paris

Lab website:<https://iees-paris.fr/>

Contact point for this topic: AgroParisTech

Advisor 1: Maïbèche Martine martine.maibeche@sorbonne-universite.fr

Advisor 2: Chertemps Thomas thomas.chertemps@sorbonne-universite.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Noctuid moths of the genus *Spodoptera* are invasive crop pests with remarkable capacities of adaptation, linked to a fine modulation of their olfactory-dependent behaviors. Great progress has been made in the understanding of their chemical ecology in our lab, using *Spodoptera littoralis* as a model. Its repertoire of olfactory genes has been established through transcriptomic approaches, allowing identifying their olfactory receptors (ORs) but also of some molecular actors of the "periofactome", i.e. genes acting upstream and downstream of the ORs and potentially involved in the transport and degradation of odorant molecules (OBPs, ODEs...). Several *S. littoralis* ORs were successfully deorphanized but the function of the periofactome genes remains to be established. Moreover, recent studies suggested that the behavioral plasticity observed in these animals (after mating or pheromone/odorant preexposure) seems to involve a modulation of expression of their periofactome genes. The goal of our project will be thus to decipher the periofactome of *S. littoralis* by identifying the complete repertoire of the genes involved (transcriptomic analysis of olfactory organs, RNAseq) and

to get insights into their function in olfaction and behavioural plasticity using a combination of in vivo (RNAi, electrophysiology and behavior) and in vitro approaches (heterologous expression systems and biochemistry).

Required background of the student: Molecular biology, biochemistry and bioinformatic skills would be appreciated. A taste for behavioral analyses would be an asset.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Gonzalez D., Rihani K., Neiers F., Poirier N., Fraichard S., Gotthard G., Chertemps T., Maïbèche M., Ferveur F., Briand L. (2020). The *Drosophila* odorant-binding protein 28a is involved in the detection of the floral odour beta-ionone. *Cell Mol Life Sci*, 77(13), 2565-2577.
2. Durand N., Pottier MA., Siaussat D., Bozzolan F., Maïbèche M., Chertemps T. (2018). Glutathione-S-Transferases in the Olfactory Organ of the Noctuid Moth *Spodoptera littoralis*, Diversity and Conservation of Chemosensory Clades. *Frontiers in Physiology*, 9(2018), DOI=10.3389/fphys.2018.01283
3. Gouin A, et al. (2017) Two genomes of highly polyphagous lepidopteran pests (*Spodoptera frugiperda*, Noctuidae) with different host-plant ranges. *Sci Rep*. Sep 25;7(1):11816.
4. Steiner C, Bozzolan F, Montagné N, Maïbèche M, Chertemps T. (2017) Neofunctionalization of "Juvenile Hormone Esterase Duplication" in *Drosophila* as an odorant-degrading enzyme towards food odorants. *Sci Rep*. Oct 3;7(1):12629.
5. Durand N, Chertemps T, Bozzolan F, Maïbèche M. (2017) Expression and modulation of neuroligin and neurexin in the olfactory organ of the cotton leaf worm *Spodoptera littoralis*. *Insect Sci*. Apr;24(2):210-221.

Illustrations :

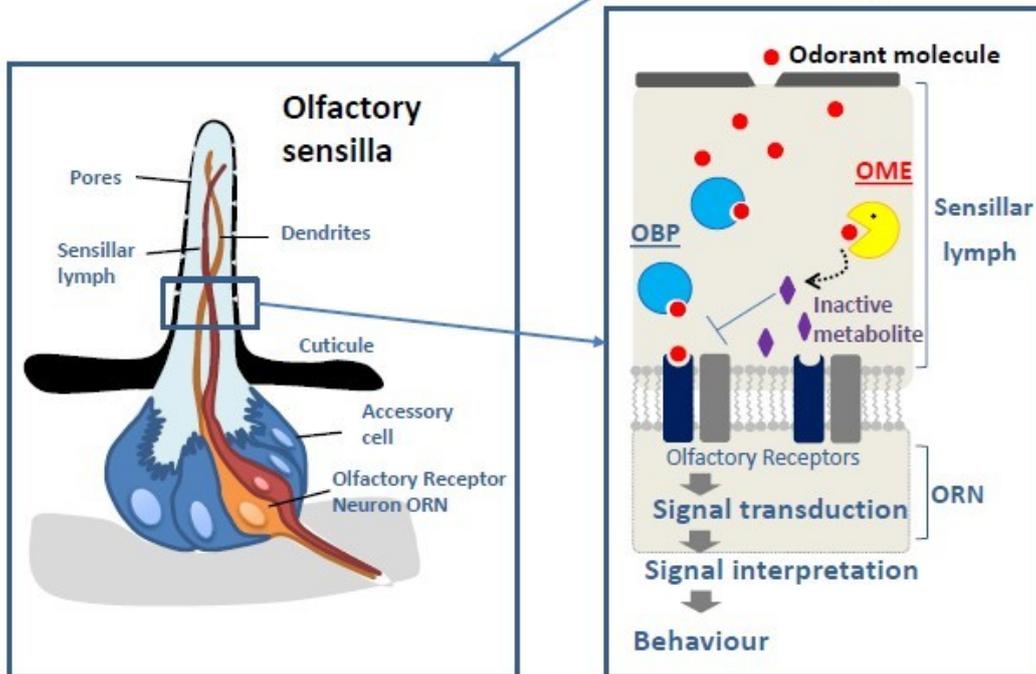
Deciphering the periofactome of a pest species

Spodoptera littoralis

- Crop pest in mediterranean countries
- Highly **polyphagous** caterpillars



antenna



Periofactome????

Odorant Binding Proteins OBP

- ✓ Odorant transport?
- ✓ Odorant buffering?

Odorant Metabolizing Enzymes OME

- ✓ Signal inactivation?
- ✓ Odorant clearance?

TITLE:IN-SILICO DESIGN OF IMPROVED ELECTRON ACCEPTORS FOR ORGANIC PHOTOVOLTAIC APPLICATIONS

Topic number : 2021_051

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes, Physics, Optics

Subfield: Theoretical and Computational Chemistry

ParisTech School: Chimie ParisTech - PSL

Research team:Theoretical Chemistry and Modeling Team

<http://www.quanhic.fr>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website:<http://www.iclehs.fr>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Adamo Carlo carlo.adamo@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Organic photovoltaics (OPV) is attracting increasing interest as an alternative to inorganic solar cells due to possible applications in low-cost, low environmental impact, light-weight and large-area flexible devices. An organic solar cell (OSC) basically consists of the hetero-junction created by putting into contact an electron donor material (D) with an electron-acceptor. The basic functioning of an OSC consists in four steps: the absorption of an incident photon by the active material (D in general) generates a bound electron-hole pair (exciton) which diffuses in the D phase and dissociates at the D/A interface. The resulting electrons and holes migrate in the D and A layers to be finally collected at the electrodes. The performance of an OSC depends on the efficiency of these four steps that is affected, in turn, by the properties of the materials employed in its fabrication. Its optimal performance requires, therefore, the improvement of the characteristics of each constituent. In this project we focus on the optimization of acceptor materials through first-principles (DFT) modeling. We apply a modern computational approach we have recently developed to shed light on the structure-properties relationships that rule the charge and exciton transport in a series of

commonly used acceptors, in both crystalline and amorphous phases. These relationships will be then used to design new acceptors with improved performances.

Required background of the student: Physical Chemistry, Chemical Physics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. D. Alberga, G.F. Mangiatordi, F. Labat, I. Ciofini, O. Nicolotti, G. Lattanzi, C. Adamo Theoretical Investigation of Hole Transporter Materials for Energy Devices J. Phys. Chem. C 119 (2015) 23890
2. D. Alberga, I. Ciofini, G.F. Mangiatordi, A. Pedone, G. Lattanzi, J. Roncali, C. Adamo, Effects of Substituents on Transport Properties of Molecular Materials for Organic Solar Cells: A Theoretical Investigation Chem. Mat 29 (2017) 673.
3. Y. Jiang, C. Cabanetos, S. Jungsuttiwong, D. Alberga, C. Adamo, J. Roncali Effects of Anthryl Groups on the Charge Transport and Photovoltaic Properties of Small Triarylamine-Based Donor-Acceptor Molecules: A Joint Experimental and Theoretical Study Chem. Selec. 2 (2017) 6296.
4. M. Turelli, D. Alberga, G. Lattanzi, I. Ciofini, C. Adamo, Theoretical insights on acceptor-donor dyads for organic photovoltaics Phys; Chem. Chem. Phys. 22 (2020) 27413.
5. M. Turelli, G. Lattanzi, I. Ciofini, C. Adamo On the Interplay between Molecular Packing and Optical Response in Thin Films for Organic Photovoltaics J. Phys. Chem. C 125 (2021) 16304.

Illustrations :

**TITLE: ROBUST ROBOTIC GRINDING CONTROL TO TAKE INTO ACCOUNT
PROCESS VARIABILITY**

Topic number : 2021_052

Field : Design, Industrialization

Subfield: Robotics & Manufacturing

ParisTech School: Arts et Métiers

Research team: Manufacturing & Control Command <http://lcfc.ensam.eu>

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://lcfc.ensam.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: BIGOT Régis regis.bigot@ensam.eu

Advisor 2: RAHARIJAONA Thibaut thibaut.raharijaona@univ-lorraine.fr

Advisor 3: CHEVRET Sandra sandra.chevret@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: The robotization of the grinding allows to reduce musculoskeletal disorders (MSD), to reduce operator injuries and allows mass production grinding and ensures repeatability of quality. The objective is to develop a robotic grinding control system able of grinding parts while controlling the grinding depth, the number of passes and obtaining the required surface finish. The work will have to allow the grinding of complex geometries with different wheel diameters and to take into account the geometrical variations of the grinding wheel during the operation. This is due to the fact that the wear of the grinding wheel affects its diameter and consequently the rate of material removal and the position of the Tool Center Point (TCP- which is generally defined at the end of the wheel). So, due to wear, the wheel diameter do not remain constant over the process. To optimize the grinding conditions of several parts it is necessary to model the variation of the grinding wheel diameter as a function of wear to enable the prediction of the grinding surface dimensions and the obtained surface roughness. To succeed a mathematically modeled is needed and will be implemented firstly to simulate the process and finally experimentally. Finally, in order to guarantee a homogeneous surface condition over the entire length of the grinding process, it is necessary to develop strategies for the entry into

contact between the workpiece and the grinding wheel and for the end of the grinding process, as the grinding wheel releases the surface. These two stages, beginning and end of grinding, often lead to slight undesired steps. The whole PhD work will be developed on an experimental robotized system (ABB robot) with a Ferrobotic head.

Required background of the student: Knowledge in robotics; manufacturing (grinding) if possible; Programming ; applied mechanics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Kolegain, K., Leonard, F., Chevret, S., Attar, A. B., & Abba, G. (2018). Off-line path programming for three-dimensional robotic friction stir welding based on Bézier curves. *Industrial Robot: An International Journal*.
2. Chaoui, M. D., Léonard, F., & Abba, G. (2019). Improving surface roughness in robotic grinding process. In *ROMANSY 22-Robot Design, Dynamics and Control* (pp. 363-369). Springer, Cham.
3. Wang, Z., Zimmer-Chevret, S., Léonard, F., & Abba, G. (2021). Prediction of bead geometry with consideration of interlayer temperature effect for CMT-based wire-arc additive manufacturing. *Welding in the World*, 1-12.
4. Venet, G., Baudouin, C., Pondaven, C., Bigot, R., & Balan, T. (2021). Parameter identification of 42CrMo4 steel hot forging plastic flow behaviour using industrial upsetting presses and finite element simulations. *International Journal of Material Forming*, 1-17
5. Wilfrido, P. Q. C., Gabriel, A., Jean-Francois, A., Thibaut, R., & Philippe, G. (2021). Load-dependent Friction Laws of Three Models of Harmonic Drive Gearboxes Identified by Using a Force Transfer Diagram. *12th International Conference on Mechanical and Aerospace Engineering (ICMAE)* (pp. 239-244). IEEE.

Illustrations :



ROBOTIC GRINDING
Arts et Metiers, Science and Technology
VULCAIN Platform, Metz Campus

TITLE: MODELING PROTON TRANSFER REACTIONS WITH BIASED AB-INITIO DYNAMICS

Topic number : 2021_053

Field : Chemistry, Physical chemistry and Chemical Engineering, Physics, Optics

Subfield: Theoretical and Computational Chemistry

ParisTech School: Chimie ParisTech - PSL

Research team: Theoretical Chemistry and Modeling Team

<http://www.quanhic.fr>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website: <http://www.iclehs.fr>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Adamo Carlo carlo.adamo@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Proton transfer (PT) reaction is undoubtedly one of “the most general and important reactions in chemistry”, being central in many physico-chemical processes and phenomena. Despite the apparent simplicity, this reaction represents a challenging playground for electronic-structure methods. This is particularly true for methods rooted in Density Functional Theory . The situation is even more complex for the Free Energy Surface (FES), which can be obtained by biasing ab-initio molecular dynamics (AIMD) trajectories with enhanced sampling algorithms such as umbrella sampling, steered MD or metadynamics. This class of simulations performs the sampling of the FES far from minima, in regions where chemical bonds are stretched and commonly used DFT approaches are less accurate . This project is focused on the development of an interface between a variant of the Atom Centered Density Matrix Propagation (ADMP) molecular dynamics model, that allows the use of any class of DFT methods , and enhanced sampling algorithms . The developed code will be used for modeling PT reactions with modern DFT approaches, including hybrid and double-hybrid functionals .

Required background of the student: Physical Chemistry, Chemical Physics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Mangiatordi, G. F.; Brémond, E.; Adamo, C. DFT and Proton Transfer Reactions: A Benchmark Study on Structure and Kinetics J. Chem. Theory. Comput. 2012, 8, 3082-3088.
2. Hait, D.; Rettig, A.; Head-Gordon, M. Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H₂, J. Chem. Phys. 2019, 150, 094115
3. Schlegel, H. B.; Millam, J. M.; Iyengar, S. S.; Voth, G. A.; Daniels, A. D.; Scuseria, G. E.; Frisch, M. J. Ab initio molecular dynamics: Propagating the density matrix with Gaussian orbitals J. Chem. Phys. 2001, 114, 9758-9763
4. Tribello, G.A.; Bonomi, M.; Branduardi, D.; Camilloni, C.; Bussi. G. PLUMED2: New feathers for an old bird, Comp. Phys. Comm. 2014, 185, 604
5. E. Brémond, I. Ciofini, J. C. Sancho-García, C. Adamo Nonempirical Double-Hybrid Functionals: An Effective Tool for Chemists Acc. Chem. Res. 2016, 49, 503

Illustrations :

TITLE: AUTOMATION OF A FLEXIBLE AND AGILE FINISHING PROCESS OF FORGED WORKPIECES WITH INDUSTRIAL ROBOTS

Topic number : 2021_054

Field : Design, Industrialization

Subfield: Manufacturing

ParisTech School: Arts et Métiers

Research team: Manufacturing <http://lcfc.ensam.eu>

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://lcfc.ensam.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: BALAN Tudor tudor.balan@ensam.eu

Advisor 2: BAUDOIN Cyrille cyrille.baudouin@ensam.eu

Advisor 3: CHEVRET Sandra sandra.chevret@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: Grinding is necessary to remove overage parts from forged workpieces (flash, surface imperfections, oxide incrustation, etc.). Finishing processes of large forged workpieces are still done manually in most cases. Automation of the finishing process is expected to eliminate the hard manual operations that can lead to musculoskeletal disorders and productivity decrease. Greater accuracy and repeatability of operations is expected. However, at the end of a forging operation, each part is unique, and is the image of the accumulation of all process variabilities. The artificial intelligence would be able to control the robot to perform grinding according to observations made on the workpiece. In the meantime, this PhD consists in creating and deploying a methodology that would allow an effective collaboration between the observation of a workpiece, the interpretation made by an operator and the realization of the expected operations by a robot in a context of industrial productivity. The robot must be able to understand human-like instructions (by gesture, graphics or digital interface). The robotic grinding must also be able to provide a desired geometry or surface roughness despite variations originating from the upstream phases of the process. Robotic grinding has to be able to master the interactions between grinding tool and material, vibrations, robot paths, and forces applied during grinding.

Required background of the student: Knowledge in robotics; manufacturing (grinding) if possible; programming; applied mechanics; mathematics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Zimmer, S., Langlois, L., Laye, J., & Bigot, R. (2010). Experimental investigation of the influence of the FSW plunge processing parameters on the maximum generated force and torque. *The International Journal of Advanced Manufacturing Technology*, 47(1), 201-215.
2. Chaoui, M. D., Léonard, F., & Abba, G. (2019). Improving surface roughness in robotic grinding process. In *ROMANSY 22-Robot Design, Dynamics and Control* (pp. 363-369). Springer, Cham.
3. Wang, Z., Zimmer-Chevret, S., Léonard, F., & Abba, G. (2021). Prediction of bead geometry with consideration of interlayer temperature effect for CMT-based wire-arc additive manufacturing. *Welding in the World*, 1-12.
4. Venet, G., Baudouin, C., Pondaven, C., Bigot, R., & Balan, T. (2021). Parameter identification of 42CrMo4 steel hot forging plastic flow behaviour using industrial upsetting presses and finite element simulations. *International Journal of Material Forming*, 1-17
5. Yang, Y., Vincze, G., Baudouin, C., Chalal, H., & Balan, T. (2021). Strain-path dependent hardening models with rigorously identical predictions under monotonic loading. *Mechanics Research Communications*, 114, 103615.

Illustrations :



ROBOTIC GRINDING

Arts et Metiers, Science and Technology

VULCAIN Platform, Metz Campus

**TITLE: SENSORLESS CONTROL FOR INTEGRATED MULTIPHASE DRIVES
APPLIED TO TRANSPORTATION SYSTEMS USING ARTIFICIAL INTELLIGENCE
POTENTIALITY**

Topic number : 2021_055

Field : Energy, Processes

Subfield: Electrical Engineering and Automation Control

ParisTech School: Arts et Métiers

Research team: Control Team of L2EP Lab

<http://l2ep.univ-lille.fr/en/groupe-de-recherche/equipe-commande/>

Research lab: L2EP - laboratoire d'Electrotechnique et électronique de puissance

Lab location: Lille

Lab website: <http://l2ep.univ-lille.fr>

Contact point for this topic: Arts et Métiers

Advisor 1: NGUYEN Ngac Ky ngacky.nguyen@ensam.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: This project aims to study a compact and performant integrated multiphase drive, including fault modes, for automotive mass market. In this context, price, reliability and compacity are the main criteria. Among the sensors, the end-shaft mechanical position sensor is the most expensive one and is consuming space. Using only current measurement could lead to a suppression of the end-shaft position sensor. Sensorless control algorithms have been proposed for three-phase drives since several decades with the increase of power calculation for signal processing. With multiphase machines, it is possible to use additionally magnetic sensors to increase the number of data of the rotor position which will be used for vector control even in fault modes. Artificial Intelligence (AI) will be investigated for sensorless algorithm development. With multiphase machines using numerous current and magnetic sensors, we propose, by coupling AI with expert knowledges on electrical multiphase machines, to obtain reliable and real-time estimation of the rotor position for a use in the vector control in healthy but also in fault mode operation.

Required background of the student: Beside a good level of English, the recruited student must have:

- A strong background of electrical machines
- A good general culture of scientific research, i.e a Master Research Diploma is helpful
- A good skill for working autonomously and within a team

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. 4. Y. Mini, N. K. Nguyen, E. Semail, "A novel Sensorless Control Strategy Based on Sliding Mode Observer for Non-Sinusoidal Seven-phase PMSM", The 10th International Conference on Power Electronics, Machines and Drives, December 2020.
2. 5. D. A. T. Guzman, N. K. Nguyen, M. Trablesi, and E. Semail, "Low Speed Sensorless Control of Non-Salient Poles Multiphase PMSM," in 2019 IEEE International Conference on Industrial Technology (ICIT), 2019, pp. 1563-1568.
3. 3. N. K. Nguyen, E. Semail, F. D. Belie, and X. Kestelyn, "Adaline Neural Networks-based sensorless control of five-phase PMSM drives," in IECON 2016 - 42nd Annual Conference of the IEEE Industrial Electronics Society, 2016, pp. 5741-5746.
- 4.
- 5.

Illustrations :

TITLE:MECHANOCHEMISTRY-ASSISTED CONTINUOUS SYNTHESIS OF ORGANOMETALLIC COMPLEXES OF MEDICINAL RELEVANCE

Topic number : 2021_056

Field : Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team: Catalysis, Synthesis of Biomolecules and Sustainable Development Team (CSB2D) <https://www.lenresearch.com>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website: <https://www.chimieparistech.psl.eu/recherche/les-laboratoires/i-clehs/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: LEN Christophe christophe.len@chimieparistech.psl.eu

Advisor 2: Cariou Kevin kevin.cariou@chimieparistech.psl.eu

Advisor 3: Gasser Gilles gilles.gasser@chimieparistech.psl.eu

Advisor 4:

Short description of possible research topics for a PhD: Over the recent years, organometallic compounds have shown enormous potential in medicinal chemistry and chemical biology.^{1,2} Ferroquine, an antimalarial drug candidate, is a ferrocenyl analogue of the antimalarial drug Chloroquine which is currently undergoing phase IIb clinical trial.³ The addition of a metal complex has allowed metal-specific modes of action to be uncovered, which has enabled resistance to be overcome and/or the bioactivity of the organic drug to be enhanced.

Among the recent advances in green chemistry and sustainable development, alternative technologies such as continuous flow and ball-milling have been reported.^{4,5} Continuous flow chemistry and alternative technology-assisted continuous flow offers significant advantages including improved thermal management, mixing control, application to a wider range of reaction conditions, scalability, energy efficiency, waste reduction, safety, use heterogeneous catalysis and multistep synthesis.

In this project, we envisage to produce novel ferrocenyl derivatives as drug candidates in either continuous flow or alternative technologies-

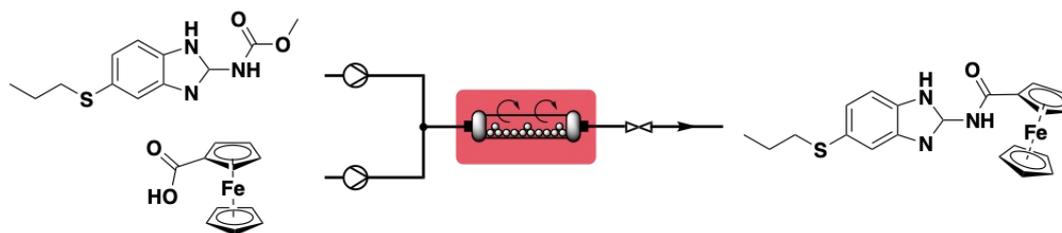
assisted continuous flow. Iron complexes have been found to be extremely promising anticancer and antiparasitic drug candidates. In order to improve the sustainability of the API production, the main tools and levers developed in this subject will be (i) the substitution of Ru(II) as noble metal by Fe(II) as non-noble metal; (ii) the use of continuous flow process and mechanochemical approach; (iii) the use of green solvent (Scheme 1).

Required background of the student: organic chemistry; catalysis; conventional analytical methods; high level written and oral communication skills; good level in English

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Patra, M.; Gasser, G. The Medicinal Chemistry of Ferrocene and its Derivatives. *Nature Rev. Chem.* 2017, 1, 0066, and references therein.
2. Jaouen, G.; Vessières, A.; Top, S. Ferrocifen type anti cancer drugs. *Chem. Soc. Rev.* 2015, 44 (24), 8802-8817, and references therein.
3. Dubar, F.; Slomianny, C.; Khalife, J.; Dive, D.; Kalamou, H.; Guérardel, Y.; Grellier, P.; Biot, C. The ferroquine antimalarial conundrum : redox activation and reinvasion inhibition. *Angew. Chem. Int. Ed.* 2013, 52, 7690-7693.
4. Su, Y.; Zhao, D.; Wang, Y.; Lu, H.; Varma, R.S.; Len, C. Innovative protocols in the catalytic oxidation of 5-hydroxymethylfurfural. *ChemSusChem* 2021, 14, 266-280.
5. Trombettoni, V.; Franco, A.; Sathicq, G.A.; Len, C.; Romanelli, G.P.; Vaccaro, L.; Luque, R. Efficient liquid -assisted grinding selective aqueous oxidation of sulfides using supported heteropolyacid catalysts, *ChemCatChem* 2019, 11, 2537-2545.

Illustrations :



TITLE: POLARIZATION SENSITIVE SINGLE PARTICLE TRACKING AND SUPER-RESOLUTION MICROSCOPY IN THE NEAR-INFRARED FOR BRAIN IMAGING

Topic number : 2021_057

Field : Biology, Biophysics and Biochemistry, Physics, Optics

Subfield:

ParisTech School: Institut d'Optique Graduate School

Research team: NanoBioMicroscopy

<https://www.lp2n.institutoptique.fr/en/teams/nanobiomicroscopy>

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab

website: <https://www.lp2n.institutoptique.fr/en/teams/nanobiomicroscopy>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: Cognet Laurent laurent.cognet@u-bordeaux.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Over the past decades, single-molecule detection and super-resolution microscopy have provided unique details of the nanoscale organization of nanostructures, with many applications in the biological sciences. For several years, our group has developed original approaches to study the nanometric structure of neuronal tissues and the diffusion of molecules involved in the functioning of the brain. In particular, our approaches are based on our expertise in the spectroscopy of carbon nanotubes and our ability to image their complex movements in the near infrared within neuronal tissues. While the study of their lateral diffusion properties are relatively well mastered their rotational diffusion properties remain to be elucidated, which would be an important step in understanding the nanoscale diffusion of physiological or pathological molecules in the brain.

The objective of this PhD project is to develop an approach based on single particle tracking microscopy and super-resolution microscopy to resolve the fast rotational diffusion of nano-objects. The method will be

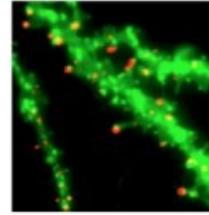
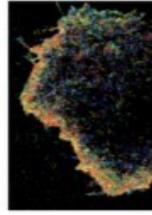
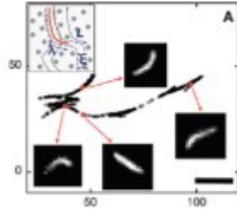
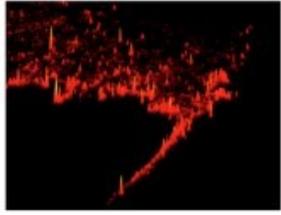
based on the use of fluorescent carbon nanotubes implanted with color centers emitting in the near infrared and on the dynamic polarization analysis of these nanotubes at the single particle level. A super-resolution microscopy study will be performed to understand the orientation of color centers and their interaction with polarized light. Applications will concern rotational diffusion of molecules in living brain slices. The better understanding of the rotational diffusion of molecules in the brain will have an impact in neurobiology, diseased brains as well as for drug delivery strategies.

Required background of the student: Optics, Photonics, Physics, Biophysics, Nanoscience

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Nature Nanotechnol. 12 (2017) 238-243, " Single-nanotube tracking reveals the nanoscale organization of the extracellular space in the live brain" A. G. Godin, J. A. Varela, Z. Gao, N. Danné, J. P. Dupuis, B. Lounis, L. Groc and L. Cognet
2. Science Advances, 5, 9, (2019) eaax1166 " Photoswitchable single-walled carbon nanotubes for super-resolution microscopy in the near-infrared " AG Godin, A. Setaro, M. Gandil, R. Haag, M. Adeli, S. Reich, L. Cognet
3. Nature Methods, 15 (2018) 449-454"Self-interference 3D super-resolution microscopy for deep tissue investigations" P. Bon, J. Linarès-Loyez, M. Feyeux, K. Alessandri, B. Lounis, P. Nassoy and L. Cognet
4. Nature Communications, 11 (2020) 3440 " Synucleinopathy alters nanoscale organization and diffusion in the brain extracellular space through hyaluronan remodeling" F.N. Soria, C. Paviolo, E. Doudnikoff, M.-L. Arotcarena, A. Lee, N. Danné, A. K. Mandal, P. Gosset, B. Dehay, L. Groc, L. Cognet* & E. Bezard*
5. Nature Scientific Reports, 10 (2020) 5286 " Fluorescent sp³ Defect-Tailored Carbon Nanotubes Enable NIR-II Single Particle Imaging in Live Brain Slices at Ultra-Low Excitation Doses " A. Mandal, X. Wu, J.S. Ferreira, M. Kim, L.R. Powell, H. Kwon, L. Groc, YH. Wang & L. Cognet

Illustrations :



TITLE:BAD METALS AND SOFT MODE IN THE QUANTUM PARAELECTRICS

Topic number : 2021_058

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team:<https://qm.lpem.espci.fr/spip.php?rubrique1>

Research lab: LPEM - Laboratoire Physique et d'études des matériaux

Lab location: Paris

Lab website:<https://www.lpem.espci.fr/spip.php?rubrique4>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Fauqué Benoit benoit.fauque@espci.fr

Advisor 2: Bourges Philippe philippe.bourges@cea.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Doped SrTiO₃ is a bad metal where the electrical resistivity does not saturate at high temperature when the mean free path is of the order of interatomic distances. Our recent preliminary results of neutron scattering show that the proximity of the ferroelectric instability, so-called quantum paraelectric phase, play an essential role in the increase of the carriers mass at high temperature (C. Collignon, Ph. Bourges, B. Fauqué and K. Behnia, Phys. Rev. X 10, 031025 (2020)). Further, the tendency towards that structural instability (associated with a soft phonon) is assumed to favour superconductivity in SrTiO₃ for dilute doping, even if both types of orders have a priori nothing in common. Motivated by these results, we propose a PhD research plan to study the effect of electronic doping in quantum paraelectric systems, that will follow two research paths: i) study of the electronic structure via electric and thermoelectric transport measurements ii) study the atomic structure and lattice dynamics by neutron scattering measurements. We will first focus on the doped SrTiO₃ compound (substitution with La and Nb, reduction in oxygen) and next to doped compounds of KTaO₃ and PbTe. These measurements will allow to understand the nature of the new electronic states of matter that occur in doped quantum paraelectric materials.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Clément Collignon, Phillipe Bourges, Benoît Fauqué, and Kamran Behnia, Phys. Rev. X 10, 031025 (2020)
2. Clément Collignon et al., Phys. Rev. Materials 5 065002 (2021)
3. C. W. Rischau et al. , Nat. Phys. 13, 643 (2017).
- 4.
- 5.

Illustrations :

TITLE:MECHANOCHEMISTRY-ASSISTED CONTINUOUS CATALYSIS IN GREEN SOLVENT

Topic number : 2021_059

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team:Catalysis, Synthesis of Biomolecules and Sustainable Development Team (CSB2D) <https://www.lenresearch.com>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website:<https://www.chimieparistech.psl.eu/recherche/les-laboratoires/i-clehs/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: LEN Christophe christophe.len@chimieparistech.psl.eu

Advisor 2: Adamo Carlo carlo.adamo@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

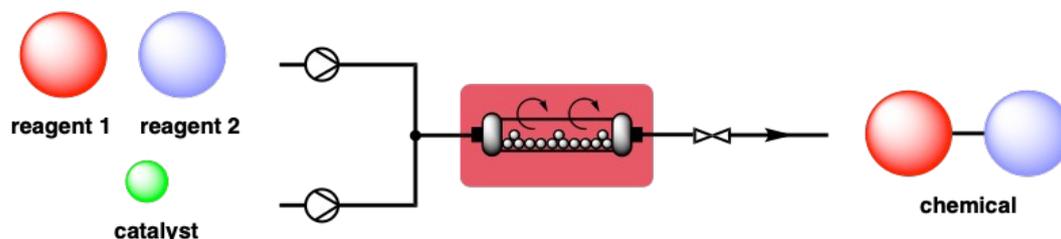
Short description of possible research topics for a PhD: The rapid depletion of non-renewable resources and the greenhouse effect have led to global environmental problems with an adverse impact on the quality of human life. In this urgent context, the search for new and greener strategies and alternative resources for the sustainable development has intensified within the scientific community and at the level of the citizen. In order to create sustainable processes in green chemistry and engineering, alternative intensification processes (continuous flow , ball-milling and mechanochemistry-assisted continuous flow) and green solvent have been explored. In this context, the development of catalysis for the production of high-value chemicals in a designed green solvent will be studied in a mechanochemistry-assisted continuous flow equipment as a high-throughput reaction platform for the first time. Moreover, the supramolecular interactions between solvents, reagents and catalysts will be explored to clearly identify the synergetic effect of this new process. Insights on the mechanism will be then gained using modern modeling approach based on Density Functional Theory , with the aim to gain insights on the whole reaction mechanism and to give some indications on the process optimization.

Required background of the student: Organic chemistry; catalysis; green chemistry; conventional analytical methods; high level written and oral communication skills; good level in English

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. C. Len, F. Delbecq, C.C. Corpas, E.R. Ramos, Continuous flow conversion of glycerol into chemicals: an overview, *Synthesis* 2018, 50, 723-741.
2. V. Trombettoni, A. Franco, A.G. Sathics, C. Len, G.P. Romanelli, L. Vaccaro, Efficient liquid-assisted grinding selective aqueous oxidation of sulfides using supported heteropolyacid catalysts, *ChemCatChem* 2019, 11, 2537-2545.
3. C. Len, M. Khodadadi, F. Lacoste, J. Thiel, Procédé de fabrication du (2,2-diméthyl-1,3-dioxolan-4-yl)méthanol, Brevet FR3103813 (A1) - 30/11/2019.
4. D. De Raffe, P. Piazzetta, N. Russo, M. Toscano, C. Adamo, Density functional determination of the energetics of the formation of trans-stilbene catalyzed by sulfenate anions *ChemCatChem* 2017 9, 278-281
5. L. Brugnoli, A. Pedone, M. C. Menziani, C. Adamo, F. Labat, O₂ Activation over Ag-decorated CeO₂(111) and TiO₂(110) surfaces: A theoretical comparative investigation *J. Phys. Chem. C* 2020, 124, 25917-25930

Illustrations :



TITLE: ELECTRONIC AND THERMOELECTRICAL PROPERTIES OF DILUTE METALS

Topic number : 2021_060

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team: <https://qm.lpem.espci.fr/spip.php?rubrique1>

Research lab: LPEM - Laboratoire Physique et d'études des matériaux

Lab location:

Lab website: <https://www.lpem.espci.fr/spip.php?rubrique4>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Fauqué Benoit benoit.fauque@espci.fr

Advisor 2: Behnia Kamran kamran.behnia@gmail.com

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: In presence of a magnetic field, the electronic spectrum of an electron gas is quantized in Landau levels. At high enough magnetic field, only one or two Landau levels are occupied, this is the quantum limit. This limit has been extensively studied in two dimension systems in the context of the quantum Hall effect. It has been however poorly studied in three dimension since this regime can only be achieved in low carrier density metals. In the last years we have shown that, beyond this limit, 3D dilute metals displays a rich variety of electronic phase transitions ranging from : a succession of a many body field induced state in the semi-metals graphite or a metal-insulator transition in the narrow gap semi-conductor InAs .

In both case this transition is accompanied by a remarkable electrical and thermoelectrical properties. To date the largest magnetoresistance has been reported in the semi-metal, Sb, at high magnetic field and a giant thermoelectrical power accompanied the field induced MI transition in InAs . In this internship/PhD we propose to understand the parameters which pinned down the amplitude of these giant responses in dilute metals. The internship/PhD work will be to measure the electrical and thermoelectrical properties in a large range of temperature, magnetic

field and to develop a new experimental set up to track the current distribution in these high mobile conductors.

Required background of the student: condensed matter, quantum and statistical mechanic

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. B.Fauqué et al, PRL, 110, 266601 (2013)
2. D. LeBoeuf, Nat. Com. 8, 1337 (2017)
3. Z. Zhu et al., PRX, 9, 011058 (2019)
4. A.Jaoui et al, arXiv:2008.06356
5. B. Fauqué and al., PRM, 2, 11420 (2018)

Illustrations :

TITLE: IMPROVING FORMABILITY OF LIGHTWEIGHT METALLIC MATERIALS USING PROCESS CHAINING: INCREMENTAL FORMING AND FRICTION STIR WELDING

Topic number : 2021_061

Field : Material science, Mechanics and Fluids

Subfield: Mechanical, Material and Process Engineering

ParisTech School: Arts et Métiers

Research team:

Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation

Lab location: Angers

Lab website: <http://lampa.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: DAL SANTO Philippe philippe.dalsanto@ensam.eu

Advisor 2: TIBA Idriss idriss.tiba@ensam.eu

Advisor 3: CHEVRET Sandra sandra.chevret@ensam.eu

Advisor 4: BALAN Tudor tudor.balan@ensam.eu

Short description of possible research topics for a PhD: The current trends of the “industry of the future” include dramatic product customization (small batch production) along with optimized lightweight construction, in particular in transportation industries. Innovative technologies to answer these challenges, include robotized forming and assembly processes like single point incremental forming (SPIF) and friction stir welding (FSW), in conjunction with sheet aluminum alloys. Developed during the last two decades, these promising processes still exhibit numerous scientific and technological challenges. Process chaining, on the same part and robot, would allow for a deeper optimization at an improved cost, allowing for the right material at the right place; however the impact of assembly on the residual formability is little known. Establishing the relationship between process parameters and part quality after welding and further forming would be a significant achievement. Controlling the sheet temperature is one of the promising directions to further improve the formability. The final objective is to propose a numerical approach to simulate the forming processes including the chaining effects. Depending on the abilities of the

candidate, one or the other of these research directions will be further developed.

Required background of the student: The student must have very good knowledge in forming processes of metallic materials and in numerical simulation. Some background in metallurgy will be also appreciated.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. D. Rou et al. Experimental and numerical investigation of the mechanical behavior of the AA5383 alloy at high temperatures. *Journal of Materials Processing Technology* (2020), 281; art. no. 116609.
2. Y. Yang and T. Balan. Prediction of the yield surface evolution and some apparent non normality effects after abrupt strain-path change using classical plasticity. *Int. Journal of Plasticity* (2019), 119; 331-343.
3. S. Boudhaouia et al. Experimental and numerical study of a new hybrid process: multi-point incremental forming (MPIF). *International Journal of Material Forming* (2018), 11; 815-827.
4. K. Kolegain et al. Off-line path programming for three-dimensional Robotic Friction Stir Welding based on Bézier curves. *Industrial Robot: An International Journal* (2018).
- 5.

Illustrations :

TITLE: SMART AND MULTIPHYSICS SOLID-SHELL FINITE ELEMENTS FOR THE SIMULATION OF 3D THIN STRUCTURES

Topic number : 2021_062

Field : Material science, Mechanics and Fluids

Subfield: Mechanical Engineering

ParisTech School: Arts et Métiers

Research team: Numerical Methods, Instabilities and Vibrations

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website: <http://www.lem3.univ-lorraine.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: ABED-MERAIM Farid Farid.Abed-Meraim@ensam.eu

Advisor 2: CHALAL Hocine Hocine.chalal@ensam.eu

Advisor 3:

Advisor 4:

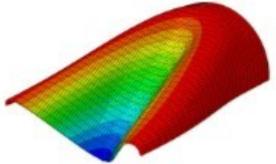
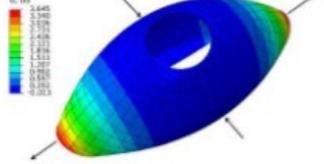
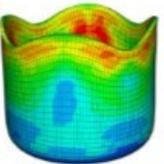
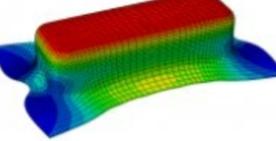
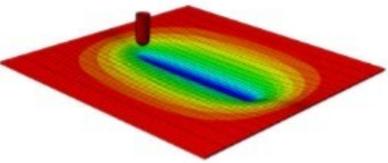
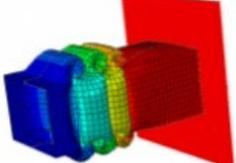
Short description of possible research topics for a PhD: In nowadays manufacturing industry, thin structures are widely designed and employed to reduce weight of products, while improving their mechanical performances (strength, crashworthiness ...). The simulation of these thin structures using the finite element method has become more and more important in the design and manufacture processes. In our research group, we have recently developed a family of solid-shell finite elements, which are capable of modeling most 3D thin structural problems using only a single element layer, while accurately describing the various through-thickness phenomena. The purpose of the present PhD thesis is to pursue the previous works on the development of solid-shell elements, by extending their formulations to advanced and multiphysics constitutive laws for the simulation of manufacturing processes. More specifically, coupled magnetic-elastic-plastic constitutive laws will be combined with the developed solid-shell elements for the simulation of magnetic pulse forming processes. Also, strong thermomechanical coupling, involving the addition of temperature degrees of freedom, will be considered in the formulation of the solid-shell finite elements, for the simulation of warm and hot sheet metal forming processes.

Required background of the student: - Solid background in finite element formulation and simulation;
- Good analytical and programming skills (e.g., Fortran, C, C++);

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Abed-Meraim F, Combescure A (2009). An improved assumed strain solid–shell element formulation with physical stabilization for geometric non-linear applications and elastic–plastic stability analysis. *International Journal for Numerical Methods in Engineering*, 80:1640–1686.
2. Wang P, Chalal H, Abed-Meraim F (2015). Efficient solid–shell finite elements for quasi-static and dynamic analyses and their application to sheet metal forming simulation. *Key Engineering Materials*, 651–653:344–349.
3. Wang P, Chalal H, Abed-Meraim F (2017). Quadratic solid–shell elements for nonlinear structural analysis and sheet metal forming simulation. *Computational Mechanics*, 59:161–186.
4. Wang P, Chalal H, Abed-Meraim F (2017). Quadratic prismatic and hexahedral solid–shell elements for geometric nonlinear analysis of laminated composite structures. *Composite Structures*, 172:282–296. 1.
5. Chalal H, Abed-Meraim F (2018). Quadratic solid-shell finite elements for geometrically nonlinear analysis of functionally graded material plates. *Materials*, 11(6), art. no. 1046.

Illustrations :

 <p data-bbox="300 398 576 465">Pinched semi-cylindrical shell</p>	 <p data-bbox="635 409 1002 477">Pinched laminate hemispherical shell</p>	 <p data-bbox="1066 398 1281 465">Deep drawing of a cylindrical cup</p>
 <p data-bbox="331 645 544 712">Deep drawing of a rectangular cup</p>	 <p data-bbox="635 667 1002 701">Single point incremental forming</p>	 <p data-bbox="1066 678 1281 712">Crash of a boxbeam</p>

TITLE: TOWARDS THE DEFINITION OF INDUSTRY 4.0 AND 5.0 KEY PERFORMANCE INDICATORS

Topic number : 2021_063

Field : Information and Communication Science and Technology

Subfield:

ParisTech School: Arts et Métiers

Research team:

Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques

Lab location: Lille

Lab website: <https://lispen.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: Klement Nathalie nathalie.klement@ensam.eu

Advisor 2: SIADAT Ali ali.siadat@ensam.eu

Advisor 3: Goepf Virginie virginie.goepf@insa-strasbourg.fr

Advisor 4:

Short description of possible research topics for a PhD: The Industry4.0 context drives the manufacturing companies towards the implementation of Reconfigurable Manufacturing Systems (RMS) enabling agility. In this context, assessing the performance of such systems becomes even more crucial. Generally, this requires to define a set of relevant KPIs (Key Performance Indicator) like these defined in the ISO 22400 standard and to manage them preferably on-line and dynamically.

Several indicators should be defined to help the manager to monitor his system: indicators about reconfigurability or performance indicators. For instance, these indicators could help the manager to decide how to reconfigure his system, or simply to modify the allocation of resources.

Nowadays, thanks to Industry 4.0 new concepts such as decentralized control system, many information, data, are available at any moment and everywhere. How to exploit these data to better define the considered system, follow it through a dashboard, help the manager to take the right decision at the right time? This can be done through Cyber Physical Production System.

Therefore, the objective of this PhD would be to define what could be

“I4.0 KPIs” that is to say which should be the relevant set of KPIs for RMSs and how to manage them dynamically that is to say how to make them change according to the system configuration.

Required background of the student: Industrial engineering, Information system, operational research

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Wu, X., Goepp, V., Siadat, A. “Concept and engineering development of cyber physical production systems: a systematic literature review” International Journal of Advanced Manufacturing Technology, 2020, 111(1-2), pp. 243-261

2. Wu, X., Goepp V., Siadat A. “The integrative link between cyber physical production systems and enterprise information systems” accepted to the 49th International Conference on Computers & Industrial Engineering conference (CIE 49), October 18-21, 2019, Beihang University, Beijing, China

3. Nieto, F. D. M., V. Goepp and E. Caillaud (2017). "From Factory of the Future to Future of the Factory: Integration Approaches." Ifac Papersonline 50(1): 11695-11700

4. Beauville dit Eynaud, A., Klement, N., Roucoules, L. et al. Framework for the design and evaluation of a reconfigurable production system based on movable robot integration. Int J Adv Manuf Technol (2021). <https://doi.org/10.1007/s00170-021-08030-1>

5. Amzil K., Yahia E., Klement N., Roucoules L. (2021) Causality Learning Approach for Supervision in the Context of Industry 4.0. In: Roucoules L., Paredes M., Eynard B., Morer Camo P., Rizzi C. (eds) Advances on Mechanics, Design Engineering and Manufacturing III. JCM 2020. Lecture Notes in Mechanical Engineering. Springer, Cham. https://doi.org/10.1007/978-3-030-70566-4_50

Illustrations :

TITLE:FORMING LIMIT PREDICTIONS FOR POROUS MATERIALS IN COLD AND WARM SHEET METAL FORMING

Topic number : 2021_064

Field : Material science, Mechanics and Fluids

Subfield: Mechanical Engineering

ParisTech School: Arts et Métiers

Research team: Numerical Methods, Instabilities and Vibrations

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website:<http://www.lem3.univ-lorraine.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: ABED-MERAIM Farid Farid.Abed-Meraim@ensam.eu

Advisor 2: CHALAL Hocine Hocine.chalal@ensam.eu

Advisor 3:

Advisor 4:

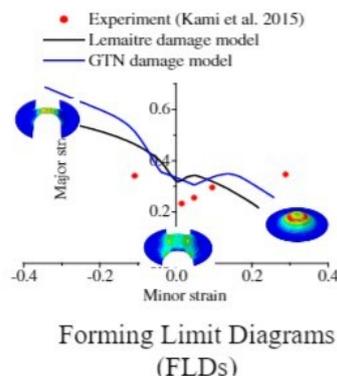
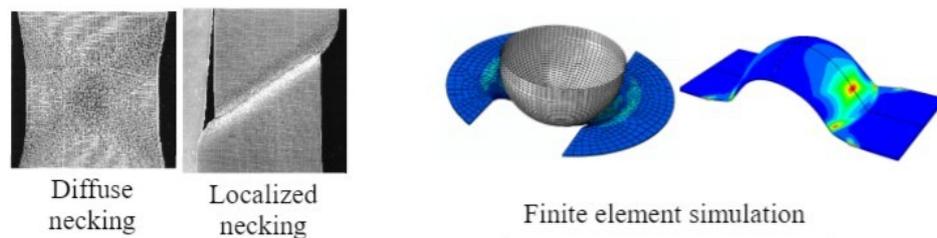
Short description of possible research topics for a PhD: In the context of sheet metal forming, the occurrence of diffuse and localized necking, which are precursors to ductile fracture, represents one of the main causes for rejection of metal parts during forming operations. In order to accurately predict the occurrence of these defects, various theoretical and numerical approaches have been developed in the literature. These approaches require, on the one hand, the introduction of appropriate constitutive models in order to reproduce the physical phenomena involved during forming operations. On the other hand, the selected constitutive models have to be combined with necking criteria for the prediction of plastic instabilities, such as diffuse and localized necking, in thin sheet metal forming. The purpose of the present PhD thesis is to combine advanced elastic-plastic-damage models with necking criteria for the prediction of formability limits of ductile materials. The resulting numerical tool is then applied for the prediction of forming limits of ductile materials under cold and warm forming conditions.

Required background of the student: - Solid background in mechanic of materials and finite element simulation;
- Good analytical and programming skills (e.g., Fortran, C, C++);

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Nasir M W, Chalal H, Abed-Meraim F (2021). Formability prediction using bifurcation criteria and GTN damage model. *International Journal of Mechanical Sciences*, 191:106083.
2. Nasir MW, Chalal H, Abed-Meraim F (2020). Prediction of forming limits for porous materials using void-size dependent model and bifurcation approach. *Meccanica*, 55(9):1829–1845.
3. Bouktir Y, Chalal H, Abed-Meraim F (2018). Prediction of necking in thin sheet metals using an elastic–plastic model coupled with ductile damage and bifurcation criteria.. *International Journal of Damage Mechanics*, 27(6):801–839.
4. Chalal H, Abed-Meraim F (2017). Numerical predictions of the occurrence of necking in deep drawing processes. H. Chalal, F. Abed-Meraim. *Metals*, 7(11), art. no. 455.
5. Chalal H, Abed-Meraim F (2017). Determination of forming limit diagrams based on ductile damage models and necking criteria. *Latin American Journal of Solids and Structures*, 14(10):1872–1892.

Illustrations :



**TITLE: HOW TO ADAPT RECONFIGURABLE PRODUCTION SYSTEMS TO
PRODUCT VARIABILITY**

Topic number : 2021_065

Field : Design, Industrialization, Information and Communication
Science and Technology

Subfield: Engineering -> Industrial Engineering

ParisTech School: Arts et Métiers

Research team: Design department

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://lcfc.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: DANTAN Jean-Yves jean-yves.dantan@ensam.eu

Advisor 2: SIADAT Ali ali.siadat@ensam.eu

Advisor 3: STIEF Paul paul.stief@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: Today's industrial environment is still marked by an ongoing trend towards more customised products. In addition, the past years have shown an increasing instability of the worldwide economy due to an accumulation of catastrophes and crises. This very fluctuating ecosystem confronts industrial production companies with serious challenges regarding the outset of their production systems. The concept of co-evolution aims to answer these challenges.

For co-evolution, product evolution and production system evolution are put into parallel to anticipate changes of both. Also, reconfigurable systems are outset to respond exactly to the adaptability need of a product family. However, there is a lack of research work concerning the evaluation of the production system capacities to be adaptable. The research question is "how to achieve a consistency between the adaptability needs induced by product variety and the adaptability capacity provided by the production system". Figure 1 (see attached files) illustrates different problematics linked to these problematics: The production system on one hand is not capable to be adapted to the entire product variety, but on the other hand has unused abilities. In a co-evolution approach, the challenge is then to orient either the product

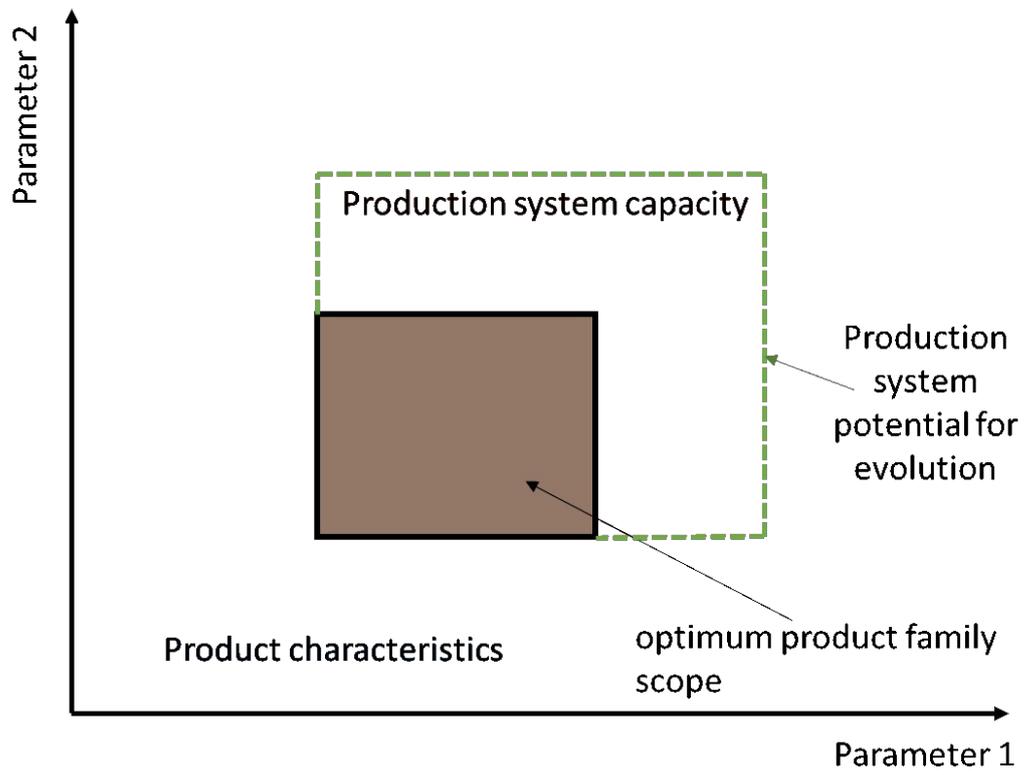
evolutions to better fit the production system abilities or to evolve the production system towards a better coverage of product variety needs. To achieve this, the thesis objective is to allow precise knowledge of production system abilities to be gathered.

Required background of the student: Industrial Engineering and/or Mechanical Engineering

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. H. A. ElMaraghy and T. AlGeddawy, 'Co-evolution of products and manufacturing capabilities and application in auto-parts assembly', *Flex Serv Manuf J*, vol. 24, no. 2, pp. 142-170, Jan. 2012, doi: 10.1007/s10696-011-9088-1.
2. P. Stief, J.-Y. Dantan, A. Etienne, A. Siadat, and G. Burgat, 'Product design improvement by a new similarity-index-based approach in the context of reconfigurable assembly processes', *Journal of Engineering Design*, vol. 31, no. 6, pp. 349-377, Jan. 2020, doi: 10.1080/09544828.2020.1748181.
3. Y. Koren, X. Gu, and Guo W., 'Reconfigurable manufacturing systems: Principles, design, and future trends', *Front. Mech. Eng.*, vol. 13, no. 2, pp. 121-136, Jan. 2018, doi: 10.1007/s11465-018-0483-0.
4. A. M. Farid and D. C. McFarlane, 'Production degrees of freedom as manufacturing system reconfiguration potential measures', *Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture*, vol. 222, no. 10, pp. 1301-1314, Jan. 2008, doi: 10.1243/09544054JEM1056.
5. A. M. Farid, 'Product Degrees of Freedom as Manufacturing System Reconfiguration Potential Measures', *Int. Trans. on Systems Science and Applications*, vol. 4, no. 3, pp. 227-242, Jan. 2008.

Illustrations :



TITLE: MODELING OF METAL NANOPARTICLES EMBEDDED IN VISCOELASTIC MEDIA USING FLUID-STRUCTURE INTERACTION APPROACH

Topic number : 2021_067

Field : Biology, Biophysics and Biochemistry, Life and Health Science and Technology , Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: Complex Fluids and Flows

[http://lampa.ensam.eu/ecoulements-complexes-132761.kjsp?](http://lampa.ensam.eu/ecoulements-complexes-132761.kjsp?RH=1415807897072&RF=1479738780674)

[RH=1415807897072&RF=1479738780674](http://lampa.ensam.eu/ecoulements-complexes-132761.kjsp?RH=1415807897072&RF=1479738780674)

Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation

Lab location: Angers

Lab website: <http://lampa.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: El Baroudi Adil adil.elbaroudi@ensam.eu

Advisor 2: Le Pommellec Jean Yves jeanyves.lepommellec@ensam.eu

Advisor 3: AMMAR Amine amine.ammar@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: Vibration modes in nanostructures present a major interest in characterization of the materials properties. In particular, virus is known to resonate in the confined-acoustic dipolar mode with microwave of the same frequency. Indeed, investigating the vibrational modes of viruses has been motivated by the possibility of using ultrasonic waves to destroy or to inactivate a virus present in a living organism. The vibration of a free homogeneous and isotropic sphere was studied by Lamb using the theory of elastic media. However the free sphere model used to interpret the experimental results is a rough approximation of the actual environmental conditions of nanoparticles. A more general theory based on nonlocal elasticity for accurately predicting the vibration modes of nanosphere embedded in a viscoelastic media is the subject of this thesis. Several constitutive laws of the viscoelastic medium must be considered in order to obtain a more realistic model.

Required background of the student: Master Mechanics, Physics, Mathematics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Le Pommellec and El Baroudi. Correlation between the toroidal modes of an elastic sphere and the viscosity of liquids, *Comptes Rendus Mécanique* (2021).
2. Billon and El Baroudi. Mathematical Modelling of Love waves propagation in viscoelastic waveguide loaded with complex fluids, *Applied Mathematical Modelling* (2021).
3. El Baroudi. A note on the spheroidal modes vibration of an elastic sphere in linear viscoelastic fluid, *Physics Letters A* (2020)
4. El Jirari, El Baroudi and Ammar. Numerical investigation of the dynamical behavior of a fluid-filled microparticle suspended in human arteriole, *Journal of Biomechanical Engineering* (2021).
5. Yang, El Baroudi and Le Pommellec. Analytical approach for predicting vibration characteristics of an embedded elastic sphere in complex fluid, *Archive of Applied Mechanics* (2020).

Illustrations :

**TITLE: A DECISION AID SYSTEM BASED ON A DECENTRALIZED ARCHITECTURE
TO FASTER THE MANAGEMENT OF HAZARDS OCCURRING UNDER
PRODUCTION AND LOGISTICS SYSTEMS**

Topic number : 2021_068

Field : Information and Communication Science and Technology

Subfield:

ParisTech School: Arts et Métiers

Research team:

Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques

Lab location: Lille

Lab website: <https://lispen.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: Klement Nathalie nathalie.klement@ensam.eu

Advisor 2: Yahia Esma esma.yahia@ensam.eu

Advisor 3: Roucoules Lionel lionel.roucoules@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: In the context of to the Industry 4.0, production and logistics systems are becoming more and more connected which help to monitor the industrial processes in order to detect hazards and then react rapidly to manage them. The problematic we would like to address is how to manage information system continuity linking the factory, its suppliers, the resources (robots or human). Second, we aim to imply some work on the decentralized information system that presents different advantages when managing planning, scheduling, resources assignment, reaction to hazards. It should answer to how to deal with a missing operator, or with a lack of raw material? How to propagate the impact of this hazard into the scheduling or assignment which was supposed to be done on the current day. Different applications are available on our lab (Lille and Aix-en-Provence) so it would be the opportunity to implement on real case study the development of such decision aid system.

Required background of the student: Industrial engineering, Information system, operational research

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Amzil K., Yahia E., Klement N., Roucoules L. (2021) Causality Learning Approach for Supervision in the Context of Industry 4.0. In: Roucoules L., Paredes M., Eynard B., Morer Camo P., Rizzi C. (eds) Advances on Mechanics, Design Engineering and Manufacturing III. JCM 2020. Lecture Notes in Mechanical Engineering. Springer, Cham.
https://doi.org/10.1007/978-3-030-70566-4_50
2. Beauville dit Eynaud, A., Klement, N., Roucoules, L. et al. Framework for the design and evaluation of a reconfigurable production system based on movable robot integration. Int J Adv Manuf Technol (2021).
<https://doi.org/10.1007/s00170-021-08030-1>
3. Derigent, W., Cardin, O. & Trentesaux, D. Industry 4.0: contributions of holonic manufacturing control architectures and future challenges. J Intell Manuf 32, 1797–1818 (2021). <https://doi.org/10.1007/s10845-020-01532-x>
4. Beauville dit Eynaud A., K. N. (2020). Risk and decision analysis for Reconfigurable Assembly System Design under uncertainties. 13th International Conference on Modeling, Optimization and Simulation-MOSIM'20-November 12-14, 2020 Agadir-Morocco" New advances and challenges for sustainable and smart industries".
- 5.

Illustrations :



**TITLE:IMPROVING SUPER-RESOLVED LOCALIZATION MICROSCOPES (PALM)
IN DEEP AND HETEROGENEOUS SAMPLES WITH CO-DESIGNED OPTIMAL
PHASE MASKS**

Topic number : 2021_069

Field : Information and Communication Science and Technology,
Physics, Optics

Subfield: Image processing - Microscopy

ParisTech School: Institut d'Optique Graduate School

Research team: Imaging and information

<https://www.lcf.institutoptique.fr/groupes-de-recherche/imagerie-et-information>

Research lab: Laboratoire Charles Fabry

Lab location: Palaiseau

Lab website:<https://www.lcf.institutoptique.fr/>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: Goudail François francois.goudail@institutoptique.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Photo-activated localization microscopy (PALM) makes it possible, thanks to sophisticated image processing techniques, to estimate the position of a fluorescent particle with a precision well above the diffraction limit and thus to reconstruct "super-resolved" images with nanometric resolution (Fig. 1). Biologists are nowadays imaging thick biological media, which requires to increase the "depth of field" (DOF) of PALM microscopes and, for some applications, to estimate the three dimensional position of the particle in the volume of the sample.

This can be done by placing optimized phase masks in the aperture stop of the microscope objective in order to "shape" the variation of the point spread function (PSF), and by applying adapted processing algorithms (Fig. 2, Fig. 3). Optimization of these masks is a tradeoff between localization precision (in 2D or 3D), depth of exploration, and photon budget (which is linked imaging frequency and phototoxicity issues) Biologists now need to be able to design the good mask for each application. The goal of this PhD project is address this concern by

developing a comprehensive phase mask optimization framework that fully takes into account the parameters and constraints linked to each PALM imaging application. The results of these studies will lead to revisit the optimization criteria of DOF enhancing and 3D estimation masks, and thus will to design new types of masks more adapted to real imaging conditions. The masks will be optimized numerically and validated by real measurements performed in collaboration with research groups recognized for their expertise in very high resolution microscopy for biology. With this interdisciplinary approach, decisive improvements in PALM imaging applied to life science and molecular biology are expected.

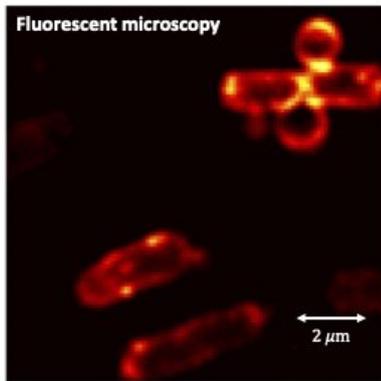
Required background of the student: This project calls upon highly interdisciplinary skills and motivation for both optical modeling and image processing. The successful candidate will ideally possess skills in both domains. However, this project is also perfectly fit for a skilled physicist eager to develop her/his knowledge about image processing, or for an image processing scientist wanting to improve her/his skills in physical modeling.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. O. Lévêque, C. Kulcsár, A. Lee, H. Sauer, A. Aleksanyan, P. Bon, L. Cognet, and F. Goudail, "Co-designed annular binary phase masks for depth-of-field extension in single-molecule localization microscopy", *Opt. Express* 28, 32426-32446 (2020)
2. O. Lévêque, R. Duverger, H. Sauer, C. Kulcsar, F. Goudail, "Influence of high numerical aperture on depth-of-field enhancing phase mask optimization in localization microscopy," *J. Opt. Soc. Am. A* 38, 1380-1390 (2021)
3. Y. Shechtman, S.J. Sahl, A.S. Backer and W.E. Moerner, "Optimal point spread function design for 3D imaging", *Physical Review Letters* 113, 133902 (2014).
4. Y. Zhou, G. Carles, "Precise 3D particle localization over large axial ranges using secondary astigmatism", *Opt. Lett.* 45, 2266 (2020)
5. A. Lee, K. Tsekouras, C. Calderon, C. Bustamante, S. Pressé, "Unraveling the Thousand Word Picture: An Introduction to Super-Resolution Data Analysis", *Chem. Rev.* 117, 7276–7330 (2017)

Illustrations :

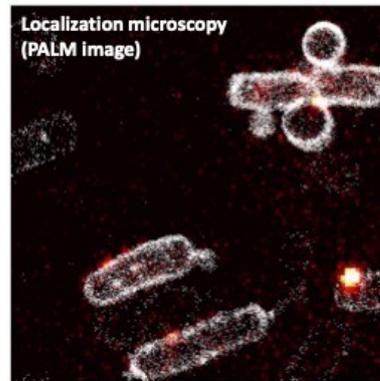
Localization microscope principle



Magnification x150
 Numerical aperture 1.45
 Sensor EMCCD
 107 nm/pixel

Crédits : Antony Lee,
 University of California,
 Berkeley

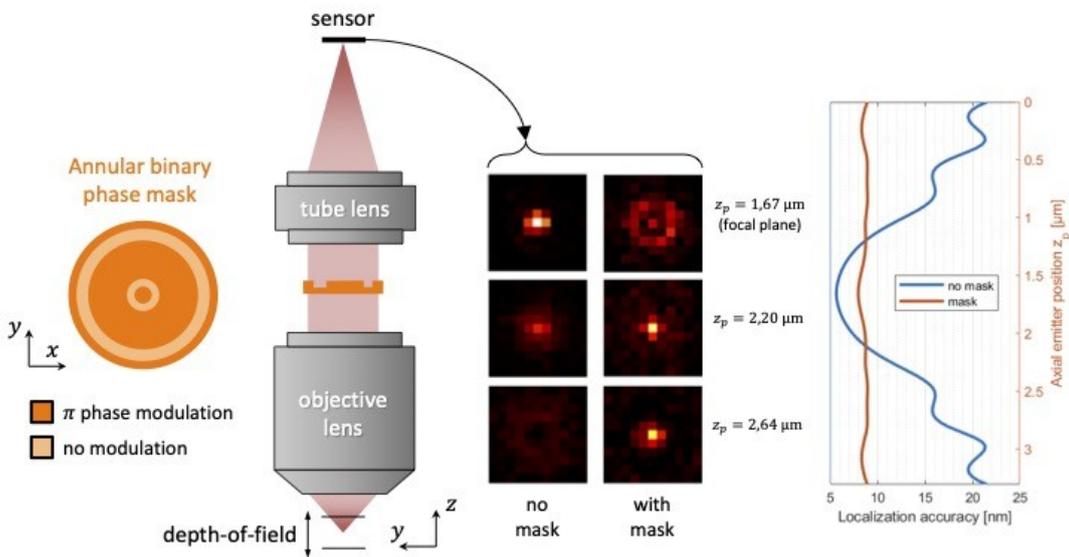
Lateral resolution ~ 200 nm
 (diffraction-limited system)



Lateral resolution ~ 10 nm
 (Estimation precision only limited by noise)



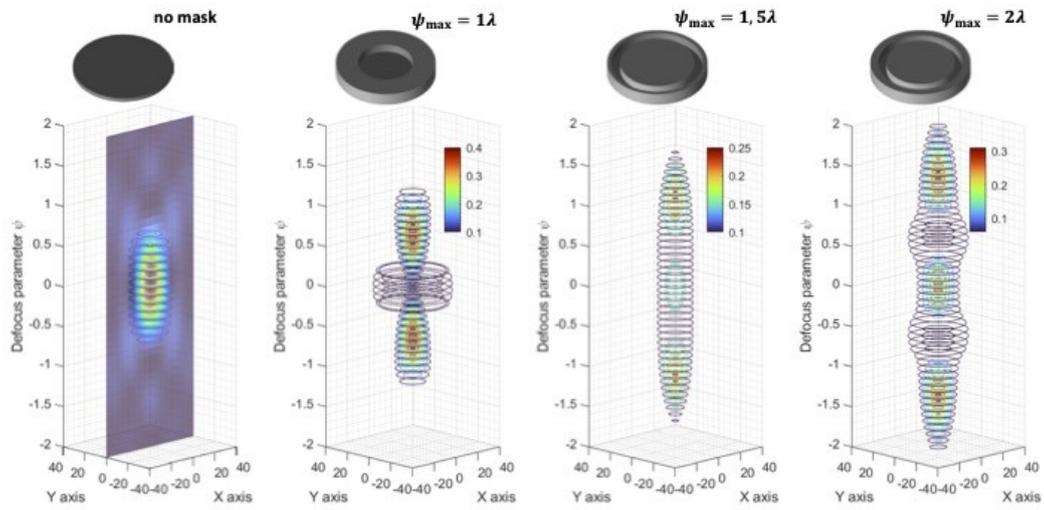
Depth-of-field enhancing phase masks



[Lévêque et al., Opt. Express 28, 32426-32446 (2020)]



Example of depth of field enhancement with optimized phase masks



TITLE:HIGH SENSITIVE ATOM INTERFEROMETRY USING MULTI-PHOTON INTERROGATION IN AN OPTICAL CAVITY

Topic number : 2021_070

Field : Physics, Optics

Subfield:

ParisTech School: Institut d'Optique Graduate School

Research team: Cold Atoms in bordeaux

<https://www.coldatomsbordeaux.org>

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab website:<https://www.lp2n.institutoptique.fr/>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: Canuel Benjamin benjamin.canuel@institutoptique.fr

Advisor 2: Bouyer Philippe philippe.bouyer@institutoptique.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The Phd project envisions to exploit the promising potential of LMT beam splitters to boost the sensitivity of atom-interferometers-based sensors and open a new class of precision measurement experiments. This project relies on the potential of optical resonators as a key technique for sensitivity improvement. Indeed, original developments achieved by a few groups worldwide have recently allowed to clearly identify multiple breakthrough brought by resonators for atom interferometry. While cavities are now considered as disruptive tools to improve AI sensitivity, the efficiency of this method will scale with resonator Finesse for both scale factor improvement and future implementation of sub shot noise measurement schemes. The PhD will therefore focus on the study of different atom interferometry geometries using high Finesse resonators with the scope of demonstrating an improved measurement scale factor thanks to the use of the cavity. Based on such developments the PdD project will enable to open new applications for fundamental physics by extending atom gradiometry applications to Dark Matter (DM) studies.

Required background of the student: Atomic Physics
Optics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. B Canuel, A Bertoldi, L Amand, E Pozzo di Borgo, T Chantrait, C Danquigny, M Dovale Álvarez, B Fang, A Freise, R Geiger, J Gillot, S Henry, J Hinderer, D Holleville, J Junca, G Lefèvre, M Merzougui, N Mielec, T Monfret, S Pelisson, M Prevedelli, S Reynaud, I Riou, Y Rogister, S Rosat, E Cormier, A Landragin, W Chaibi, S Gaffet, P Bouyer, Exploring gravity with the MIGA large scale atom interferometer; Scientific Reports, 8 1 14064, 2018
2. Chaibi, Walid; Geiger, Remi; Canuel, Benjamin; Bertoldi, Andrea; Landragin, Arnaud; Bouyer, Philippe; Low frequency gravitational wave detection with ground-based atom interferometer arrays; Physical Review D 93 021101, 2016
3. Riou, Isabelle; Mielec, Nicolas; Lefèvre, Grégoire; Prevedelli, Marco; Landragin, Arnaud; Bouyer, Philippe; Bertoldi, Andrea; Geiger, Remi; Canuel, Benjamin; Atom interferometry in a marginally stable optical resonator; Journal of Physics B: Atomic, Molecular and Optical Physics, 50 155002 (2017)
4. B Canuel et al, ELGAR—a European Laboratory for Gravitation and Atom-interferometric Research, Class. Quantum Grav. 37 225017 (2020)
- 5.

Illustrations :

TITLE: PLASTICS CONVERSION IN MOLTEN SALTS

Topic number : 2021_071

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team: Interfaces, Electrochimie-Energie Team and Matériaux, Interface et Matière Molle Team

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <https://www.ircp.cnrs.fr>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: LAIR Virginie virginie.lair@chimieparistech.psl.eu

Advisor 2: SEMETÉY Vincent vincent.semety@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: In recent decades, the world has been concerned about the environmental impact of waste plastic requiring their recycling. The mechanical recycling techniques fails to treat the majority of waste plastics. Only 32% of plastics are recycled in EU. The recycling of plastic wastes (particularly low grade plastics) is challenging in the absence of a strong economic driving force. Such a driving force can be achieved through the low-cost conversion of plastic wastes into highly valuable outputs like the production of fuel. In this project we want to investigate the conversion of plastics employing molten salts to valuable materials such as hydrogen (Flandinet et al.), carbonates, carbon nanomaterial (Kamali), fuel (Bertolini et al.)... To achieve this goal, model molecules as well as polymers will be studied to properly identify the products and optimize the conditions as well as the reactor. Simulations taking into account the enthalpies of reactions that can be carried out and associated with DSC-ATG analyzes. The effects of temperature, salt composition will be studied, and the yield and the composition of solid/liquid/gas products will analyzed. The system will be design in order to be able to check the mass balance and an energy balance would be carried out as well.

Required background of the student: Chemistry, Physical chemistry, Polymer chemistry, Chemical engineering

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Flandinet L., Tedjar F., Ghetta V., Fouletier J. J Hazard Mater. 2012, 485-490.
2. Kamali A. Green Production of Carbon Nanomaterials in Molten Salts and Applications. Springer 2020, 109-140.
3. Bertolini J., Fontaine J. Conservation & Recycling 1987, 10, 331-343.
4. Zhao L., Semetey V. ACS Omega 2021, 6, 6, 4175-4183
5. Meskine H., Albin V., Cassir M., Ringuedé A., Lair V. International Journal of Hydrogen Energy 2021, 46, 14944-14952

Illustrations :

TITLE: DEVELOPMENT OF UV LASER SOURCES FOR APPLICATIONS IN QUANTUM PHYSICS

Topic number : 2021_072

Field : Physics, Optics

Subfield: lasers

ParisTech School: Institut d'Optique Graduate School

Research team: Photonics Systems

<https://www.lp2n.institutoptique.fr/en/teams/photonics-systems>

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab website: <https://www.lp2n.institutoptique.fr/>

Contact point for this topic: Institut d'Optique Graduate School

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Advisor 2: Santarelli Giorgio giorgio.santarelli@institutoptique.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Tunable high power laser sources in the 300 to 320nm UV range are required for different applications, ranging from atmospheric physics to quantum computing. For these applications, high level of power as well as low noise figures are required (from hundreds of milliwatt to several Watt). This PhD thesis aims at developing new lasers sources based on nonlinear conversion (both resonant and non-resonant) of high-power fibred laser systems in the Infrared range. A study of the noise characteristics and transfers will be pursued, to actively reduce it. This work will be realized in close collaboration with the company AzurLight Systems and the technology centre Alphanov.

Required background of the student: optics / lasers

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. D. Darwich, Y.V. Bardin, C. Dixneuf, M. Goepner, G. Guiraud, N. Traynor, G. Santarelli and A. Hilico "Ultra low-intensity noise, 10 W all-fiber single frequency tunable laser system around 1550 nm," Appl. Opt. 60,, 8550-8555 (2021). 10.1364/AO.435274
2. C. Dixneuf, G. Guiraud, H. Ye, Y. Bardin, M. Goepner, G. Santarelli and N. Traynor, "Robust 17 W single-pass second-harmonic-generation at 532 nm and relative-intensity-noise investigation," Opt. Lett. 46, 408-411 (2021). 10.1364/OL.415532
3. B. Gouhier, Clément Dixneuf, Adèle Hilico, G. Guiraud, N. Traynor, and G. Santarelli, "Low intensity noise high-power tunable fiber-based laser around 1007 nm", IEEE Journal of Lightwave Technology, 37, 3539-3543, (2019). 10.1109/JLT.2019.2917651
4. C. Dixneuf, G. Guiraud,, Y. Bardin, Q, Rosa, M. Goepner, A. Hilico, C. Pierre, J. Boulet, N. Traynor and G. Santarelli, "Ultra-Low intensity noise allfiber 365 W linearly polarized single frequency laser at 1064 nm," Opt. Expr. 28, 10960-10969 (2020). 10.1364/OE.385095
- 5.

Illustrations :

**TITLE: DEVELOPMENT OF ADVANCED MULTISCALE COMPUTATIONAL TOOLS
FOR THE MULTIPHYSICS PREDICTION OF CARBON NANOTUBES (CNTs)
FUZZY FIBER COMPOSITES**

Topic number : 2021_073

Field : Material science, Mechanics and Fluids

Subfield: Mechanical engineering, Computational mechanics, Mechanics of Materials

ParisTech School: Arts et Métiers

Research team:

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website: <http://www.lem3.univ-lorraine.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: Chatzigeorgiou George georges.chatzigeorgiou@ensam.eu

Advisor 2: Meraghni Fodil fodil.meraghni@ensam.eu

Advisor 3: BENAARBIA Adil adil.benaarbia@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: Modern engineering applications require the development of composite materials with advanced mechanical, thermal, electrical etc. properties that provide high performances when employed for structural components. Carbon nanotubes (CNTs) have shown excellent characteristics when introduced in composite structures. A relatively new type of material system considers matrices reinforced with “fuzzy fibers” (fibers with CNTs grown on their surfaces). SiC fibers with grown CNTs are embedded in ceramic matrices towards developing lightweight high-heat engine parts in aerospace applications . These complicated heterogeneous materials cannot be studied with the classical multiscale methodologies and they require appropriate micromechanics tools .

The proposed Ph.D. is going to investigate and design computational homogenization strategies (both full-field and mean-field) for composite structures reinforced with fuzzy fibers. The examined multiphysical properties will include mechanical, thermal and electrical properties as well as their coupling. Nonlinear and damage mechanisms will also be taken into account.

Required background of the student: Mechanical engineering, Computational mechanics, Mechanics of Materials

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. A.H.C. Hart, R. Koizumi, J. Hamel et al. (2017), “Velcro-Inspired SiC Fuzzy Fibers for Aerospace Applications”, ACS Applied Materials & Interfaces, Vol. 9(15), pp. 13742–13750.

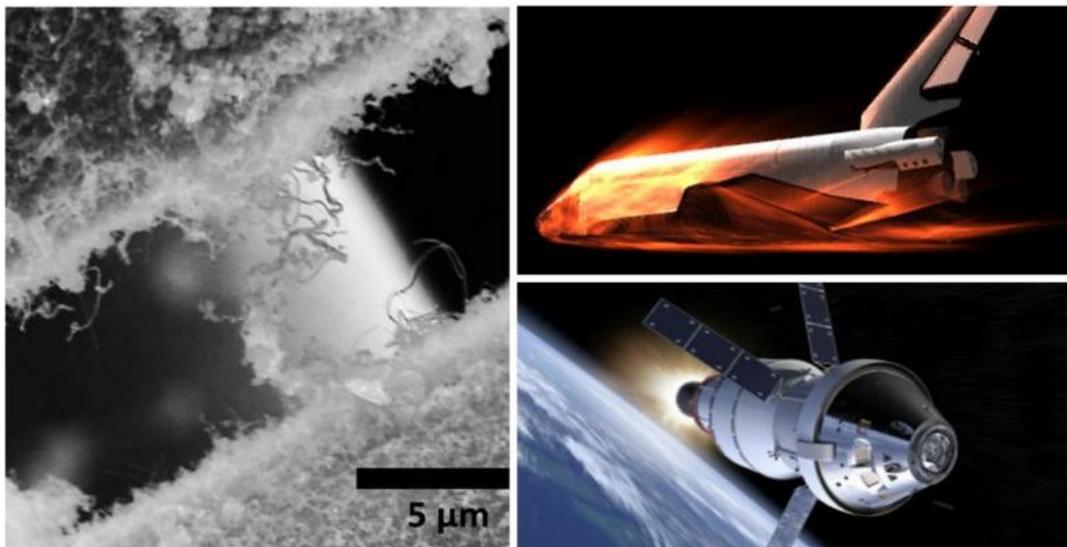
2. G. Chatzigeorgiou, F. Meraghni, N. Charalambakis, A. Benaarbia (2020), “Multiscale modeling accounting for inelastic mechanisms of fuzzy fiber composites with straight or wavy carbon nanotubes”, International Journal of Solids and Structures, Vol. 202, pp. 39–57.

3. Q. Chen, G. Chatzigeorgiou, F. Meraghni (2021), “Hybrid hierarchical homogenization theory for unidirectional CNTs-coated fuzzy fiber composites undergoing inelastic deformations”, Composites Science and Technology, Vol. 215, pp. 109012.

4.

5.

Illustrations :



TITLE:LEARNING WITH IMMERSIVE TECHNOLOGIES

Topic number : 2021_074

Field : Information and Communication Science and Technology

Subfield:

ParisTech School: Arts et Métiers

Research team: Presence & innovation <http://lampa.ensam.eu/equipe-p-i-132195.kjsp?RH=1415871394252&RF=1478611858411>

Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation

Lab location: Angers

Lab website:<http://lampa.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: RICHIR SIMON simon.richir@ensam.eu

Advisor 2: Gorisse Geoffrey geoffrey.gorisse@ensam.eu

Advisor 3: Fleury Sylvain sylvain.fleury@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: The proposed research project aims at investigating the potential of immersive technologies (virtual reality, augmented reality) to learn technical and/or scientific contents. Virtual and augmented reality have developed rapidly over the last twenty years, both in terms of hardware and software quality, which offers several potentialities and use cases. However, these technologies remain under-exploited in several fields. The digital learning transformation, particularly in higher education and professional training, requires further investigations in order to adapt to the cognitive characteristics of learners and to develop pedagogical approaches that integrate these technologies in a relevant way. Today, the main obstacles to the use of immersive technologies for learning are not only technical, but also ergonomics and pedagogical. It is necessary to identify the conditions of effectiveness of these devices by working on a better understanding of users' cognitive functioning in learning situations. More specifically, we want to study how virtual agents (autonomous characters controlled by the computer) can be used to facilitate learning. For instance, we could investigate how a virtual agent acting as a tutor could facilitate the learning of a technical procedure.

We could also study how to "capture" a teacher's lesson and how to reproduce it in a virtual environment, through a virtual agent (using the "CAPLAB" platform being installed in Laval).

In this context, experiments could be carried out to identify the optimal characteristics of this virtual tutor, in terms of realism, attractiveness and behavior, in order to enhance learners' motivation. Evaluations could focus on learning performance (memorization, understanding, ability to reproduce the task in realistic context), participant involvement, but also on learners' satisfaction in order to guarantee the acceptability of the technologies used in such contexts.

The use of artificial intelligence modules could be considered if this subject interests the selected candidate for the thesis.

This work will lead to high-level international publications that will shed light on relevant pedagogical tools and good practices for learning using immersive technologies.

Required background of the student: Master's degree in computer science with extended knowledge of virtual reality. We are looking for a candidate with an interest in multidisciplinary research, at the frontier of virtual reality and experimental psychology. A strong interest for experimental research is required: production of protocols, conducting experiments, data analysis and writing. Applicants are expected to read, speak and write academic english.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Buttussi, F., & Chittaro, L. (2017). Effects of different types of virtual reality display on presence and learning in a safety training scenario. *IEEE transactions on visualization and computer graphics*, 24(2), 1063-1076.
2. Hamilton, D., McKechnie, J., Edgerton, E., & Wilson, C. (2021). Immersive virtual reality as a pedagogical tool in education: a systematic literature review of quantitative learning outcomes and experimental design. *Journal of Computers in Education*, 8(1), 1-32.
3. Hew, K. F., & Cheung, W. S. (2010). Use of three-dimensional (3-D) immersive virtual worlds in K-12 and higher education settings: A review of the research. *British journal of educational technology*, 41(1), 33-55.
4. Makransky, G., Andreasen, N. K., Baceviciute, S., & Mayer, R. E. (2020). Immersive virtual reality increases liking but not learning with a science simulation and generative learning strategies promote learning in immersive virtual reality. *Journal of Educational Psychology*.

5. Parong, J., & Mayer, R. E. (2018). Learning science in immersive virtual reality. *Journal of Educational Psychology*, 110(6), 785.

Illustrations :



TITLE: ANALYSIS, MODELING AND SIMULATION OF PARAMETRIC RESONANCES OF PIEZOELECTRIC STRUCTURES. APPLICATION TO NANOSYSTEMS AND ENERGY HARVESTING

Topic number : 2021_075

Field : Information and Communication Science and Technology, Material science, Mechanics and Fluids, Mathematics and their applications

Subfield: Nonlinear Dynamics, Intelligent Systems, Micro/Nano Electromechanical Systems

ParisTech School: Arts et Métiers

Research team: Olivier THOMAS group <https://lispen.ensam.eu/user/87>

Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques

Lab location: Lille

Lab website: <https://lispen.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: THOMAS Olivier olivier.thomas@ensam.eu

Advisor 2: GIRAUD-AUDINE Christophe christophe.giraud-audine@ensam.eu

Advisor 3: BENACCHIO Simon simon.benacchio@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: With the developments of sensors networks and the internet of things, the problem of powering such autonomous or dormant systems becomes critical and avoiding the use of batteries could be interesting. Therefore, ongoing researches focus on ambient energy conversion thanks to phenomena such as photoelectricity, thermoelectricity or piezoelectricity. The latter conversion offers the possibility to harvest energy from vibrations and also becomes a widely used technique in the field of micro and nano electromechanical systems (M/NEMS), to replace traditional electrostatic transduction. For both energy harvesting and M/NEMS applications, parametric resonances can enhance the performance of the system. A parametric driving of a resonant system is observed if the external forcing is equivalent to the periodic modulation of a system's parameter, its stiffness for instance. In this context, this PhD proposal aims at solving some open scientific and technological

questions, in the field of numerical simulation of those nonlinear structural systems as well as on the use of the properties of parametric resonances. In particular, it aims at:

- (1) produce and exploit pertinent structural models able to predict parametric resonances in a structure, coming from either a mechanical action or a piezoelectric action. Numerical models using the finite-element methods will be at the core of the process;
- (2) use those models to optimize piezoelectric resonators;
- (3) design an electronic circuit able to enhance as much as possible the performance of a parametric harvester, in particular with switch strategies or power electronics techniques

This work will be based on theory (nonlinear oscillations, structural mechanics), numerical simulations (finite-elements, matlab) and experimental tests with up to date devices (scanning laser vibrometer, shaking table).

Required background of the student: Mechanical engineering, finite-element simulations, engineering vibrations, electronics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. O. Thomas, F. Mathieu, W. Mansfield, C. Huang, S. Trolrier-McKinstry, and L. Nicu. Efficient parametric amplification in micro-resonators with integrated piezoelectric actuation and sensing capabilities. *Applied Physics Letters*, 102(16) :163504, 2013.
2. V. Denis, M. Jossic, C. Giraud-Audine, B. Chomette, A. Renault, and O. Thomas. Identification of nonlinear modes using phase-locked-loop experimental continuation and normal form. *Mechanical Systems and Signal Processing*, 106 :430–452, 2018.
3. A. Givois, C. Giraud-Audine, J.-F. Deü, and O. Thomas. Experimental analysis of nonlinear resonances in piezoelectric plates with geometric nonlinearities. *Nonlinear Dynamics*, 102 :1451–1462, 2020. 10.1007/s11071-020-05997-6.
4. A. Givois, J.-F. Deü, and O. Thomas. Dynamics of piezoelectric structures with geometric nonlinearities : A non intrusive reduced order modelling strategy. *Computers & Structures*, 253 :106575, 2021
5. M. Berardengo, O. Thomas, C. Giraud-Audine, and S. Manzoni. Improved resistive shunt by means of negative capacitance : new circuit,

performances and multi-mode control. Smart Materials and Structures, 25(7) :075033, 2016.

Illustrations :

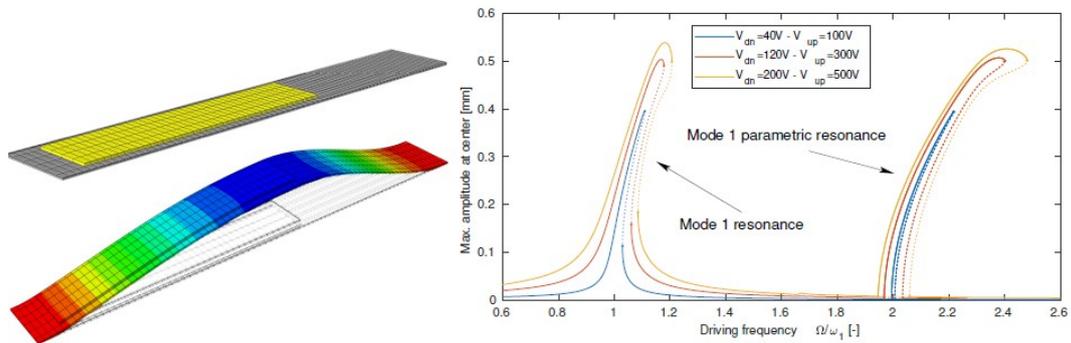
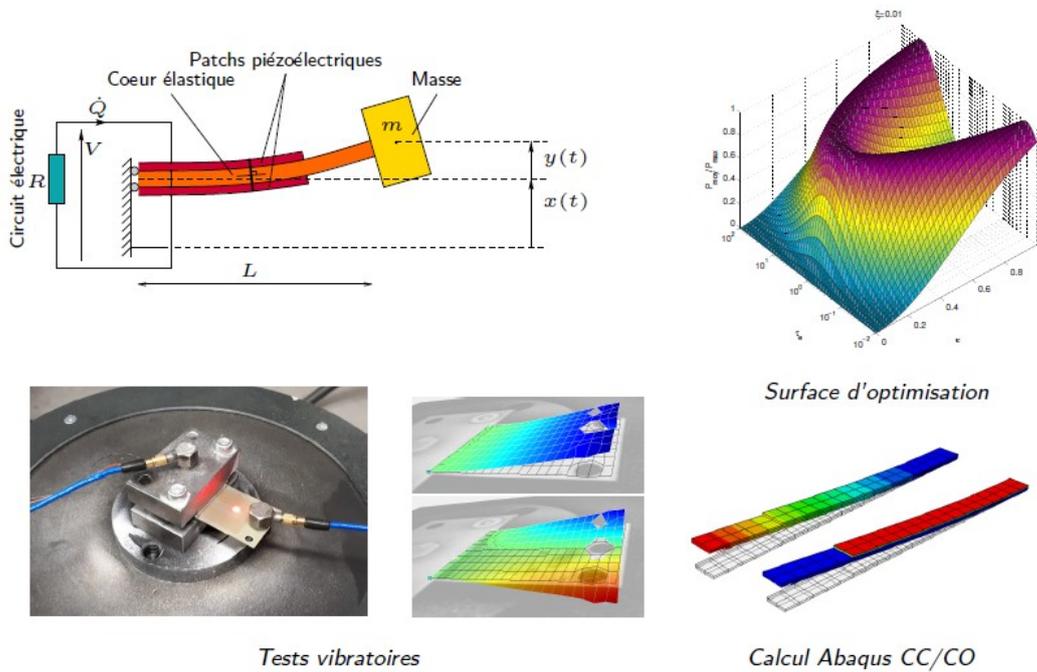


FIG. 1 – Piezoelectric laminated structure in bending subjected to piezoelectric actuation



**TITLE: MULTI-SCALE DATA-DRIVEN MODELLING OF SHORT-FIBRE
REINFORCED COMPOSITES FOR AUTOMOTIVE APPLICATIONS**

Topic number : 2021_076

Field : Material science, Mechanics and Fluids, Mathematics and their applications

Subfield:

ParisTech School: Arts et Métiers

Research team: SMART Research Group

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website: <http://www.lem3.fr>

Contact point for this topic: Arts et Métiers

Advisor 1: Meraghni Fodil fodil.meraghni@ensam.eu

Advisor 2: PRAUD Francis francis.praud@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Short-fibre reinforced composites have shown to be among the best candidates to replace the actual metallic structural components in a view to reduce the mass of vehicles in the automotive industry. This is due to their remarkable properties induced by the association of stiff and tough glass fibre reinforcements with lightweight thermoplastic matrices. However, the use of such composites gives rise to highly complex mechanical responses that strongly depend on the fibre orientation, itself linked with the moulding process as fibres tends to be oriented along the moulding flow direction. Furthermore, the mechanical behaviour of these composites is also strongly influenced by the thermoplastic matrix, which exhibits both fluid and solid properties coupled to damage mechanisms . For these reasons, short-fibre reinforced composites have an anisotropic and time-dependent behaviour resulting from the microstructure arrangement, the complex rheological behaviour of the matrix and the fibre/matrix interface degradation mechanisms occurring at the scale of the microstructure.

Over the past years, many experimental and modelling efforts have been undertaken to better understand this type of composite. On the modelling

side, multi-scale modelling techniques either employing mean-field or full-field theories have been developed to predict the macroscopic response of these composites in relation with the local behaviour of the constituents and the arrangement of the microstructure. Although these approaches provided promising results in good agreement with experimental data, the significant computational cost and the important number of microstructural parameters hamper its practical use in structure analysis.

To overcome this limitation, the objective of the proposed PhD thesis is to investigate the use of data-driven modelling techniques such as non-intrusive PGD (Proper Generalized Decomposition) to efficiently deal with the simulations of short-fibre reinforced composites for which many microstructural parameters are involved. Indeed, PGD has been used in different multi-parametric problems involved in science and engineering fields, by assuming each parameter as an extra-coordinate of the model. Therefore, approximated responses of the composite can be determined by multi-dimensional regression using a precomputed dataset of offline solutions.

Required background of the student: Mechanical engineering, Mechanics of materials, Finite element method, Mathematics

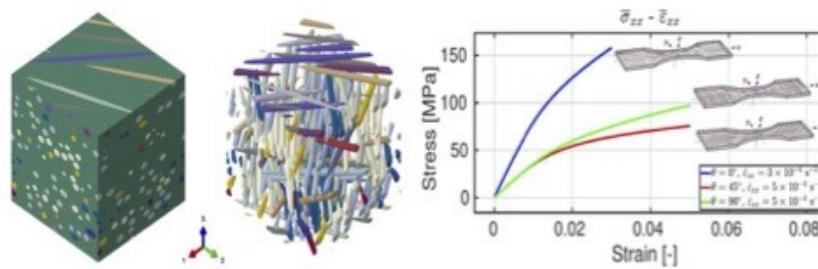
A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. F. Praud, G. Chatzigeorgiou, J. Bikard and F. Meraghni, Phenomenological multimechanisms constitutive modelling for thermoplastic polymers, implicit implementation and experimental validation, *Mechanics of Materials*, 114:9-29, 2017.
2. M. Barral, G. Chatzigeorgiou, F. Meraghni, R. Léon, Homogenization using modified Mori-Tanaka and TFA framework for elastoplastic-viscoelastic-viscoplastic composites: Theory and numerical validation, *International Journal of Plasticity*, 127:102632, 2020.
3. Q. Chen, G. Chatzigeorgiou and F. Meraghni, Extended mean-field homogenization of viscoelastic-viscoplastic polymer composites undergoing hybrid progressive degradation induced by interface debonding and matrix ductile damage, *International Journal of Solids and Structures*, 210-211:91-17, 2021.
4. F. Praud, G. Chatzigeorgiou, and F. Meraghni, Fully integrated multi-scale modelling of damage and time-dependency in thermoplastic-based

woven composites, International Journal of Damage Mechanics, 30:163–195, 2021.

5. Tikkarouchine E., Benaarbia A., Chatzigeorgiou G., Meraghni F., (2020). Non-linear FE2 multiscale simulation of damage, micro and macroscopic strains in polyamide 66-woven composite structures: analysis and experimental validation. Composite Structures: 255: 112926.

Illustrations :



**TITLE:EFFICIENT COMPUTATIONAL FRAMEWORK TO MODEL SIZE EFFECTS IN
MINIATURIZED PRODUCTS**

Topic number : 2021_077

Field : Material science, Mechanics and Fluids

Subfield: Computational mechanics, Nonlinear mechanics, Generalized continua

ParisTech School: Arts et Métiers

Research team:Méthodes Numériques, Instabilités et Vibrations
(Numerical Methods, Instabilities and Vibrations)

Research lab: LEM3 - Laboratoire d'étude des microstructures et de
mécanique des matériaux

Lab location: Metz

Lab website:<http://www.lem3.fr>

Contact point for this topic: Arts et Métiers

Advisor 1: ABED-MERAIM Farid Farid.Abed-Meraim@ensam.eu

Advisor 2: Jebahi Mohamed mohamed.jebahi@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Due to the increasing trend towards miniaturization, micro-scaled products have become widely used in various high technology fields, such as microelectronics and microbotics. However, when decreasing the geometrical size, several parameters, e.g., grain size and number of shallow grains, remain unchanged. This may result in modifying the mechanical properties of materials. As experimentally observed, in the size range between hundreds of nanometers and few tens of micrometers, the strength of materials is no longer scale-independent and the peculiar phenomenon “smaller is stronger” appears. Conventional plasticity theories cannot predict size-dependent behavior of materials, due to the lack of internal length scale(s). To overcome limitations of these theories, gradient-enhanced plasticity approaches have been proposed. These approaches, which are relatively recent, present very attractive features in capturing different kinds of size effects, making them one of the major scientific focuses of today. In this context, a flexible 2D gradient-based numerical tool has been developed in small and finite deformation frameworks. This tool has been successfully applied to study challenging

size-dependent phenomena in ultra-thin sheet metals. The very interesting results obtained by this tool have motivated the present PhD project, which aims at developing an optimized 3D extension of this numerical tool. To achieve its objectives, this project is divided into three parts. First, an enhanced gradient-plasticity model will be developed, considering the recent progress made on the gradient-based description of size effects. Then, the proposed model will be implemented using accurate numerical techniques within the gradient-based numerical platform (COMAP) developed by the project team. Finally, the implemented model will be applied to study challenging small-scale problems, particularly formability of ultra-thin sheet metals. The project developments will offer to the scientific and industrial communities an original and powerful numerical tool that can be used for numerous breakthrough applications, like numerical optimization of the microstructure of miniaturized products. This has numerous economic, environmental, and social benefits in terms of design and fabrication of more effective industrial components.

Required background of the student: - Solid background in non-linear solid mechanics and finite element formulation and simulation;
- Good analytical and programming skills (e.g., Fortran, C, C++);
- Excellent English level

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Jebahi M., Cai L., Abed-Meraim F. (2020). Strain gradient crystal plasticity model based on generalized non-quadratic defect energy and uncoupled dissipation. *International Journal of Plasticity*, 126:102617. DOI: <https://doi.org/10.1016/j.ijplas.2019.10.005>.
2. Cai L., Jebahi M., Abed-Meraim F. (2021). Strain localization modes within single crystals using finite deformation strain gradient crystal plasticity. *Crystals*, in Press. DOI: <https://doi.org/10.3390/cryst1010000>.
3. Jebahi M., Forest S. (2021). Scalar-based strain gradient plasticity theory to model size-dependent kinematic hardening effects. *Continuum Mechanics and Thermodynamics*. DOI: <https://doi.org/10.1007/s00161-020-00967-0>.
4. Jedidi M. Y., Ben Bettaieb M., Abed-Meraim F. , Khabou M. T., Bouguecha A., Haddar M. (2020). Prediction of necking in HCP sheet metals using a two-surface plasticity model. *International Journal of Plasticity*, 128 :102641

5. Ben Bettaieb M. Abed-Meraim F. (2021). Formability prediction of substrate-supported metal layers using a non-associated plastic flow rule. *Journal of Materials Processing Technology*, 287:116694

Illustrations :

TITLE:ENGINEERING OF MULTIMODAL MAGNETIC RESONANCE AND OPTICAL IMAGING USING TARGETED THERANOSTIC NANOPARTICLES FOR DIAGNOSIS AND THERAPEUTIC STUDIES AGAINST CANCER IN PRECLINICS.

Topic number : 2021_078

Field : Biology, Biophysics and Biochemistry, Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team:SEISAD Synthesis Electrochemistry Imaging and Analytical System for Diagnosis <https://iclehs.fr/research/seisad/>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website:<https://www.chimieparistech.psl.eu/recherche/les-laboratoires/i-clehs/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: DOAN Bich-Thuy bich-thuy.doan@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Cancer is a major public health problem worldwide. Clinical cancerology therefore needs the development of both: i) sensitive and efficient diagnostic methods such as bioimaging and ii) effective but better tolerated new therapies. In this context, the research for innovative and efficient systems to effectively diagnose and treat cancers is highly active: development of new nanoparticles (NP) with bioimaging features allows to consider the design of multi-functional chemical objects. These objects are probes able to be vectorized to target tumoral tissues or additionally to encapsulate medicine for therapeutical purpose.

We propose to develop quantitative multimodal and multiscale molecular bioimaging methods based on MRI and optical imaging to codevelop innovative nanomedicine based on various nanoparticles : bimodal fluorescent and magnetic liposomes, luminescent and magnetic nanoparticles synthesized in collaboration with chemists team at the Université PSL and Sorbonne Université. The task is to gather

multiparametric imaging data (molecular, anatomic, diffusion, perfusion...) to create new diagnostic imaging biomarkers applied to the study of cancer on tumor murine models.

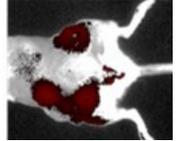
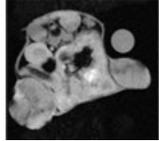
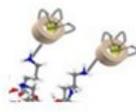
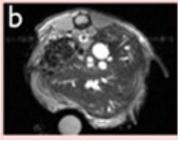
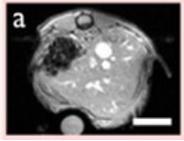
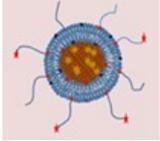
The different tasks will be : participation in the synthesis, physicochemical and imaging characterization of the theranostic probes in vitro, MRI and optical biomimaging developments adapted to the probes for antitumor therapy in preclinics.

Required background of the student: Biophysics, Imaging, Chemistry, Biology

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Ramniceanu G., Doan B.-T., Vezignol C., Graillot A., Loubat C., Mignet N. and Berret J.-F. Delayed hepatic uptake of multi-phosphonic acid poly(ethylene glycol) coated iron oxide measured by real-time Magnetic Resonance Imaging, RSC Adv., 2016,6, 63788
2. Thébault CJ, Ramniceanu G, Boumati S, Michel A, Seguin J, Larrat B, Mignet N, Ménager C, Doan BT. Theranostic MRI liposomes for magnetic targeting and ultrasound triggered release of the antivascular CA4P. J Control Release. 2020 4;322:137-148.
3. Thébault C., Ramniceanu G. , Michel A. , Beauvineau C. , Girard C. , Seguin J. , Mignet N. , Ménager C. , Doan B-T. . In Vivo Evaluation of Magnetic Targeting in Mice Colon Tumors Monitored by MRI with Ultra-Magnetic Liposomes, Mol Imaging Biol. 2019 Apr;21(2):269-278. doi: 10.1007/s11307-018-1238-3
4. Khaled W, Piraquive J, Leporq B, Wan JH, Lambert SA, Mignet N, Doan BT, Lotersztajn S, Garteiser P, Van Beers BE In vitro distinction between proinflammatory and antiinflammatory macrophages with gadolinium-liposomes and ultrasmall superparamagnetic iron oxide particles at 3.0T. J Magn Reson Imaging. 2019;49(4):1166-1173
5. Do HD, Couillaud BM, Doan BT, Corvis Y, Mignet N Advances on non-invasive physically triggered nucleic acid delivery from nanocarriers. Adv Drug Deliv Rev. 2019;138:3-17

Illustrations :



TITLE:CONTINUUM SOLVATION FOR EXTENDED PERIODIC SYSTEMS

Topic number : 2021_079

Field : Chemistry, Physical chemistry and Chemical Engineering, Life and Health Science and Technology

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team:Theoretical Chemistry and Modelling Team
<https://www.quanthic.fr>

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website:<https://iclehs.fr>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: LABAT FREDERIC frederic.labat@chimieparistech.psl.eu

Advisor 2: Adamo Carlo carlo.adamo@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Solvation effects play a fundamental role in many physical and chemical processes, with a strong influence in the photophysical properties of some molecules as well as in homogeneous and heterogeneous catalysis for instance. To consider solvation effects in quantum-mechanical calculations, continuum solvation replaces the solvent molecules by a structure-less and polarizable media characterized solely by its static relative permittivity. While continuum solvation has long been established in the molecular field, with robust models reproducing almost quantitatively the experimental data with the possibility to compute many response properties, the situation is completely different for solid-state calculations. Indeed, only very recently have some approaches been proposed to tackle continuum solvation of periodic systems such as polymers and surfaces. One such approach is the generalized Finite-Difference Poisson-Boltzmann (FDPB) approach which has been developed and implemented in our group in the Crystal code , allowing continuum solvation to be applied to various systems ranging from molecules, helices, nanotubes, polymers to surfaces . The aim of this project is to better understand, from a modeling viewpoint, the solvation of various extended periodic systems such as

oxide surfaces involved in energy-related processes, and how solvation influences the relative stability of such surfaces and their related reactivity towards simple model reactions. Care will be devoted to the selection of surfaces and reactions for which solvation plays a key role, to better understand fundamental steps in such processes and to improve them, using periodic ab-initio approaches rooted on Density Functional Theory.

Required background of the student: Physical Chemistry, Chemical Physics and, if possible, theoretical chemistry and previous programming experience.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. R. Dovesi et al. WIREs Comput Mol Sci. 8, e1360 (2018).
2. F. Labat et al. J. Chem. Theory Comput., 14, 5969 (2018).
3. D. Vassetti et al. J. Comput. Chem., 41, 1464 (2020).
4. D. Vassetti et al. J. Chem. Theory Comput., 17, 6432 (2021).
- 5.

Illustrations :

TITLE: GRAPH-BASED UNBOUNDED CONSTRAINED MODELS SEARCH FOR HIGH-LEVEL LOGICAL REASONING

Topic number : 2021_080

Field : Information and Communication Science and Technology, Mathematics and their applications

Subfield: Computer science, combinatorial algorithms, constraint programming, finite model search, graph theory, cyber-physical systems engineering.

ParisTech School: Arts et Métiers

Research team:

Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques

Lab location: Aix-en-Provence

Lab website: lispen.ensam.eu

Contact point for this topic: Arts et Métiers

Advisor 1: Pernot Jean-Philippe Jean-Philippe.Pernot@ensam.eu

Advisor 2: Kleiner Mathias mathias.kleiner@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The project is a fundamental research proposal involving algorithms and software

development. The project aims at providing an original reasoning approach for hard combinatorial problems based on the generation of finite graphs under a set of structural constraints.

More precisely, we are interested in problems where knowledge is represented in the form of an object-oriented model with additional constraints expressed in first-order predicate logic (for instance, metamodels conforming to OMG's MOF and their associated OCL constraints). In this context, a classical problem is to be able to generate an instance of the object model which satisfies all the

constraints. For instance, it can be used to automatically explore cyber-physical systems engineering alternatives given a loosely defined partial solution.

Existing approaches mostly rely on the mapping between the model and its

constraints to a lower-level constraint programming paradigm (e.g. SAT, CSP) where

resolution (e.g. constraint-based solving) is achieved. However the translations

induce drawbacks such as the loss of structure knowledge about the problem, they require to

bound the solutions potential number of elements (since real first-order logic is rarely

supported by current solvers), and some constraints are hard (or even impossible) to

translate efficiently.

The main idea behind this project is that resolution at a graph-level, using graph

generation techniques, may allow for a more efficient resolution. Indeed it is then

possible to exploit the structure of the object-model and its solutions to guide the

search more efficiently (for instance graph-based heuristics), discard unsatisfiable

partial solutions that could not be detected otherwise (for instance graph

isomorphisms), and it is not necessary to bound the number of solution elements (by

generating structures of a priori unknown size). On a more practical level, another

benefit of the approach is that it reduces the gap between the original knowledge

representation and the reasoner paradigms, hence allowing for a more integrated use

of the solver in a software chain (e.g. reverse mapping of the solution, understandable

structure-based explanations, etc.). Advances in the theoretical aspects, novel

algorithms, usecases and integration of a free software library in a model-based

software environment (such as Eclipse Modelling Framework) are among the expected

outputs of the project.

The proposed approach will be validated on multiple case studies ranging from literature toy prob-

lems to more complex applications (cyber-physical systems engineering, 3D geometry, natural lan-

guage parsing and texts generation, etc.)

Required background of the student: Computer science, excellent programming skills, combinatorial algorithms, constraint programming.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Laurent Hénocque, Mathias Kleiner, Nicolas Prcovic, “Advances in polytime isomorph elimination for configuration”, Principles and Practice of Constraint Programming-CP 2005, p. 301-313, Springer, 2005.
2. Mathias Kleiner, Marcos Didonet Del Fabro, “A generic approach to model generation operations”, Journal of Systems and Software, p 136-155, Elsevier, 2018.
3. Hu H., Kleiner M., Pernot J-P., “Over-constraints detection and resolution in geometric equation systems”, Computer-Aided Design (2017), vol. 90, pp. 84-94.
4. Gilles Gouaty, Lincong Fang, Dominique Michelucci, Marc Daniel, Jean-Philippe Pernot, Romain Raffin, Sandrine Lanquetin, Marc Neveu, “Variational geometric modeling with black box constraints and DAGs”, Computer-Aided Design 75, p. 1-12, 2016
- 5.

Illustrations :

**TITLE:PHYSICALLY INFORMED AND DATA-DRIVEN APPROACHES TOWARDS
RELIABLE SIMULATION OF THERMOPLASTIC COMPOSITE AUTOMOTIVE
COMPONENTS**

Topic number : 2021_081

Field : Design, Industrialization, Material science, Mechanics and Fluids

Subfield: Mechanical engineering, Computational mechanics, Mechanics of Materials.

ParisTech School: Arts et Métiers

Research team:Mécanique des Matériaux, des Structures et du Vivant (MMSV) / Milieux Multiphasés et couplages multiphysiques

Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux

Lab location: Metz

Lab website:<http://www.lem3.univ-lorraine.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: BENAARBIA Adil adil.benaarbia@ensam.eu

Advisor 2: Meraghni Fodil fodil.meraghni@ensam.eu

Advisor 3: NACHTANE Mourad mourad.nachtane@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: In the industry, the challenge of confronting the structural behaviour of lab tests and real structures with a thorough understanding calls for further improvement regarding the scientific tools required for the interpretation and implementation of the material behavior within commercial simulation software. Whatever the scale of description chosen, the quality and validity of simulation results naturally depend on the relevance of the behaviour equations chosen to account for the physics. The phenomenological nature of these constitutive equations generally introduces modelling errors, leading to mismatches between simulations and experimental results. The main objective of this PhD project is to propose alternative ways to overcome this limitation by merging classical simulation tools with data coming from experimental measures in a dynamic way. Several numerical algorithms, based on parameter identification and data-driven techniques, will be designed throughout the project in order to strengthen the link between data and computational mechanics, notably for automotive applications, through a holistic

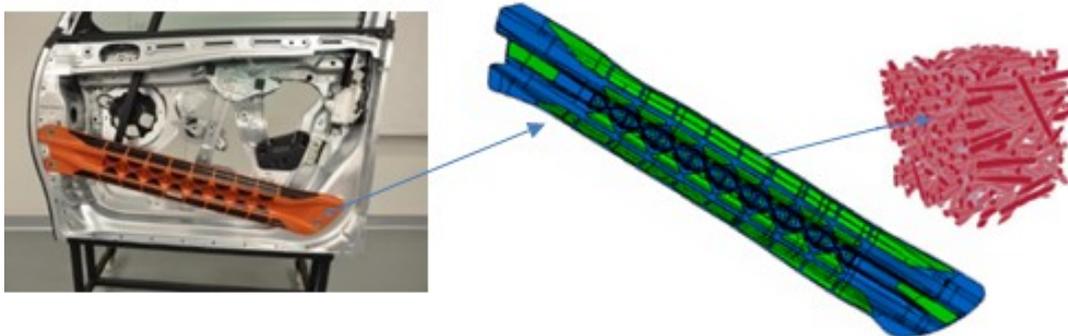
approach based on digital twin concept (simulation environments in which the designed composite properties can virtually be tested without the need for costly and time-expensive physical mock-ups). This will be coupled with Model Order Reduction techniques to overcome the computation costs and achieve computations at the real time.

Required background of the student: Applicants should have, or expect to achieve at least a Master's degree (or an equivalent overseas degree) in Mechanical Engineering. Candidates with suitable experience in computational mechanics and/or data-driven programming are welcome to apply.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Benaarbia A., Chrysochoos A. (2017). Proper orthogonal decomposition application for estimating heat sources within thermoplastic composite materials. *Quantitative Infrared Thermography Journal*, 14: 132-152.
2. Benaarbia A., Chatzigeorgiou G., Kiefer B., Meraghni F., (2019). A fully coupled thermo-viscoelastic-viscoplastic-damage framework to study the cyclic variability of the Taylor-Quinney coefficient for semi-crystalline polymers. *International Journal of Mechanical Sciences* 163: 105128.
3. Tikkarouchine E., Benaarbia A., Chatzigeorgiou G., Meraghni F., (2020). Non-linear FE2 multiscale simulation of damage, micro and macroscopic strains in polyamide 66-woven composite structures: analysis and experimental validation. *Composite Structures*: 255: 112926.
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- 5.

Illustrations :



**TITLE: SUSTAINABILITY ASSESSMENT AND MULTI-PHYSICAL/MULTI-SCALE
MODELLING OF SURFACE INTEGRITY IN MACHINING OF INCONEL 718
SUPERALLOY USING ADVANCED CUTTING TOOLS MATERIALS**

Topic number : 2021_082

Field : Material science, Mechanics and Fluids

Subfield: Mechanical Engineering, Manufacturing Processes

ParisTech School: Arts et Métiers

Research team: High Speed Machining

Research lab: LABOMAP - Laboratoire Bourguignon des matériaux et procédés

Lab location: Cluny

Lab website: <http://labomap.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: OUTEIRO Jose jose.outeiro@ensam.eu

Advisor 2: Birembaux Hélène helene.birembaux@ensam.eu

Advisor 3: Besnard Aurélien aurelien.besnard@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: The machining industry is constantly looking for new solutions to increase the productivity and the quality of products, but also to reduce the environmental footprint and cost of the process. Today, cemented carbides are the most used cutting tool material in the industry. In 2017, the worldwide production of cemented carbide exceeded 90,000 tons, being about 65% used by the machining industry. There is a need to reduce the amount of carbide materials used in the cutting tool and replace them by other high performance tool materials, such as PCBN and PCD materials.

The project is focused on the sustainable machining of Inconel 718, a superalloy largely used in the aerospace industry, using advanced tool materials and environmentally friendly metalworking fluids (MWF). The objective is to investigate and optimize the turning operation of Inconel 718 alloy using ceramic and PCBN cutting tools, and environmentally friendly MWF like liquid CO₂, for an enhanced surface integrity of aerospace components made on Inconel 718. To reach this objective multi-physical/multi-scale modelling and experimental approaches will be applied. A sustainability assessment will be conducted considering the

results obtained by these advanced tool materials and those obtained using traditional cemented carbide tools.

Required background of the student: We are looking for a highly motivated candidate with a Master's degree in Mechanical Engineering or Materials Science. A knowledge of manufacturing processes, continuum mechanics and finite element method will be considered a strong merit.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. R. M'Saoubi, T. Larsson, J.C. Outeiro, Y. Guo, S. Suslov, C. Saldana, S. Chandrasekar, "Surface integrity analysis of machined Inconel 718 over multiple length scales", CIRP Annals - Manufacturing Technology, Vol. 61/1, pp. 99-102, 2012.
2. X. Xu, J.C. Outeiro, J. Zhang, B. Xu, W. Zhao, "Machining simulation of Ti6Al4V using coupled Eulerian-Lagrangian approach and a constitutive model considering the state of stress", Simulation Modelling Practice and Theory, Vol. 110, pp. 102312, 2021.
3. I. Hamm, G. Poulachon, F. Rossi, H. Birembaux. Innovative experimental measurements of cutting temperature and thermal partition during Ti-6Al-4V orthogonal cutting. Procedia CIRP, volume 102, 2021, p. 281-286.
4. X. Xu, Jun Zhang, J.C. Outeiro, B. Xu, W. Zhao, Multiscale simulation of grain refinement induced by dynamic recrystallization of Ti6Al4V alloy during high speed machining, Journal of Materials Processing Technology, Vol. 286, pp. 116834.
5. J. C. Outeiro, J. C. Pina, R. M'Saoubi, F. Pusavec, I. S. Jawahir, "Analysis of Residual Stresses Induced by Dry Turning of Difficult-to-machine Materials", CIRP Annals - Manufacturing Technology, Vol. 57, pp. 77-80, 2008.

Illustrations :

TITLE:RECYCLING POLYURETHANE USING

Topic number : 2021_083

Field : Chemistry, Physical chemistry and Chemical Engineering, Material science, Mechanics and Fluids

Subfield:

ParisTech School: Chimie ParisTech - PSL

Research team: Matériaux, Interfaces et Matière Molle

<https://www.ircp.cnrs.fr/la-recherche/equipe-mim2/>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <https://www.ircp.cnrs.fr>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: LAIR Virginie virginie.lair@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Polyurethane (PU) is one of the most used polymers all over the world. The global production of PU was 22.9 million tons in 2017 and is increasing by 4.5% per year (Cornille et al.). As a result of the increasing quantity of PU demand, a large amount of PU waste, particularly foams, was disposed of by landfilling in the last decades. PU recycling could constitute an alternative approach to incineration or landfilling. We have recently developed a new strategy to recycle polyurethanes Rhone et al.) using base-catalyzed transurethanisation (Guichard et al.). PUs are depolymerized qualitatively in the presence of MeOH (methanol)/tetrahydrofuran as a solvent and tert-butoxide as a base catalyst (Zhao et al.). The resulting depolymerized mixture constituted by O-dimethylcarbamates and polyols can either be used as the starting material to synthesize new PUs with the transurethanisation approach or be purified to recover polyols and diisocyanates. The versatility and easy scaling-up of the experimental procedures and high depolymerization outcomes of this method make this strategy very attractive for PU recycling. We will particularly investigate the recycling of different PUs (thermoset as well as thermoplastic polyurethane) to provide high quality

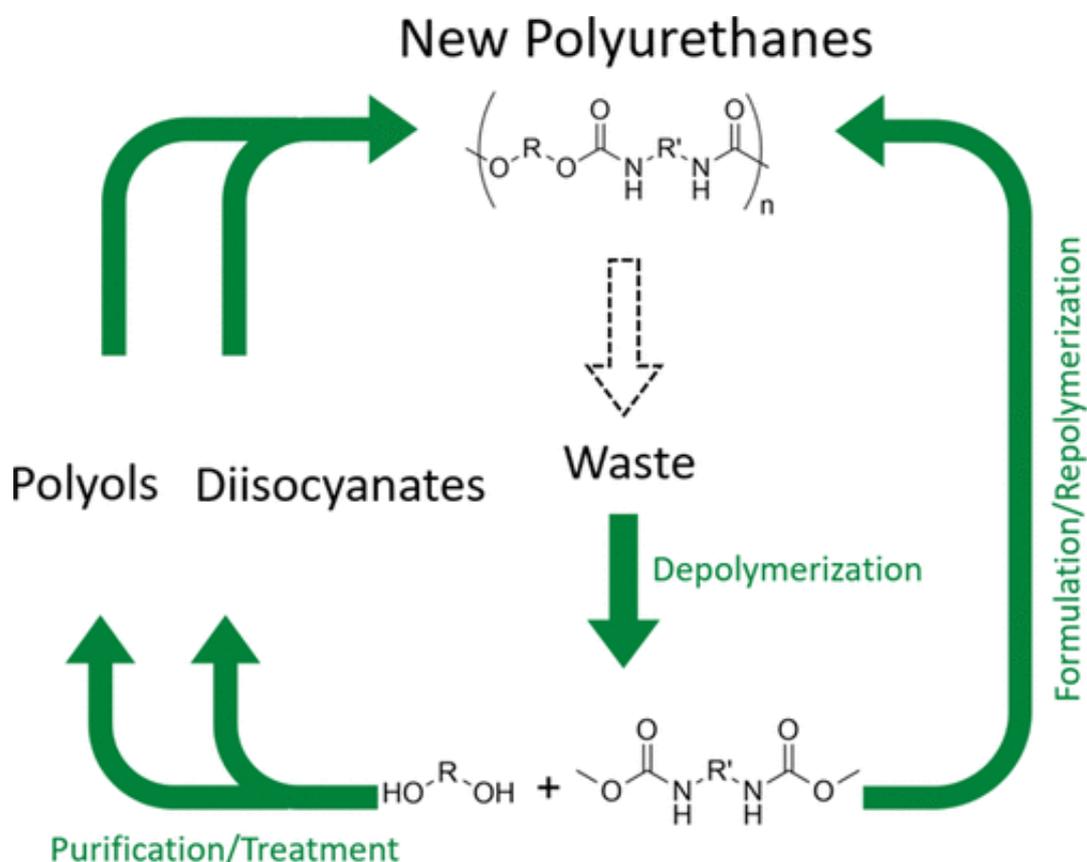
diisocyanates and polyols or high performance polyurethanes and smart materials.

Required background of the student: Chemistry, Physical Chemistry, Polymer Chemistry, Chemical engineering

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Cornille A., Auvergne R., Figovsky O., Boutevin B., Caillol S. Eur. Polym. J. 2017, 87, 535- 552.
2. Guichard G., Semetey V., Didierjean C., Aubry A., Briand J.-P., Rodriguez M. J. Org. Chem. 1999, 64, 8702-8705.
3. Rhone B., Semetey V. Synlett 2017, 28, 2004-2007.
4. Zhao L., Semetey V. ACS Omega 2021, 6, 6, 4175-4183.
5. Piñeiro-García A., Vega-Díaz S. M., Mutton G., Tristán F., Meneses-Rodríguez D., Semetey V., ChemNanoMat 2021, 7, 842-850

Illustrations :



TITLE: SPATIO-TEMPORAL VARIABILITY OF RAINFALL DROP SIZE DISTRIBUTION ACROSS SCALES: RETRIEVAL, CHARACTERIZATION AND USES

Topic number : 2021_084

Field : Environment Science and Technology, Sustainable Development, Geosciences

Subfield:

ParisTech School: Ecole des Ponts ParisTech

Research team:

Research lab: HM & Co - Hydrologie Météorologie et Complexité

Lab location: Champs-sur-Marne

Lab website: hmco.enpc.fr/

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: Tchiguirinskaia Ioulia ioulia.tchiguirinskaia@enpc.fr

Advisor 2: Gires Auguste auguste.gires@enpc.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Rainfall is a geophysical field extremely variable over wide range of spatio-temporal scales which makes it complex to analyse and even to measure. Weather radars are currently the only devices providing a spatio-temporal insight into this field. Radars basically analyse the signal backscattered by the hydrometeors of the atmosphere and derive rainfall maps from it. These conversion algorithms rely on assumed features of the rain Drop Size Distribution (DSD), and notably its homogeneity within a radar gate. DSD is also directly measured with the help of disdrometers.

The student will review and implement techniques to generate DSD maps from radar data. After, he/she develop an appropriate theoretical framework based on Universal Multifractal to explore and quantify the spatio-temporal variability of DSD. This will enable the development and validation of innovative algorithms for rain rate retrieval with weather radars which will account for the variability DSD from large scale to sub-radar gate scale.

Required background of the student: geophysics, statistics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Brandes, E.A., G. Zhang, and J. Vivekanandan, 2004: Comparison of Polarimetric Radar Drop Size Distribution Retrieval Algorithms. *J. Atmos. Oceanic Technol.*, 21, 584–598, [https://doi.org/10.1175/1520-0426\(2004\)021<0584:COPRDS>2.0.CO;2](https://doi.org/10.1175/1520-0426(2004)021<0584:COPRDS>2.0.CO;2)
2. Gires, A., Tchiguirinskaia, I., and Schertzer, D.: Multifractal comparison of the outputs of two optical disdrometers, *Hydro. Sci. J.*, 6, 1641–1651, <https://doi.org/10.1080/02626667.2015.1055270>, 2015.
3. Schertzer, D. and Lovejoy, S., 2011. Multifractals, generalized scale invariance and complexity in geophysics. *International Journal of Bifurcation and Chaos*, 21 (12), 3417–3456.
[doi:10.1142/S0218127411030647](https://doi.org/10.1142/S0218127411030647)
- 4.
- 5.

Illustrations :

TITLE: DESIGN A SAFE WORK-CELL FOR HUMAN-ROBOT CO-ACTIVITY IN INDUSTRY

Topic number : 2021_085

Field : Design, Industrialization

Subfield:

ParisTech School: Arts et Métiers

Research team:

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://lcfc.ensam.eu>

Contact point for this topic: Arts et Métiers

Advisor 1: RAHARIJAONA Thibaut thibaut.raharijaona@univ-lorraine.fr

Advisor 2: WU Yier yier.wu@ensam.eu

Advisor 3: SAVIN Jonathan jonathan.savin@inrs.fr

Advisor 4:

Short description of possible research topics for a PhD:

Collaboration between a human operator and a robot is a key feature of the “industry of the future”. The increasing interactions between humans and robots raise questions in terms of occupational risk prevention. For instance, how can we ensure, at the earliest stage of a work-cell design, that protective devices are properly chosen and placed at the appropriate safety distances? Conventional design methods rely on the “worst-case hypothesis” given by the robot manufacturer to implement safety equipment and strategies. These methods often lead to over-evaluation of the safety criteria, typically an overestimated breaking distance, which drastically reduces the system performance.

We need to know how to combine robot performance and human safety in a cobotic cell. The thesis aims at: (i) Identifying the potential hazardous zones according to the manufacturing task (robot trajectory, external loading, etc), in order to optimize the placements of safety equipment. (ii) Developing the perception of the human presence in the shared work-cell by sensor implementation (eg. with a depth camera and/or distance sensors), and adapting the robot’s control strategy accordingly. (iii) Developing the human operator perception by using an augmented reality of the work-cell in order to distinguish the safe and dangerous working area in real-time. The overall aim of the thesis is to develop real-time

robot simulation and control according to human presence in the work-cell via sensor data fusion technologies. We will validate the design method on robots working in a real industrial scenario.

Required background of the student: Robotic modeling and control, Sensor implementation, Data fusion

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. J. Savin, J. Baudoin, J.P. Bello and Y. Wu, "Dynamic simulation of the stopping performance of an industrial robot for the design of a safe work-cell", 10th international conference on safety of industrial automated systems, 2021.

2. P. Martin, B. Daille-Lefèvre, J. Marsot, X. Godot, G. Abba, A. Siadat, and M. Gomez-Echeverri. "New Issues for Workers Safety in the Factory of the Future." In Advances on Mechanics, Design Engineering and Manufacturing II, 402-411, 2019.

3. B. Tahar-Hakim, M. Bounouar, R. Bearee, and A. Siadat. "Industry of the Future, Future of Work: The Case of Collaborative Robotics." In Proceedings of the 21st Congress of the International Ergonomics Association (IEA 2021), 29-35, 2021.

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Illustrations :

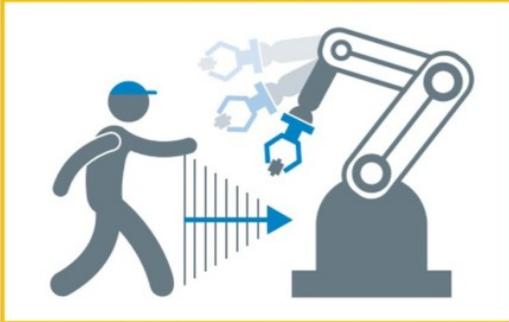
MODE 1 - Safety-rated monitored stop



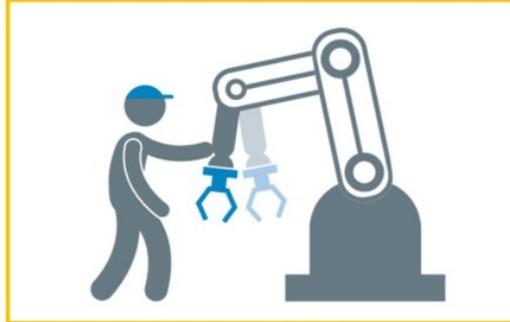
MODE 2 - Hand-guiding



MODE 3 - Speed and separation monitoring



MODE 4 - Power and force limiting



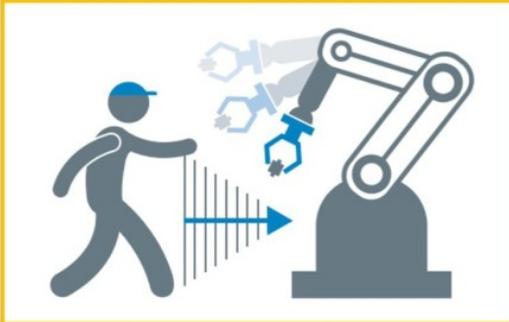
MODE 1 - Safety-rated monitored stop



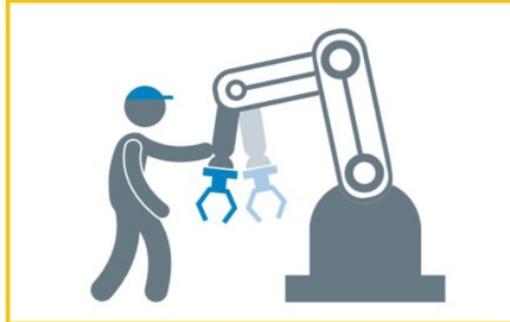
MODE 2 - Hand-guiding



MODE 3 - Speed and separation monitoring



MODE 4 - Power and force limiting



TITLE:INTELLIGENT VISUAL ANALYTICS FOR THE DESIGN AND MONITORING OF TURBO ENGINE SYSTEMS

Topic number : 2021_086

Field : Design, Industrialization, Information and Communication Science and Technology, Material science, Mechanics and Fluids

Subfield: Intelligent Design and monitoring of Sustainable Systems

ParisTech School: Arts et Métiers

Research team:Turbomachines

<https://lifse.artsetmetiers.fr/equipes/turbomachines>

Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques

Lab location: Paris

Lab website:<https://lifse.artsetmetiers.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: GARBAYA Samir samir.garbaya@ensam.eu

Advisor 2: KHELLADI Sofiane sofiane.khelladi@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Turbomachines are complex machines with components that could fail or develop faults when operating. These problems could be difficult to handle and can have an impact on other components in the case of failure. The prediction of the machine states and the remaining useful life (RUL) in real time mode are important objectives. This could allow reducing maintenance costs and the stock of spare parts. The main objective of this PhD thesis is to develop innovative methodologies of visual analytics and machine learning to support the design and monitoring of the functioning of turbo engine systems. Real-time monitoring and data capture such as noise/vibration, energy consumption, heat/temperature, pressure, wear, etc. are necessary to extract the knowledge to optimize the machine design at the virtual prototyping stage and take proactive actions to prevent the machine failure during the operation of the physical systems.

Required background of the student: Applicants must have completed a Master of Engineering in a discipline related to mechanical

engineering. Prospective applicants must have skills in Computational fluid dynamics, Experimental fluid dynamics and Turbomachines, Machine learning, Sensor technologies and Real-time data capture and analysis.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Maryam Boumrah, Samir Garbaya and Amina RADGUI, "Real-Time Visual Analytics for Patient's Health Monitoring", Visualization of Information and Scientific data, Visu 2021, 8 June 2021, (<https://journee-visu.github.io/2021/documents/boumrah.pdf>)
2. Garbaya, S., Romano, D. and Hattar, G. (2019), "Gamification of assembly planning in virtual environment", Assembly Automation, Vol. 39 No. 5, pp. 931-943. <https://doi.org/10.1108/AA-10-2018-0147>
3. Samir Garbaya and Vincent Hugel, "Modelling Movement Time for Haptic-enabled Virtual Assembly", the International Conference on Human Computer Interaction Theory and Applications (HUCAPP), 27-29 February 2020, Valletta, Malta
4. OUZANI R., Khelladi S., Danlos A., (2020) Mixing in turbulent compressible heated coaxial jets: a numerical study - International Journal of Hydrogen Energy, Vol.45, Issue 33, pp. 16816-16837, 2020. <https://doi.org/10.1016/j.ijhydene.2020.01.194>
5. H. Vanaei, M. Deligant, K. Raissi, S. Khelladi, A. Tcharkhtchi, (2020) Influence of process parameters on thermal and mechanical properties of PLA fabricated by Fused Filament Fabrication - Polymer Engineering and Science

Illustrations :

**TITLE:ULTRASONIC IMAGING OF SOFT GRANULAR MATERIALS
AND BIOMEDICAL APPLICATIONS**

Topic number : 2021_087

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield: Applied Physics, Physical acoustics

ParisTech School: ESPCI Paris - PSL

Research team:Wave in complex media

Research lab: Institut Langevin

Lab location: Paris

Lab website:<https://www.institut-langevin.espci.fr>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: JIA Xiaoping xiaoping.jia@espci.fr

Advisor 2: GENNISSON Jean-Luc jean-luc.gennisson@universite-paris-saclay.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Understanding the microscopic origin of behavior in particulate and particle-fluid systems such as granular media, foams, and emulsions are of practical and fundamental importance (A. Liu and S. Nagel, Jamming is not just cool anymore, Nature 21, 396 (1998)). In this PhD project, we will investigate the mechanical behavior of an assembly of immersed gel beads (isodense) by ultrasound imaging (transient elastography) and rheology. Such a soft granular medium or suspension makes it possible to study a material not only close to the concerns of the biomedical field (muscles and tissues) but also relevant to the physics of complex systems such as the transition from a liquid state to a solid state .

In this work, we first use an ultrafast ultrasound scanner (Aixplorer, Supersonic Imagine) to monitor the oscillatory shear wave inside optically opaque, dense gel beads packing generated by a vibrating metallic plate (Fig. 1). We are particularly interested by the nonlinear response such as shear elastic softening and fracture dynamics as a function of the shear impact (Fig. 2a). Such transient elastography was originally developed in our laboratory to track tissue motion induced by low-speed shear waves for the medical imaging . Moreover, we will also use the dynamics by the

oscillatory or stationary rheology (Fig. 2b) , combined with the ultrasonic imaging of the structure change with plastic rearrangements of particles.

Finally, we will investigate the effects of the particle shape (e.g., granular dimers/trimers) and the anisotropic force chains, responding to external load (M. Miskin and H. Jaeger, Adapting granular materials through artificial evolution, *Nature Materials* 12, 326 (2013)). This investigation concerns the study of a possible system for the production of artificial skeletal muscles whose mechanical properties can be modified and produce the desired force to dissipate the mechanical energy of external impact. We will also explore the idea of a nematic phase transition of liquid crystals (Fig. 2b) which cause a sudden contraction beyond a certain temperature (P. G. de Gennes, A semi-fast artificial muscle, *C. R. Acad. Sci. Paris* 324, 343 (1997)).

This work will be carried out, in collaboration with the Biomaps, Laboratoire d'Imagerie Biomédicale Multimodale at Paris-Saclay University.

Required background of the student: A good background in physics and particularly acoustics and mechanics. The management and interpretation of images generally use the MATLAB and /or Python language with which the candidate should be familiar.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. X. Jia, C. Caroli, and B. Velicky, "Ultrasound propagation in externally stressed granular media", *Phys. Rev. Lett.* 82, 1863 (1999) & *Phys. Rev. Focus* 3, story 12
2. P. Johnson and X. Jia, "Nonlinear dynamics, granular media and dynamics earthquake triggering", *Nature* 437, 871 (2005)
3. J. Brum, J.-L. Gennisson, M. Fink, A. Tourin & X. Jia, "Drastic slowdown of the Rayleigh-like wave in unjammed granular suspensions", *Phys. Rev. E* 84, 020301 (2019)
4. S. Catheline, J.-L. Gennisson, M. Tanter, and M. Fink, "Observation of shock transverse waves in elastic media", *Phys. Rev. Lett.* 91, 164301 (2003)
5. J. Léopoldès and X. Jia, "Probing intermittency and reversibility in a dense granular suspension under shear using multiply scattered ultrasound", *Soft Matter* (2020), DOI: 10.1039/D0SM01427C

Illustrations :

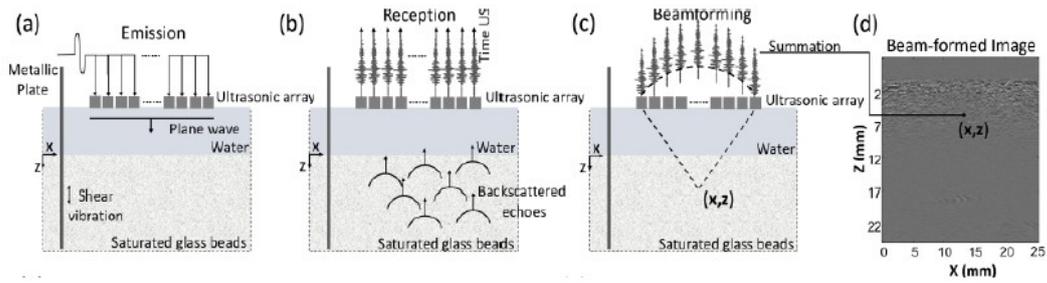


Fig. 1 (a) Ultrasound emission step: all elements in the array emit simultaneously a short pulse centered at 4 MHz, thus generating a pulsed plane ultrasonic wave (b) Ultrasound reception step: the backscattered echoes coming from different locations within the medium are recorded by each element of the transducer array. (c) Beam-forming step: relate the arrival time of an ultrasound echo to a given position within the imaging plane, each point (x, z) in the image is obtained by adding coherently the backscattered signals originating from it (d).

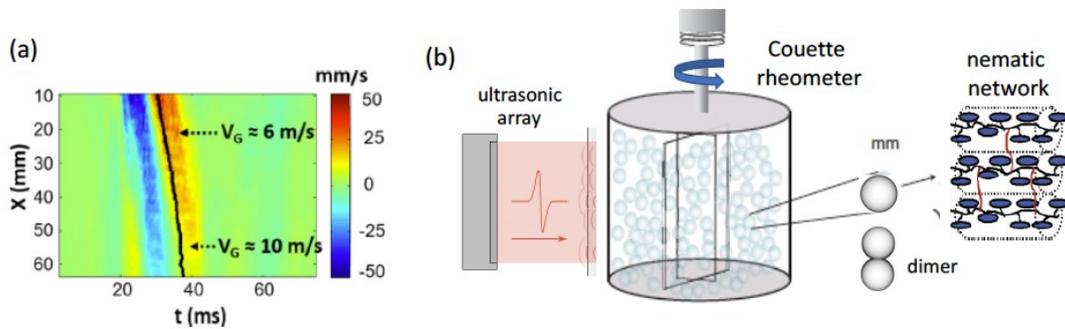


Fig. 2 (a) Particle velocity fields associated with a shear wave propagation inside a granular medium (Fig. 1). (b) The gel bead packing is sheared at constant speed in a Couette-like rheometer and analyzed using ultrasound imaging.

TITLE:PHYSICS AND ALGORITHMS FOR MOLECULAR MODELING

Topic number : 2021_088

Field : Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team: Theory <https://turner.pct.espci.fr/~amaggs/index2.html>

Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle

Lab location: Paris

Lab website: <https://www.gulliver.espci.fr/?-home-&lang=en>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Maggs Anthony anthony.maggs@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Molecular modeling (research rooted in particle-based computation) is central to our understanding of the material world. Its methods allow one to investigate complex phenomena in biophysics and materials research, and to describe the fundamental phase behavior of the universe that surrounds us. Molecular modeling has provided methods for many other fields, from astrophysics to hydrodynamics, statistical mechanics and field theory. Molecular modeling is an interdisciplinary research field, in which the development of algorithms plays an important role. Improved sampling methods, constrained ensembles, and novel approaches beyond molecular dynamics stand out in their promise for the future.

Although the principal methods have been developed for over half a century, disruptive development continues to take place. An example is the irreversible Markov-chain Monte Carlo methods which violate the fundamental detailed-balance condition yet converge towards equilibrium. They illustrate that past algorithms were overly restrictive. Radically new Markov-chain Monte Carlo algorithms have already led to the resolution of long-standing controversies (as for example in two-dimensional melting studied through the use of irreversible Markov chains). We wish to extend these methods to standard interaction potentials in soft-matter physics, in the belief that this can lead to highly

efficient codes that explore equilibrium configurations under irreversibility conditions.

Required background of the student: Physics, applied mathematics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Event-chain Monte Carlo with factor fields

Z Lei, W Krauth, AC Maggs

Physical Review E 99 (4), 043301

2. Sparse hard-disk packings and local Markov chains

P Hoellmer, N Noirault, B Li, AC Maggs, W Krauth

arXiv preprint arXiv:2109.13343

3. All-atom computations with irreversible Markov chains

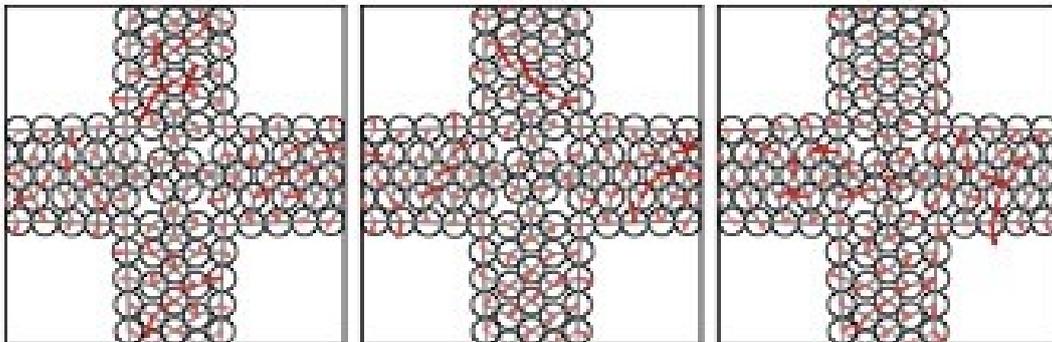
MF Faulkner, L Qin, AC Maggs, W Krauth

The Journal of chemical physics 149 (6), 064113

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Illustrations :



**TITLE:ARTIFICIAL GROUND FREEZING : FROM LABORATORY EXPERIMENTS
DEVELOPMENT TO IN-SITU SCALE PREDICTIONS**

Topic number : 2021_089

Field : Environment Science and Technology, Sustainable Development, Geosciences, Material science, Mechanics and Fluids

Subfield:

ParisTech School: MINES ParisTech - PSL

Research team:Géologie de l'Ingénieur et Géomécanique

Research lab: GEOSCIENCES - Centre de Géosciences

Lab location: Fontainebleau

Lab website:<https://www.geosciences.minesparis.psl.eu/>

Contact point for this topic: MINES ParisTech - PSL

Advisor 1: Rouabhi Ahmed emad.jahangir@mines-paristech.fr

Advisor 2: Jahangir emad emad.jahangir@mines-paristech.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Artificial ground freezing (AGF), a technique that allows to temporarily waterproof and consolidate the ground, is becoming an increasingly relevant solution for underground construction in urban areas as well as for mining operations.

Mines-Paristech team has taken part formerly in study of the thermo-hydro-mechanical coupling effect on the ground artificial freezing (Tounsi thesis 2019).

The current proposed subject is on the continuity of the Tounsi works, where the newly developed tri-axial cell will be used to impose a more realistic thermo-mechanical stress path of ground artificial freezing. For in-situ scale, the freezing process starts and progress from inside (near to the freezing pipe) towards the outside of the frozen zone. In laboratory scale (except for some rare experiences performed by gas injection) the freezing is generally obtained by placing the soil/rock sample in a cold (air-conditioned) chamber. By doing so, the outer part of sample freezes first and imposes an undrained condition during the rest of the test. This can modify the frozen materials behavior and make them less sensitive to confining pressure effect. To overcome this issue, a new test facility will be added to the used cell during this proposed thesis to promote the

freezing process from inside to outside of sample.

The successful candidate will participate actively on the enhancement of the above-mentioned laboratory test and eventually on improvement of the existent constitutive model formulation that will be finally integrated into a numerical finite element code.

Required background of the student: Rock and soil mechanics, Solid mechanics, Finite element method.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Rouabhi, A., Jahangir, E., and Tounsi, H. (2018). Modeling heat and mass transfer during ground freezing taking into account the salinity of the saturating liquid. *International Journal of Heat and Mass Transfer*, 120 :523-533.
2. Tounsi H., Rouabhi A., Jahangir E., Guérin F. (2020-a). Mechanical behavior of frozen metapelite: Laboratory investigation and constitutive modeling, *Cold Regions Science and Technology*, Volume 175, 2020, 103058.
3. Tounsi, H., Rouabhi, A., & Jahangir, E. (2020-b). Thermo-hydro-mechanical modeling of artificial ground freezing taking into account the salinity of the saturating fluid. *Computers and Geotechnics*, Volume 119, 103382.
4. Vitel, M., Rouabhi, A., Tijani, M., & Guérin, F. (2015). Modeling heat transfer between a freeze pipe and the surrounding ground during artificial ground freezing activities. *Computers and Geotechnics*, 63, 99-111. doi:10.1016/j.compgeo.2014.08.004.
5. Vitel, M., Rouabhi, A., Tijani, M., Guérin, F. (2016). Modeling heat and mass transfer during ground freezing subjected to high seepage velocities. *Computers and Geotechnics*, 2016, 73, pp. 1-15.

Illustrations :



Artificial ground freezing : from laboratory experiments development to in-situ scale predictions

Ecole Doctorale 398 Géosciences et Ressources Naturelles
Centre de GEOSCIENCES de Mines ParisTech
35, Rue Saint Honoré, 77305 Fontainebleau Cedex
Director: Ahmed Rouabhi
Co-director: Emad Jahangir
Contact: Emad.Jahangir@mines-paristech.fr

Approach:

Artificial ground freezing (AGF), a technique that allows to temporarily waterproof and consolidate the ground, is becoming an increasingly relevant solution for underground construction in urban areas as well as for mining operations. AFG is done by circulating coolant fluid through freezing tubes that are in contact with the ground. The freezing process is a time and cost dependent operation, where for a quick need to create a frozen area (such as stop ground contamination, e.g. Fukushima nuclear disaster) a supercooling refrigerant, as liquid nitrogen (~ -196 °C), should be used. However, when slower freezing kinetics are sufficient, brine between -20 °C and -30 °C could be used at lower cost.

Through heat exchange between the soil (initially fully or partially saturated with water) and the freezing tube, a thermo-hydro-mechanical (THM) process occurs and an adequate modelling approach is usually necessary to obtain reliable predictions of the process.

This THM coupled process gives rise to the following principal scientific challenges:

- estimation of the extent of the frozen area ;
- phase change problem in the ground and evolution of the thermo-hydraulic characteristics;
- mechanical behavior of the frozen area.

Mines-Paristech team has taken part formerly in study of these themes in the context of different applications as freezing of rocky aquifers for the exploitation of uranium mines, construction of an ice wall for the exploitation of an open pit mine, tunnel stability, etc., through both numerical and experimental investigations. The performed research highlighted the importance of the hydro-mechanical coupling (Vitel, 2015), heat exchange throughout freeze pipe wall (Vitel et al, 2015), high flow velocity due to the hydraulic gradient during freezing (Vitel, 2016), the hyper salinity of the natural water contained in the porous medium (Rouabhi et al, 2018) and the thermo-hydro-mechanical coupling effect on the ground artificial freezing (Tounsi et al, 2020-a&b). This latter was treated through Tounsi Ph.D thesis (2019) performing temperature controlled tri-axial tests where the strain gauges measurements for low temperatures were developed and validated.

**TITLE: COHERENT DIPOLE-DIPOLE COUPLING OF QUANTUM EMITTERS AND
MANIPULATION OF THEIR DEGREE OF ENTANGLEMENT**

Topic number : 2021_090

Field : Physics, Optics

Subfield: Quantum optics

ParisTech School: Institut d'Optique Graduate School

Research team: Nanophotonics group

Research lab: LP2N - Laboratoire Photonique, numérique et
nanosciences

Lab location: Bordeaux

Lab

website: <https://sites.google.com/site/bordeauxnanophotonicsgroup/home>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: LOUNIS Brahim brahim.lounis@u-bordeaux.fr

Advisor 2: TREBBIA Jean-Baptiste jean-baptiste.trebbia@u-bordeaux.fr

Advisor 3:

Advisor 4:

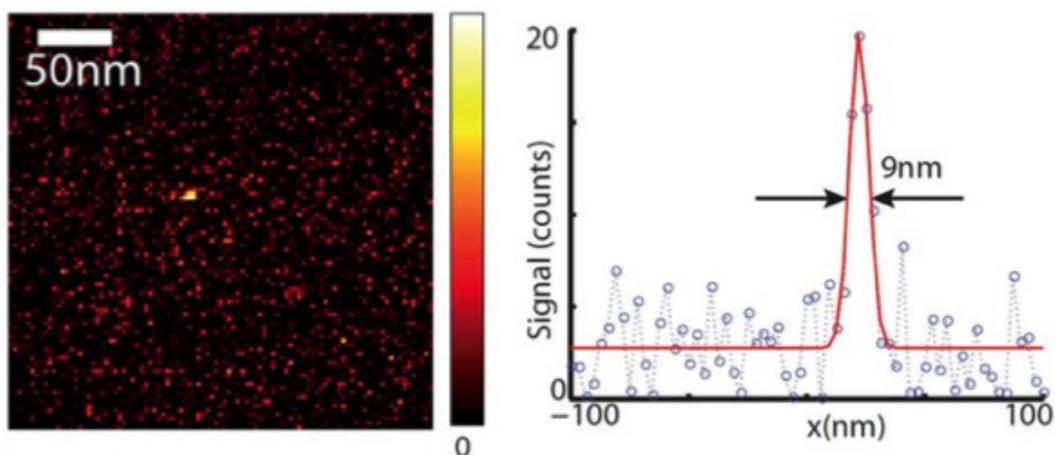
Short description of possible research topics for a PhD: The controlled, coherent manipulation of quantum systems is an important challenge in modern science, with significant applications in quantum technologies. Solid-state quantum emitters such as single molecules, quantum dots and defect centers in diamond are promising candidates for the realization of entangled quantum bits and quantum networks. Collective quantum dynamics resulting from coherent dipole-dipole coupling is challenging, since they require nanometric distances between emitters, the degeneracy of their optical resonances and low temperatures. We will aim at developing experimental schemes to find coupled quantum emitters and manipulate their degree of entanglement with external fields. The optical super-resolution nanoscopy technique built in the group (with sub 10-nm far-field optical resolution at cryogenic temperatures) will be used to reveal the rich space-frequency signatures of coherent coupled quantum emitters. The formation of collective quantum states from coupled optical emitters being a general phenomenon, these experimental schemes can also be useful for the study of many other systems including light harvesting complexes polymer conjugates, quantum dots molecules and hybrid systems.

Required background of the student: Quantum physics, optics, light-matter interaction, lab training. The thesis will be mainly experimental. The candidate will also develop theoretical simulations and acquire a strong background in laser spectroscopy, single photon detection, quantum optics...

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Optical Nanoscopy with Excited State Saturation at Liquid Helium Temperatures B. Yang, et al.,
Nature Photonics, 9 (2015) 658-662.
2. Indistinguishable near-infrared single photons from an individual organic molecule J.-B. Trebbia et al.,
Phys. Rev. A. 82 (2010) 063803.
3. 3D optical nanoscopy with excited state saturation at liquid helium temperatures, J.-B. Trebbia, R. Baby, P. Tamarat, and B. Lounis, Optics Express, 27 (2019) 23486
4. A solid state source of photon triplets based on quantum dot molecules, M. Khoshnegar et al.,
Nature Communications 8 (2017) 15716.
5. Optical Manipulation of Single Flux Quanta, I. S. Veshchunov et al., ,
Nature Communications 7 (2016) 12801.

Illustrations :



**TITLE: ACTIVE LIQUID CRYSTALS: CONTROLLING ACTIVE FLOWS THROUGH
"SMART CONFINEMENT"**

Topic number : 2021_091

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield:

ParisTech School: ESPCI Paris - PSL

Research team: Lopez-Leon's team

Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle

Lab location: Paris

Lab website: <https://www.gulliver.espci.fr/>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Lopez-Leon Teresa teresa.lopez-leon@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Active liquid crystals are bio-inspired materials combining biofilaments and motor proteins. When confined to an interface, these biofilaments form bundles that locally orient parallel to each other, developing long-range orientational order, also called nematic order. The motor proteins bring the biofilaments bundles into motion by consuming ATP. This results in a fascinating system with autonomous motion, which continuously reorganizes its structure and flows over time. This distinctive behavior conceals another significant feature of active liquid crystals: their capability to adapt to the environments where they reside. For instance, geometrical confinement tends to control active flows, replacing the bulk chaotic dynamics usually observed in unconstrained situations, by more regular flow configurations. Preliminary studies in the lab have shown encouraging pathways to control active flows using curvature and wall patterning. The goal of this PhD is to take advantage of these findings to design "smart" confining geometries, using high-resolution 3D-printing, which will allow us to induce pre-designed dynamical states in the system. This study will be relevant for potential applications, including autonomous microfluidic devices or bio-inspired micro-machines, and in assessing the pertinence of the concepts of active matter in the

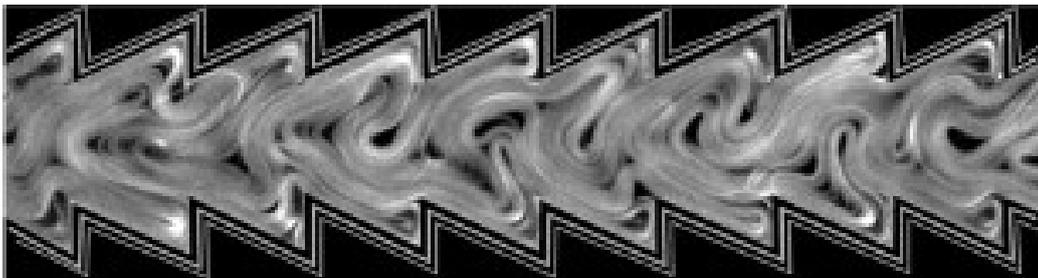
description of biological systems. This work will be done in the Gulliver lab at ESPCI, in collaboration with the University of Barcelona and the University of Chicago.

Required background of the student: physics/physical chemistry/biophysics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. J. Hardoüin, R. Hughes, A. Doostmohammadi, J. Laurent, T. Lopez-Leon, J. M. Yeomans, J. Ignés-Mullol, F. Sagués, *Commun. Phys.* 2, 121 (2019)
2. J. Hardouin, J. Laurent, T. Lopez-Leon, J. Ignés-Mullol, F. Sagues, *Soft Matter* 16, 9230 (2020)
3. L. Tran, M. O. Lavrentovich, G. Durey, A. Darmon, M. F. Haase, N. Li, D. Lee, K. J. Stebe, R. D. Kamien and T. Lopez-Leon, *Physical Review X*, 7, 041029 (2017)
4. F. Serra, U. Tkalec, T. Lopez-Leon "Editorial: Topological Soft Matter" *Frontiers in Physics* 8, 373 (2020)
- 5.

Illustrations :



Active nematic confined to a ratchet channel: the pattern of the wall induces directional flows and transport along the channel.

**TITLE: EXPLORING THE OPTICAL PROPERTIES OF PEROVSKITE SINGLE
NANOCRYSTALS AND SUPERLATTICES**

Topic number : 2021_092

Field : Physics, Optics

Subfield: Nanophysics

ParisTech School: Institut d'Optique Graduate School

Research team: Nanophotonics group

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab

website: <https://sites.google.com/site/bordeauxnanophotonicsgroup/home>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: LOUNIS Brahim brahim.lounis@u-bordeaux.fr

Advisor 2: TAMARAT Philippe philippe.tamarat@u-bordeaux.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Lead halide perovskites exhibit outstanding optical and electronic properties for a wide range of applications in optoelectronics and for light-emitting devices. Yet, the physics of the band-edge exciton, whose recombination is at the origin of the photoluminescence, is the subject of ongoing debate. In particular, the long-lived ground exciton of lead halide perovskite nanocrystals plays a major role in the quantum properties of the emitted light, since it promotes the formation of biexcitons and thus the emission of correlated photon pairs. Future investigations will aim at reducing the dephasing rate and spectral diffusion in these materials and improve the indistinguishability character of the emitted photons. With a view to the realization of ideal sources of entangled photons, we will aim at achieving degenerate bright triplet emission. We will also study the quantum optical properties of the photoluminescence stemming from lead halide NCs that are self-organized into highly ordered three-dimensional superlattices. We will investigate the spectroscopic and temporal signatures of collective coupling of the nanocrystals, which should give rise to the many-body quantum phenomenon of superfluorescence. Such entangled multi-photon quantum light sources should fuel the

development of next-generation devices for quantum technologies. These activities will be led in close collaboration with the group of chemists of M. Kovalenko (ETH Zürich).

Required background of the student: Quantum physics, optics, solid-state physics, lab training.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. « Revealing the Exciton Fine Structure in Lead Halide Perovskite Nanocrystals»

L. Hou, P. Tamarat, B. Lounis

Nanomaterials 11 (2021) 1058.

2. « The dark exciton ground state promotes photon-pair emission in individual perovskite nanocrystals »

P. Tamarat, L. Hou, J.-B. Trebbia, A. Swarnkar, L. Biadala, Y. Louyer, M.

I. Bodnarchuk, M. V. Kovalenko, J. Even, B. Lounis

Nature Communications 11 (2020) 6001.

3. « The ground exciton state of formamidinium lead bromide perovskite nanocrystals is a singlet dark state »

Philippe Tamarat, Maryna I. Bodnarchuk, Jean-Baptiste Trebbia, Rolf Erni,

Maksym V. Kovalenko , Jacky Even and Brahim Lounis

Nature Materials, 18 (2019) 717-724.

4. “Unraveling exciton-phonon coupling in individual FAPbI₃ nanocrystals emitting near-infrared single photons”

M. Fu, P. Tamarat, J.-B. Trebbia, M. I. Bodnarchuk, M. V. Kovalenko, J.

Even, B. Lounis

Nature Communications, 9, 3318 (2018).

5. « Neutral and charged exciton fine structure in single lead halide perovskite nanocrystals revealed by magneto-optical spectroscopy »

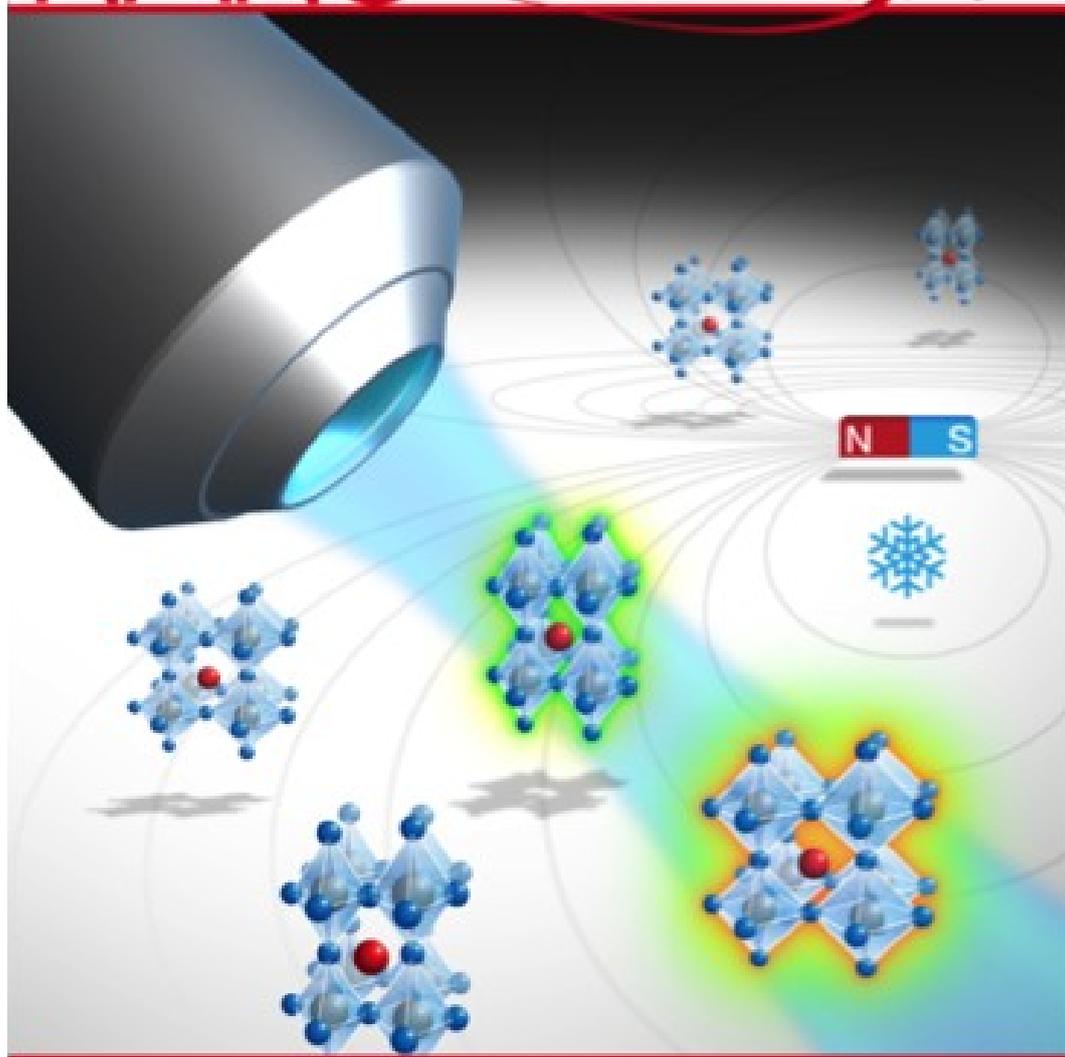
Ming Fu, Philippe Tamarat, He Huang, Jacky Even, Andrey L. Rogach, and Brahim Lounis

Nano Letters, 17 (2017) 2895-2901.

Illustrations :

NANO LETTERS

June 2015
Volume 21, Number 6
pubs.acs.org/nanoltr



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TITLE: FAST JOSEPHSON-JUNCTION CONTROL BY OPTICAL MANIPULATION OF A FLUX QUANTUM

Topic number : 2021_093

Field : Physics, Optics

Subfield: Superconductivity

ParisTech School: Institut d'Optique Graduate School

Research team: Nanophotonics group

Research lab: LP2N - Laboratoire Photonique, numérique et nanosciences

Lab location: Bordeaux

Lab

website: <https://sites.google.com/site/bordeauxnanophotonicsgroup/home>

Contact point for this topic: Institut d'Optique Graduate School

Advisor 1: LOUNIS Brahim brahim.lounis@u-bordeaux.fr

Advisor 2: TAMARAT Philippe philippe.tamarat@u-bordeaux.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The miniaturization of semiconductor-based electronic components could reach its limits within a decade. Superconducting electronics, based on quantum flux superconducting logic circuits (Josephson junctions), is a promising alternative offering both high operating rates and low switching energies. Full optical control of Josephson junctions would enable low-power, wideband communication between logic circuits at cryogenic temperatures and room-temperature mass memories. In this context, the thesis objective is the fundamental exploration of the interplay between optics, magnetism and superconductivity, an emerging research field. Innovative optical methods of individual Abrikosov vortex manipulation recently developed in our group offer promising perspectives such as fast optical Josephson junction control by moving a quantum of flux near a junction by photo-thermal effect. We will also aim at creating the Josephson junction itself by photo-thermal effect, by illuminating the section of a superconducting ribbon. The Josephson electrical transport signatures will be studied according to the geometry and power of the laser beam used to locally weaken the superconductivity. Finally, in the perspective of an all-optical control of

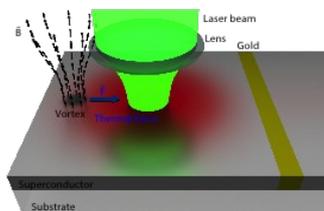
superconducting electronic devices, part of the thesis will be dedicated to the creation of flux quanta with a laser pulse, using the inverse Faraday effect.

Required background of the student: Quantum physics, optics, light matter interaction, superconductivity and magnetism.

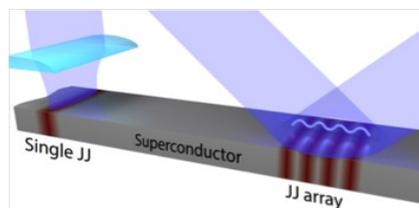
A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. « Optical Manipulation of Single Flux Quanta», I. S. Veschunov et al. Nature Communications 7 (2016) 12801.
2. “Anomalous Josephson effect controlled by an Abrikosov vortex”, S. Mironov et al., PRB 96, 214515 (2017).
3. “On-Demand Optical Generation of Single Flux Quanta” A. Rochet et al. Nano Letters 20 (2020) 6488.
4. Patent "Control of the displacement of an individual Abrikosov vortex », A. Bouzdine, B. Lounis, P. Tamarat.
- 5.

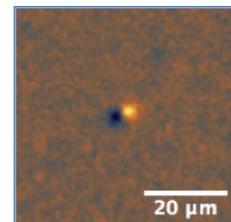
Illustrations :



Control of a Josephson junction with a single vortex.



Sculpting a normal region in a superconductor with light.



Generation of a vortex-antivortex pair with a laser pulse.

**TITLE: IDENTIFICATION OF PARAMETERS CONTROL AND IMPROVEMENT
FROM THIXOFORGING PROCESS OF ALUMINUMS (VS STEEL)**

Topic number : 2021_094

Field : Design, Industrialization, Material science, Mechanics and Fluids

Subfield: New Forming Process and Processus Eng., and material Eng,

ParisTech School: Arts et Métiers

Research team: Forming Process department

Research lab: LCFC - Laboratoire de conception, fabrication, commande

Lab location: Metz

Lab website: <http://lcfc.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: BIGOT Régis regis.bigot@ensam.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Thixoforging is a manufacturing process of metal alloys at semisolid state. Semisolid state is obtained by heating the material from the solid state, up to a temperature within the solidus-liquidus temperature range. Since always, Industry minimizes manufacturing process plan and increases mechanical behaviour. In this topic, the thixoforging process offers important perspectives. It is on the way of industrial development between casting and forging process thanks the typical rheological behaviour of the semisolid material.

This research work must contribute to improve comprehension of the aluminium behaviour during thixoforging and define the application field for this process. To achieve this goal, experimental testing with device will must be use and develop. The main thixoforging parameters to shape these alloys will be identify and study such as the forming speed, the initial steel temperature, the initial tool temperature, etc. The quality of the thixoforged parts must be study and characterize by the macrographic and micrographic observations of their metallurgical structure and mechanical tests or with other means that will be choice. The tests can be compared with simulations in order to determine and improve the predictive model capacity implemented.

Required background of the student: The student must have preferably a background in forming process, steel or aluminum material and perhaps eng. Software Catia®, Forge® or Abaqus®. Knowledge of metallurgy may also be a plus. He need have a good approach with experimental studies and numerical simulation. The use of numerical inverse models to improve the simulation models can be useful.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Aba-perea, P., Becker, E., Recherche, I. De, Matériaux, T., Procédés, M., & Metz, F. F.-. (2020). Measurement and modeling of thermal evolution during induction heating and thixoforming of low carbon steel. *Journal of Materials Processing Tech.*, 283(April), 116717. <https://doi.org/10.1016/j.jmatprotec.2020.116717>

•

2. Becker, E., Bigot, R., Rivoirard, S., Faverolle, P. (2017). EXPERIMENTAL INVESTIGATION OF THE THIXOFORGING OF TUBES OF LOW-CARBON STEEL. *Journal of Materials Processing Technology*, 1 Oct 2017, PROTEC15423

3. Balan, T., Becker, E., Langlois, L., & Bigot, R. (2017). CIRP Annals - Manufacturing Technology A new route for semi-solid steel forging. *CIRP Annals - Manufacturing Technology*, 66(1), 297-300. <https://doi.org/10.1016/j.cirp.2017.04.111>

4. Gu, G., Pesci, R., Langlois, L., Becker, E., Bigot, R., & Guo, M. X. (2014). Microstructure observation and quantification of the liquid fraction of M2 steel grade in the semi-solid state, combining confocal laser scanning microscopy and X-ray microtomography. *Acta Materialia*, 66, 118-131. <https://doi.org/10.1016/j.actamat.2013.11.075>

5. Gu, Guochao, Pesci, R., Langlois, L., Becker, E., & Bigot, R. (2015). Microstructure investigation and flow behavior during thixoextrusion of M2 steel grade. *Journal of Materials Processing Technology*, 216, 178-187. <https://doi.org/10.1016/j.jmatprotec.2014.09.009>

Illustrations :

STEEL THIXOFORGING or SEMISOLID STEEL FORGING

E. BECKER, L. LANGLOIS, T. BALAN, R. BIGOT
Arts et Métiers ParisTech, Université de Lorraine, LCFC, F-57000 Metz

Context

➤ Forging in semisolid state significantly extends the possibilities of classical hot forging. In order to fully exploit its potential, the process requires a specific and demanding environment, penalizing its industrial deployment. In this context, an alternative route is proposed. In the proposed process, semisolid zones at the heart of the material coexist with surrounding solid zones within the part. The outcome is an optimized process where the benefits of thixoforging are reached at a significant extent within the classical process framework of hot forging.

Hypotheses and objectives

EXPECTED IMPROVEMENTS

- Product
 - Complex shapes
 - Thin walls
 - Tighter dimensional tolerances
 - Improved mechanical properties compare to casting
 - Good surface
- Process
 - Reducing Forming Route
 - Decrease forming effort
 - Near Net Shape product

* Approximate temperatures for C38 Steel (JRWTH Aachen 2008)

Methods

Liquid fraction and his volume distribution	Influence of the forming parameters	Modelling and simulation	KNOWLEDGES TRANSFER / QUALIFICATION OF SCIENTIFIC AND TECHNOLOGICAL KNOWLEDGE
<p>TRL 1 →3</p> <p>Characterization of the liquid fraction and its evolution in the thixoforging process</p> <p>- Reliable determination of the liquid fraction of some steels containing alloying elements acting tracer - For other steels the minimum liquid fractions according to the heating rate → temperature</p>	<p>TRL 3 →4</p> <p>Identify and define the parameters allowing the mastering of SSF</p> <p>Influence of: - The forming speed - From the slug temperature - Tool temperature → heat exchanges impact on the product</p>	<p>TRL 3 →4</p> <p>Develop a two phases model and implemented in Forge® to simulate shapes by thixoforging, liquid and solid.</p> <p>Micro-macro model developed and improved since 2003 and implemented in Forge® giving satisfactory results according to the conditions</p>	<p>TRL 4 →6</p> <p>Study and realization, by the thixoforging process, of a piston of internal combustion engine made of steel.</p> <p>Steel SSF process development</p> <p>Process industrialization / industrial demonstrator</p> <p>10000 PARTS 1 PART EACH 8 SECONDS</p> <p>2 blocs of 8 induction heat-cells, with a power of 600kW Production rate 450 part/hour Temperature reached around 1430°C in 120 seconds</p>

Recent Results

Backward Thixoextrusion of SAE1006 steel

Exploration of a new steel for the thixoforging domain and its limits

Steel Grade	SAE1006	C38
Carbon Percentage	0.05	0.38
Crush temperature start	1456	1430
Semi-Solid Temperature start	63	100

Usually steel thixoforging for LCFC

Thixoextrusion of a high fusion temperature steel

Geometry	nominal	min	max	bearing
D _o outside diameter +57mm	57mm	56.78	56.91	56.83
Zα: clearance angle 1°	1°	1.01	1.23	1.11
d _i inside diameter +45mm	45mm	44.14	44.31	44.19
b: bottom +15mm	15mm	15.44	17.01	15.87

Exploration of the thixoforging domain and its limits → Determination of thixoforging rules

Different part geometry (wall thickness) thixoforging with the same parameters →

- Determination of thixoforging rules
- Verification of the robustness and repeatability of the process

Geometry	Thickness e = 5mm	Thickness e = 7mm
Maximum load [kN]	519	550
Average [kN]	527	213
Mean deviation [kN]	19	15
Maximum deviation [kN]	67	45

Conclusion

- ✓ Define the application domain of thixoforging for different alloys
- ✓ Define the associated rules
- ✓ Qualification of scientific and technological knowledge for an industrial transfer of thixoforging process

Perspectives

- ✓ Thixoforging of aluminium alloys and the possibilities of reinforcing with fiber

References

Balan, T., Becker, E., Langlois, L., Bigot, R., 2023. A new route for semisolid steel forging. CRP AACT. 16-17.
 Bigot, R., Becker, E., Langlois, L., Balan, T., Bigot, R., Gao, M., 2024. Microstructure observation and quantification of the liquid fraction of A52 steel grade in the semi-solid state, combining confocal laser scanning microscopy and X-ray microtomography. Acta Materialia.
 Bigot, R., Becker, E., Langlois, L., 2022. Some approaches on industrialization of steel thixoforging processes. Proceedings 129th Int. Conf. S31. Oct 2022. Cape Town, South Africa.
 Becker, E., Favier, V., Bigot, R., Ollard, F., Langlois, L., 2020. Impact of experimental conditions on material response during forming of steel in semi-solid state. JMAP.

TITLE: CONSEQUENCES OF CLIMATE CHANGE ON THE STRUCTURAL INTEGRITY OF BURIED LARGE-DIAMETER WATER-TRANSMISSION MAINS

Topic number : 2021_095

Field : Environment Science and Technology, Sustainable Development, Geosciences, Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team:

Research lab: I2M - Institut de Mécanique et d'ingénierie

Lab location: Bordeaux

Lab website: <https://www.i2m.u-bordeaux.fr>

Contact point for this topic: Arts et Métiers

Advisor 1: YANEZ GODOY Humberto humberto.yanez-godoy@u-bordeaux.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Les stratégies de gestion des systèmes d'eau potable, notamment les conduites de transport d'eau potable de grand diamètre, sont basées généralement sur l'avis d'experts. Parmi ces stratégies quelques unes sont difficilement formalisées et ne répondent que partiellement aux priorités. En effet, les cinétiques de dégradation pour ce type de conduites sont mal connues et les modèles numériques de prédiction des dégradations sont rarement disponibles. En outre, les effets du changement climatique dans des zones à fort stress hydrique doivent être mieux maîtrisés. En effet, s'ils sont plus ou moins connus sur les sols qui reçoivent ces conduites, peu de lien est fait dans les études avec l'impact sur les ouvrages eux mêmes. Ces aspects sont de nature à compliquer de plus en plus la gestion des priorités des actifs hydrauliques. Les variations dimensionnelles provoquées par les grands cycles d'hydratation-séchage et leurs répercussions en terme de gonflement ou de retrait peuvent induire la rupture des ouvrages par des tassements différentiels en particulier. Ce travail devrait nous amener à l'acquisition d'une meilleure connaissance des grands déterminants du comportement mécanique des conduites principales d'alimentation en eau par une

meilleure connexion entre l'étude sur le sol et l'impact généré sur ces structures. Ce projet de thèse a pour but de développer un modèle géomécanique-fiabiliste pour étudier le comportement des conduites d'eau potable sous contraintes qui dépendent fortement des conséquences du changement climatique. Ce modèle permettrait d'envisager la construction d'outils dédiés à la gestion de la maintenance des systèmes d'eau potable dans des régions à fort stress hydrique.

Required background of the student: Civil engineering

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Yáñez-Godoy H., Elachachi S.M., Darwich G. "Geomechanical behaviour of large diameter pressure water pipelines in unidimensional heterogeneous soils". Safety, Reliability, Risk, Resilience and Sustainability of Structures and Infrastructure: Proceedings of the 12th International Conference on Structural Safety and Reliability (ICOSSAR2017), Vienna, Austria, 6-10 August 2017. Christian Bucher, Bruce R. Ellingwood, Dan M. Frangopol (Ed.): TU Verlag, ISBN: 978-3-903024-28-1, pp. 386-395, 2017.
2. Yáñez-Godoy H, Elachachi S-M, Chesneau O, Feliers C. Identification of key determinants of geo-mechanical behavior of an instrumented buried pipe. In: Proceedings of the 13th International Conference on Applications of Statistics and Probability in Civil Engineering (ICASP13). Korean Institute of Bridge and Structural Engineers; 2019. p. 1297-304.
3. Yanez-Godoy H, Darwich G, Elachachi SM, Chesneau O, Feliers C. Suivi du comportement mécanique d'une conduite d'eau potable enterrée et instrumentée : analyse des premières mesures. Acad J Civ Eng. 2018;36(1):629-32.
- 4.
- 5.

Illustrations :

TITLE:OPTIMAL IMPLEMENTATION OF NATURE-BASED SOLUTIONS TO MITIGATE URBAN HEAT ISLANDS

Topic number : 2021_096

Field : Environment Science and Technology, Sustainable Development, Geosciences

Subfield: Hydrology

ParisTech School: Ecole des Ponts ParisTech

Research team:

Research lab: HM & Co - Hydrologie Météorologie et Complexité

Lab location: Champs-sur-Marne

Lab website:<https://hmco.enpc.fr/>

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: Versini Pierre-Antoine pierre-antoine.versini@enpc.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Urban Heat Island (UHI) is a microclimatic phenomenon occurring in urbanized spaces that tend to have higher temperatures than their surrounding countryside. In a context of climate change, the increase of heat waves, in terms of frequency and intensity, has placed the mitigation of UHI as a priority in many cities. Nature Based Solutions (NBS) as rain garden, green roofs, and parks represent some relevant infrastructures to address this challenge and make cities more resilient. As urban environments are complex and very heterogeneous in space, the implementation of NBS regarding the most vulnerable (hot) areas represents a difficult task. The objective of this PhD subject is therefore to develop a methodology, which helps to optimize NBS implementation with regard to UHI. First, temperature fields and their space-time variability will be analysed at the urban scale. For this purpose, every available data will be used, that they are produced by observation devices (satellite, public and private sensors networks) or models (simulations). A particular effort will be made to valorize crowdsourced and remote sensing data. Second, existing NBS spatial distribution will be studied. Finally, based on both fields' properties, some prospective (urban and climate) scenarios will be proposed to optimize NBS cooling effect.

Required background of the student: Have skills in the modelling of mechanics (graduated in fluid mechanics or environmental physics), capabilities in computer simulations, and be of interest to urban geophysics.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Versini, P.-A., Kotelnikova, N., Poulhes, A., Tchiguirinskaia, I., Schertzer, D. and Leurent, F., 2018. A distributed modelling approach to assess the use of Blue and Green Infrastructures to fulfil stormwater management requirements. *Landscape and Urban Planning*, 173: 60-63
2. Versini, P.-A., Gires, A., Schertzer, D. and Tchiguirinskaia, I., 2020. Fractal analysis of green roof spatial implementation in European cities. *Urban Forestry & Urban Greening*, 49, 126629
3. Foissard, X., Dubreuil, V., Quénol, H. 2019. Defining scales of the land use effect to map the urban heat island in a mid-size European city: Rennes (France), *Urban Climate*, Volume 29, 100490
- 4.
- 5.

Illustrations :

TITLE: DEVELOP AN INNOVATIVE FRAMEWORK TO ASSESS THE ENVIRONMENTAL PERFORMANCES OF A NEW TRAIN STATION OVER TIME

Topic number : 2021_097

Field : Environment Science and Technology, Sustainable Development, Geosciences

Subfield:

ParisTech School: Ecole des Ponts ParisTech

Research team:

Research lab: HM & Co - Hydrologie Météorologie et Complexité

Lab location: Champs-sur-Marne

Lab website: <https://hmco.enpc.fr/>

Contact point for this topic: Ecole des Ponts ParisTech

Advisor 1: Versini Pierre-Antoine pierre-antoine.versini@enpc.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Train stations appear as complex infrastructures as they can no longer be considered just as some transit points, but rather as systems advocating multimodality and multi-functionality. This complexity should also be considered when studying their environmental impacts. In this context, this PhD subject aims to study, through the example of a particular station of the Greater Paris (Grand Paris Express under construction), the necessary consideration of the interactions between the different geophysical fields (temperature, precipitation), urban form (transport network, planning and green spaces) and human flows, as well as their space-time variability. Coupling literature review, measured observations, and distributed model simulations (New tools should also be developed if necessary) will lead to identify and assess the main environmental issues concerning the station. They will aim to capture the space-time variability of the involved processes and variables, but also their interactions. This work should illustrate the necessity to adopt a complex system and multi-scale approach to well understand the interaction of an infrastructure with its surrounding urban environment.

Required background of the student: Have skills in the modelling of mechanics (graduated in fluid mechanics or environmental physics), capabilities in computer simulations, and be of interest to urban geophysics.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Versini, P.-A., Kotelnikova, N., Poulhes, A., Tchiguirinskaia, I., Schertzer, D. and Leurent, F., 2018. A distributed modelling approach to assess the use of Blue and Green Infrastructures to fulfil stormwater management requirements. *Landscape and Urban Planning*, 173: 60-63
2. Versini, P.-A., Gires, A., Schertzer, D. and Tchiguirinskaia, I., 2020. Fractal analysis of green roof spatial implementation in European cities. *Urban Forestry & Urban Greening*, 49, 126629
3. Samuel A. Markolf, Christopher Hoehne, Andrew Fraser, Mikhail V. Chester, B. Shane Underwood, Transportation resilience to climate change and extreme weather events – Beyond risk and robustness, *Transport Policy*, Volume 74, 2019, Pages 174-186,
- 4.
- 5.

Illustrations :

**TITLE: PHASE FIELD MODELING OF DAMAGE AND FRACTURE IN
POLYCRYSTALLINE MATERIALS UNDER THERMOMECHANICAL LOADING**

Topic number : 2021_098

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: DIPPE

Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation

Lab location: Angers

Lab website: <http://lampa.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: AMMAR Amine amine.ammar@ensam.eu

Advisor 2: EL AREM Saber saber.elarem@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: In the present work, we are interested in the development of a model which is

dedicated to the description of damage in polycrystalline metallic materials. This study aims at building a model that would describe how cracks initiate,

propagate and interact with each other at the micro-scale.

To reach this objective, it is proposed to use the phase field method (PFM)

within the context of polycrystalline plasticity. Indeed, within the framework of

irreversible thermodynamics, the phase-field method has proved to be extremely

powerful in the description of microstructural transformations without having to

track the evolution of individual interfaces, as in the case of sharp interface

models. In the present case, it is expected that the introduction of an order

parameter associated with damage will allow for capturing some complex phenomena like crack kinking or crack branching.

The proposed study would therefore consist of:

(1) Defining an appropriate set of internal variables (and the associated energy potential) to deal with both elasticity, plasticity and damage in crystalline

materials at the micro-scale

(2) Deriving the evolution equations associated with the different internal

variables within the context of the phase field method

(3) Implementing the constitutive equations within an appropriate numerical

solver (finite element solver for instance)

(4) Validating the proposed formulation by testing its ability to reproduce some

known experimental results.

At the end of this PhD research program, the numerical model will allow for

investigating the interactions between various physical mechanisms governing

the macroscopic behavior (e.g. plasticity, damage) at different length scales.

Required background of the student: Solid Mechanics, numerical mechanics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Gmati, H. "Phase field modelling of fracture of elastic and elastoviscoplastic solid materials", Thèse de doctorat ENSAM, 2020
2. Gmati, H, Mareau, C, Ammar, A, El Arem, S. A phase-field model for brittle fracture of anisotropic materials. Int J Numer Methods Eng. 2020;

121: 3362- 3381. <https://doi.org/10.1002/nme.6361>

3. H. Gmati C. Mareau, S. El Arem, A. Ammar. « Phase field modeling of damage and fracture in polycrystalline materials », MECAMAT, Aussois, France, 2019

4. C. Mareau, « A non-local damage model for the fatigue behaviour of metallic polycrystals», Philo. Mag., 100(8), 955-981, 2020

5.

Illustrations :

TITLE: TOP-DOWN REGULATION OF OLFACTORY SENSITIVITY IN THE INSECT BRAIN

Topic number : 2021_099

Field : Biology, Biophysics and Biochemistry, Environment Science and Technology, Sustainable Development, Geosciences, Life and Health Science and Technology , Life Science and Engineering for Agriculture, Food and the Environment

Subfield:

ParisTech School: AgroParisTech

Research team: Sensory Ecology department; NeO (Neuro-ethology of Olfaction) team <https://iees-paris.fr/teams/neuroethology-of-olfaction/>

Research lab: IEES Paris - Institut d'Ecologie et des Sciences de l'Environnement de Paris

Lab location: Versailles

Lab website: <https://iees-paris.fr/en/>

Contact point for this topic: AgroParisTech

Advisor 1: Chatterjee Abhishek abhishek.chatterjee@inrae.fr

Advisor 2: Anton Sylvia sylvia.anton@inrae.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Internal physiological state calibrates our perception of the outside world; for example, mated animals temporarily downregulate their physiological and behavioural response to pheromones. Similarly, a male moth's sensitivity to the female's sex-pheromone troughs when it's time for him to sleep. The internal circadian clock, on a daily basis, tunes the functioning of the sensory circuits that inform the brain about the external environment. While periodic regulation of sleep-wake cycles has long been an area of active research, much less is known about the clock-driven sensory rhythms. Our preliminary data suggest that a neuropeptide, corazonin (Crz), which is already known to be an effector of the lunar clock in annelids, could link the insect circadian clock with olfactory processing. The PhD student's work should elucidate how Crz signalling encodes the time-of-the-day and how olfactory information at the level of the antennal lobe is modified by Crz. The student will use

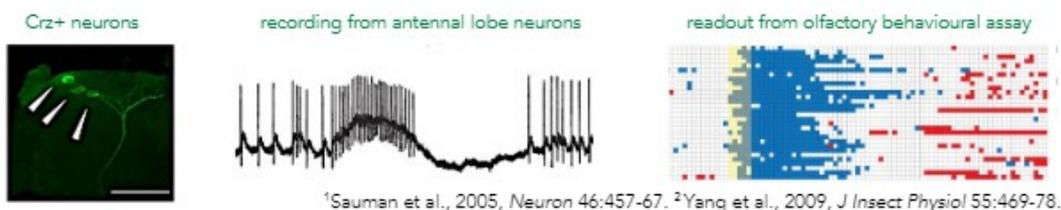
both *Drosophila* and pest moth model to gain fundamental mechanistic insights, and subsequently apply the knowledge for plant protection.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Andreatta G., et al., (2020), Corazonin signaling integrates energy homeostasis and lunar phase to regulate aspects of growth and sexual maturation in *Platynereis*. PNAS Jan 14;117(2):1097-1106. doi: 10.1073/pnas.1910262116
2. Flyer-Adams JG., et al., (2020), Regulation of Olfactory Associative Memory by the Circadian Clock Output Signal Pigment-Dispersing Factor (PDF). J Neurosci. 2020 Nov 18;40(47):9066-9077. doi: 10.1523/JNEUROSCI.0782-20.2020.
3. Miller JE., et al., (2014), Vasoactive intestinal polypeptide mediates circadian rhythms in mammalian olfactory bulb and olfaction. J Neurosci. Apr 23;34(17):6040-6. doi: 10.1523/JNEUROSCI.4713-13.2014
4. Gadenne C. et al., (2016), Plasticity in Insect Olfaction: To Smell or Not to Smell? Annu Rev Entomol. 61:317-33. doi: 10.1146/annurev-ento-010715-023523.
5. Tanoue S, et al., (2008), G protein-coupled receptor kinase 2 is required for rhythmic olfactory responses in *Drosophila*. Curr Biol. Jun 3;18(11):787-94. doi: 10.1016/j.cub.2008.04.062.

Illustrations :



TITLE:NONLINEAR DYNAMICS OF CRACKED STRUCTURES: APLICATION TO WIND TURBINES

Topic number : 2021_100

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team:DIPPE

Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation

Lab location: Angers

Lab website:lampa.ensam.eu

Contact point for this topic: Arts et Métiers

Advisor 1: AMMAR Amine amine.ammar@ensam.eu

Advisor 2: EL AREM Saber saber.elarem@ensam.eu

Advisor 3: El Baroudi Adil adil.elbaroudi@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: For rotating shafts, a propagating fatigue crack can have detrimental effects on the reliability of a steam, gas or wind turbines where these vital parts are subjected to very arduous working conditions in harsh environment. The vibration analysis and modeling of the shaft and cracks are necessary for a reliable identification of the crack location and depth to avoid catastrophic failures. In fact, cracks can develop and propagate to relevant depths without affecting consistently the normal operating conditions of the shaft. We recently have presented a systematic approach in dealing with the problem of modeling cracked rotating shafts. The breathing mechanism identification is the crucial step in the process and has been made with the greatest care. The approach presented is original and its implementation in industrial context is straight forward. The objective, based on previous development we have

recently proposed, is to apply our approach to develop a new and systematic methodology combining finite elements (1D and 3D) and modal analysis to analyzing the nonlinear dynamics of wind turbines. We will be focusing on the effect of the cracks presence on the behaviour of the turbine to develop tools for early online crack detection.

suggest an analysis methodology.

Required background of the student: solid mechanics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. S. El Arem. On the mechanics of beams and shafts with cracks : A standard and generic approach. Eur Jou Mechanics-A/Solids 85,104088, 2020
2. S. El Arem. Nonlinear analysis, instability and routes to chaos of a cracked rotating shaft. Nonlinear Dynamics , 96(1) :667-683, 2019
3. S. El Arem and M. Ben Zid. On a systematic approach for cracked rotating shaft study : breathing mechanism, dynamics and instability. Nonlinear Dynamics , 88(3) :2123-2138, 2017
4. S. El Arem and Q.S. Nguyen. Nonlinear dynamics of a rotating shaft with a breathing crack. Annals of Solid and Structural Mechanics , 3(1-2) :1-14, 2012
5. S. El Arem and H. Maitournam. A cracked beam finite element for rotating shaft dynamics and stability analysis. J. of Mechanics of Materials and Structures , 3(5) :893-910, 2008

Illustrations :

TITLE: MODELING OF THE FLUID-SOLID INTERACTIONS DURING STEADY AND TRANSIENT FLOWS OF NON-NEWTONIAN FLUIDS THROUGH DEFORMABLE POROUS MEDIA

Topic number : 2021_101

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes, Environment Science and Technology, Sustainable Development, Geosciences, Life and Health Science and Technology , Material science, Mechanics and Fluids

Subfield: Transfer in porous media

ParisTech School: Arts et Métiers

Research team: Porous Media team

<https://www.i2m.u-bordeaux.fr/Recherche/TREFLE-Transfert-Fluide-Energetique>

Research lab: I2M - Institut de Mécanique et d'ingénierie

Lab location: Bordeaux

Lab website: <https://www.i2m.u-bordeaux.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: Ahmadi-Senichault Azita azita.ahmadi@ensam.eu

Advisor 2: Rodriguez de Castro Antonio

antonio.rodriquezdecastro@ensam.eu

Advisor 3: Omari Abdelaziz Abdelaziz.Omari@enscbp.fr

Advisor 4:

Short description of possible research topics for a PhD: The mechanical interactions between non-Newtonian fluids and deformable porous media are at the interface between fluid physics and solid mechanics, and are of interest in many applications, including health and materials fields. For example, the flow of blood throughout the entire vascular network of arteries, veins and vessels of varying sizes plays a key role in the functioning human body by supplying our cells with oxygen and nutrients. A partial or total blockage (thrombus) in this vascular network due to an atheroma deposit consisting of cholesterol and cellular debris on the walls of the arteries can lead to atherosclerosis and heart attack or to a stroke. A detailed understanding of blood flow both at the local level and at the level of the capillary network is therefore essential for the development of preventive and therapeutic strategies. Moreover, blood is a shear-thinning complex fluid, which

exhibits non-Newtonian rheology. Its unsteady circulation through the vascular tree is pulsatile. This situation therefore raises the question of how to accurately represent the interactions between a complex fluid and a deformable capillary. In the field of material sciences, improving our knowledge of physical phenomena occurring during the processing of fiber-reinforced polymer composite is equally crucial in order to produce optimized structural or functional components. In particular, understanding the flow of the liquid polymer through the fibrous reinforcements requires still further research. The objective of this PhD thesis is to develop a macroscopic model for the flow of a shear-thinning fluid through a deformable porous medium by using pore network modelling methods. The accuracy of the model will be assessed through cutting-edge laboratory experiments and numerical simulations.

Required background of the student: Fluid and solid mechanics, numerical simulations, experimental skills, spoken and written English or French

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Kirst, C., Skriabine, S., Vieites-Prado, A., Topilko, T., Bertin, P., Gerschenfeld, G., Verny, F., Topilko, P., Michalski, N., Tessier-Lavigne, M., Renier, N (2020). Mapping the Fine-Scale Organization and Plasticity of the Brain Vasculature. *Cell* 180, 780-795
2. Peyrounette, M., Davit, Y., Quintard, M., Lorthois, S. (2018). Multiscale modelling of blood flow in cerebral microcirculation: Details at capillary scale control accuracy at the level of the cortex. *PLoS One* 13(1), e0189474.
3. Rodríguez de Castro, A., Goyeau, B. (2021). A pore network modelling approach to investigate the interplay between local and Darcy viscosities during the flow of shear-thinning fluids in porous media. *Journal of Colloid and Interface Science* 590, 446 - 457.
4. Rodríguez de Castro, A., Agnaou, M., Ahmadi-Sénichault, A., Omari, A., Numerical investigation of Herschel-Bulkley fluid flows in 2D porous media: yielding behaviour and tortuosity, *Computers and Chemical Engineering*, Volume 140, 2 September 2020, 106922.
5. Weibel, E. R. (2009). What makes a good lung? Review article. *Swiss Medical Weekly* 139(27-28), 375-386.

Illustrations :

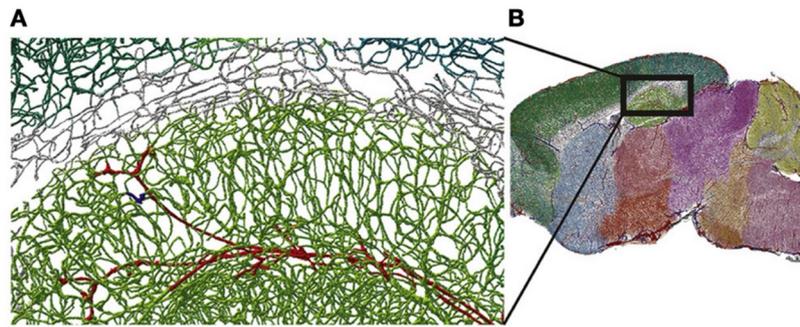


Figure 1. Multiscale architecture of microvascular networks in a mouse brain obtained by light sheet microscope. (A) Microscopic scale of interconnected capillaries. (B) Macroscopic scale where the network of capillaries can be represented by a continuous equivalent medium. (Adapted from Kirst et al. 2020)

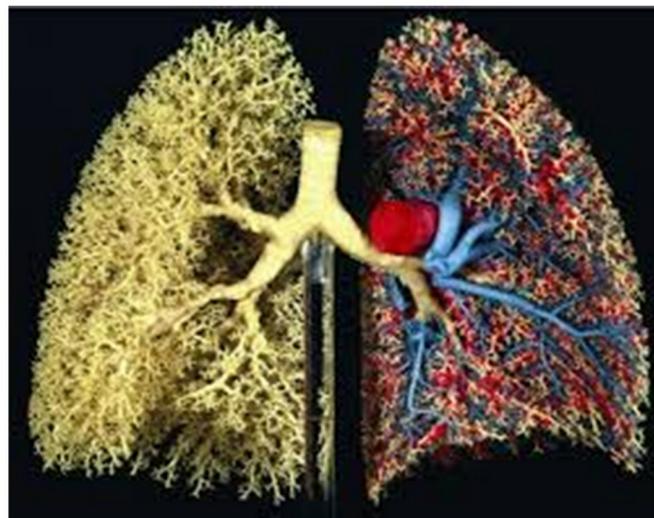


Figure 2. Resin cast of the human respiratory tree showing the dyadic branching of the bronchi from the trachea and the systematic reduction in the diameter and length of the airways with progressive branching. In the left lung, pulmonary arteries (red) and veins (blue) are also represented (Weibel 2009).

**TITLE: MULTI-SCALE APPROACH FOR THE DEVELOPMENT OF EFFECTIVE SOIL
REMEDICATION METHODS BASED ON FOAM INJECTION**

Topic number : 2021_102

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes, Environment Science and Technology, Sustainable Development, Geosciences, Material science, Mechanics and Fluids

Subfield: Transfer in porous media

ParisTech School: Arts et Métiers

Research team: Porous Media team

<https://www.i2m.u-bordeaux.fr/Recherche/TREFLE-Transfert-Fluide-Energetique>

Research lab: I2M - Institut de Mécanique et d'ingénierie

Lab location: Bordeaux

Lab website: <https://www.i2m.u-bordeaux.fr>

Contact point for this topic: Arts et Métiers

Advisor 1: Ahmadi-Senichault Azita azita.ahmadi@ensam.eu

Advisor 2: Rodriguez de Castro Antonio
antonio.rodriguezdecastro@ensam.eu

Advisor 3: Omari Abdelaziz Abdelaziz.Omari@enscbp.fr

Advisor 4:

Short description of possible research topics for a PhD:

Hydrocarbon spills can seep through the unsaturated zone of aquifers due to gravity and capillary forces, polluting water from the phreatic zone and the areas covered during their passage. Since most hydrocarbons are toxic and carcinogenic, the clean-up of these sites is a major challenge. Unlike site remediation processes by excavation, "in situ" treatments have the major advantage of not requiring soil movement. However, injecting a displacing fluid into heterogeneous or fracture-containing polluted soil generates preferential flow, leading to low sweeping efficiency. The use of foams has proven to be a relevant solution to overcome this problem. This method consists in saturating the high permeability area with foam, which produces a significant pressure loss by viscous dissipation and diverts the flow to less permeable regions, thereby improving the rate of pollutant recovery. In addition, the ability of foams to effectively invade the less permeable strata of heterogeneous makes them suitable as mobility control agents. They can also be used to

convey clean-up products (such as phosphates or iron nanoparticles). Therefore, mastering the rheology of foams when injected in porous media is essential to design an effective clean-up strategy. In this PhD thesis, multi-scale numerical and experimental approaches will be combined to relate process conditions to the efficacy of the soil remediation technique. This will allow for the optimization of pollutant recovery. In particular, the choice of the surfactant will be addressed, and microfluidic experiments will be carried out to assess the mechanisms of stability and coalescence in the presence and absence of the polluting phase.

Required background of the student: Fluid mechanics, numerical simulation, experimental skills, knowledge of physical chemistry would be appreciated

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. EPA. "Monitored natural attenuation of petroleum hydrocarbons. U.S. EPA Remedial Technology Fact Sheet, EPA/600/F-98/021", May 1999.
2. Forey, N., Atteia, O., Omari, A., Bertin, H. (2021). Use of saponin foam reinforced with colloidal particles as an application to soil remediation: Experiments in a 2D tank. *Journal of Contaminant Hydrology* 238. 103761
3. Hernando, L., Satken, B., Omari, A., Bertin, H. (2018). Transport of polymer stabilized foams in porous media: Associative polymer versus PAM. *Journal of Petroleum Science and Engineering* 169, 602 - 609.
4. Omirbekov, S., Davarzani, H., Colombano, S., Ahmadi-Senichault, A. (2020). Experimental and numerical upscaling of foam flow in highly permeable porous media. *Advances in Water Resources* 146, 103761
5. Shojaei, M. J., Rodríguez de Castro, A., Méheust, Y., Shokri, N. (2019). Dynamics of foam flow in a rock fracture: Effects of aperture variation on apparent shear viscosity and bubble morphology, *Journal of Colloid and Interface Science* 552, 464 - 475.

Illustrations :

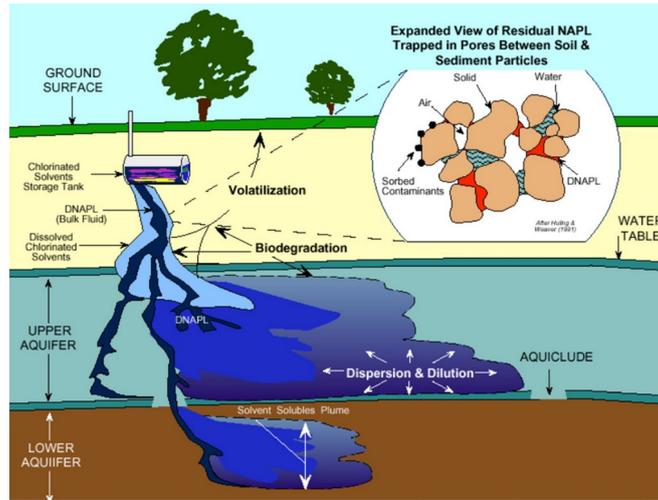


Figure 1. As a Dense NonAqueous Phase liquid (DNAPL) moves through the subsurface, some of the liquid may be trapped in the soil or sediment pores (residual saturation); some may evaporate (volatilization); some may become sorbed to the surface of the soil particles (sorption) and some may dissolve in the ground water (dissolved plume). Since DNAPL are denser than water, they will move down the aquifer until they become trapped in the less permeable layers.

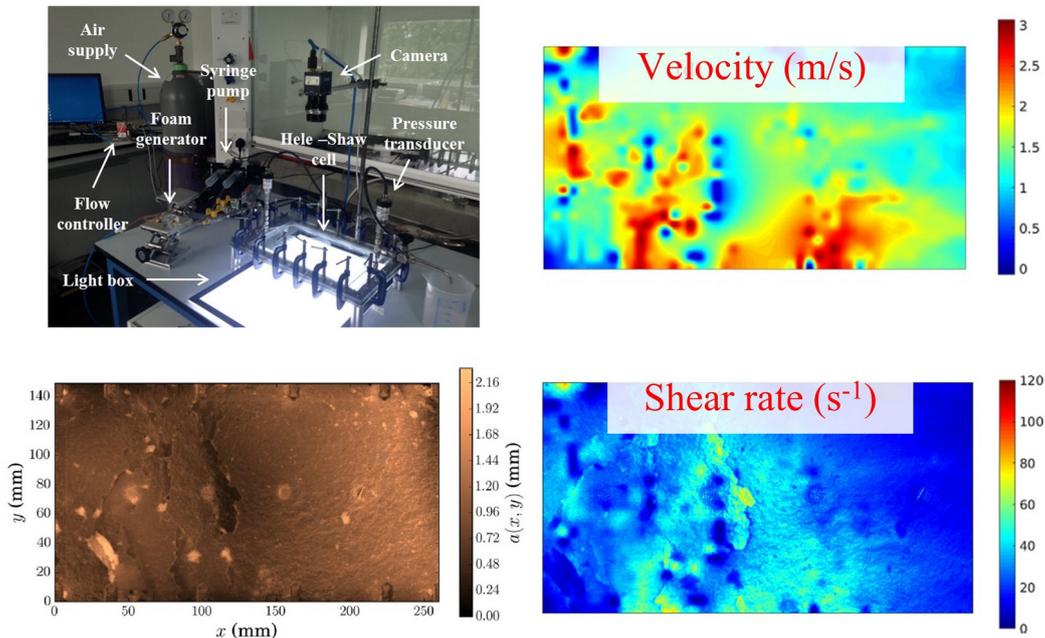


Figure 2. (a) Experimental setup used to inject pre-generated foam through a replica of a rough-walled rock fracture. (b) aperture map (c) Velocity map obtained by PIV. (d) Shear-rate map. From Shojaei et al. (2019)

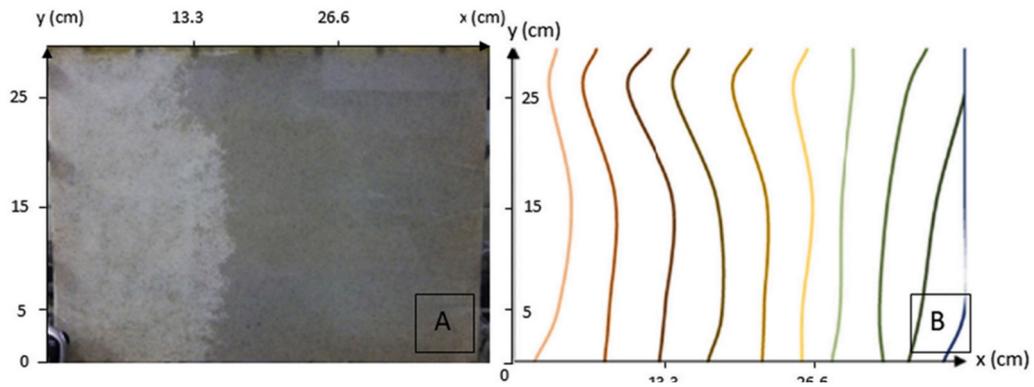


Figure 3 (A) Injection of a dyed foam (in white) through a 2D tank filled with sand and saturated with surfactant. (B) Subsequent positions of the invasion front. From Forey et al. (2021).

TITLE: NANO-RHEOLOGY OF CHARGED SOLID/LIQUID INTERFACES

Topic number : 2021_104

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield: Nanomechanics, Interfaces, Ionic Double Layer

ParisTech School: ESPCI Paris - PSL

Research team: <https://blog.espci.fr/jcomtet/>

Research lab: SIMM - Sciences et ingénierie de la matière molle

Lab location: Paris

Lab website: <https://www.simm.espci.fr/-Home-.html>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Comtet Jean jean.comtet@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Most solid/liquid interfaces are characterized by a net spatial separation of charges, due to the dissociation of surface charges on the solid surface, which get screened by a diffuse layer of counter-ions in the liquid. The dynamics of this “Electric Double Layer” of typical nanometric size, has fundamental importance for diverse domains such as energy storage (super-capacitors, batteries), energy harvesting, or nanofiltration... However, the dynamic couplings between ionic charge transport and liquid flow at these interfaces (“electrokinetic effects”) remain poorly understood, with e.g. long-standing discrepancies between static and dynamic surface charges, controversial reports of flow-induced shift of the surface charges or peculiar “electro-viscous” over-dissipation during deformation of the electric double layer. These observations call for the development of novel experimental methodology to quantitatively probe the dynamic response of charged solid/liquid interfaces. The aim of this PhD is to investigate the full out-of-equilibrium response of the ionic double layer over decades of dynamic range, by developing new dynamic Atomic Force Microscopy methodology, based on Tuning-Fork AFM (see Fig. 1A). These techniques have recently demonstrated their potential for the investigation of the nano-rheology of non-volatile liquids, and will be here adapted to study dynamic process in aqueous solutions. In particular, we will probe the

dynamic response of these charged interfaces under the flow induced by an oscillating colloidal probe (Fig. 1B), to extract the full conservative and dissipative rheological response associated with the deformation of the double layer, and gain novel insights on the coupled electro-kinetic effects taking place at the interface. These measurements will be carried out by systematically varying the physicochemistry of the aqueous solution, and the properties of the solid surfaces, shedding new lights on the molecular processes taking place at the intimate scale of the solid/liquid interface. We will finally probe how electronic capacitive couplings between the tip and the surface can affect interfacial ionic dynamics. The PhD student will acquire expertise in nano-assembly and micro-fabrication, signal processing for dynamic Atomic Force Microscopy, as well as fundamental knowledge of electrokinetic effects at solid/liquid interface, of relevance for a broad class of micro and nanofluidic problems of interest.

J. Comtet, A. Niguès, V. Kaiser, B. Coasne, L. Bocquet, and A. Siria, "Nanoscale capillary freezing of ionic liquids confined between metallic interfaces and the role of electronic screening," *Nature Materials*, 2017.

J. Comtet, G. Chatté, A. Niguès, L. Bocquet, A. Siria, and A. Colin, "Pairwise frictional profile between particles determines discontinuous shear thickening transition in non-colloidal suspensions," *Nature Communication*, 2017.

R. Hartkamp, A. L. Bianco, L. Fu, J. F. Dufrêche, O. Bonhomme, and L. Joly, "Measuring surface charge: Why experimental characterization and molecular modeling should be coupled," *Curr. Opin. Colloid Interface Sci.*, 2018.

D. Lis, E. H. G. Backus, J. Hunger, S. H. Parekh, and M. Bonn, "Liquid flow along a solid surface reversibly alters interfacial chemistry," *Science*, 2014.

F. Liu, A. Klaassen, C. Zhao, F. Mugele, and D. Van Den Ende, "Electroviscous Dissipation in Aqueous Electrolyte Films with Overlapping Electric Double Layers," *J. Phys. Chem. B*, 2018.

Figure : (A) Schematic of the experimental set-up. (B) Dynamic electrokinetic couplings between ionic and fluidic transport in confinement, induced by the oscillation of the colloidal AFM.

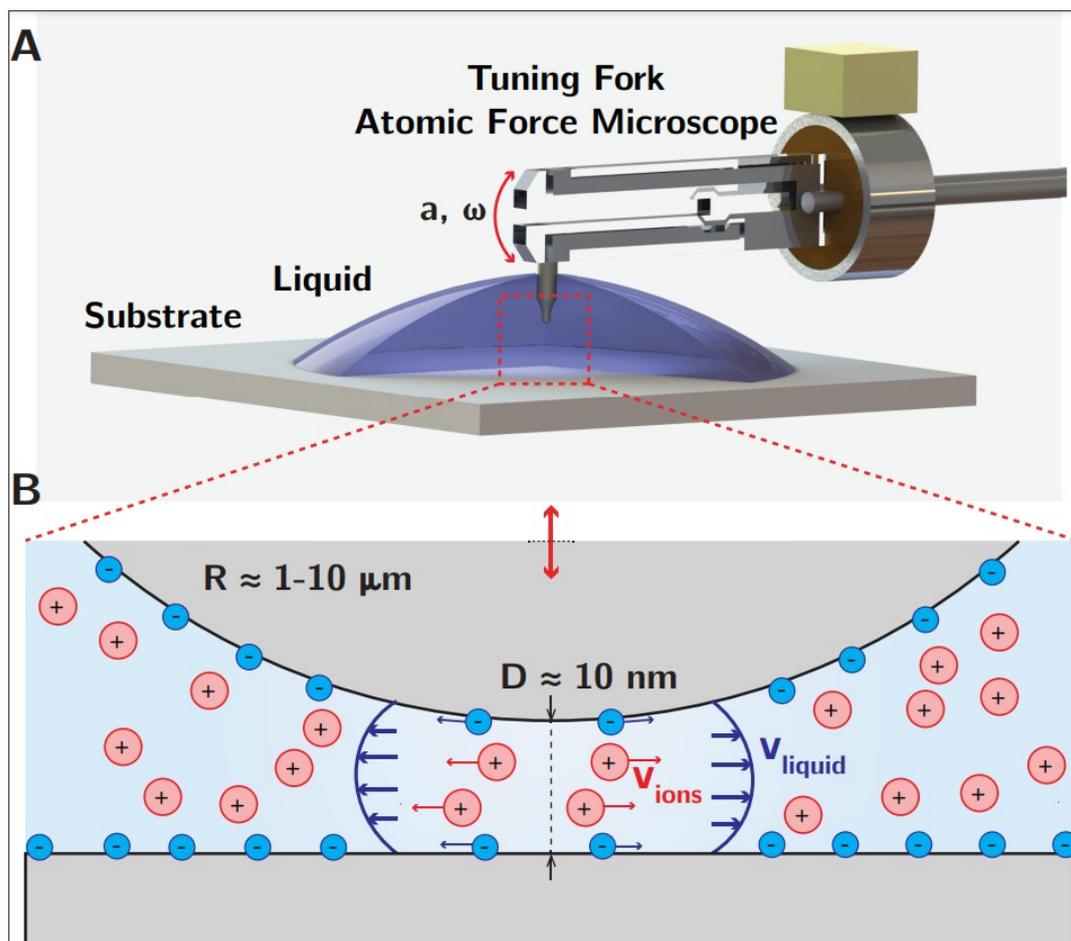
Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. J. Comtet, A. Niguès, V. Kaiser, B. Coasne, L. Bocquet, and A. Siria, "Nanoscale capillary freezing of ionic liquids confined between metallic interfaces and the role of electronic screening," *Nature Materials*, 2017.

2. J. Comtet, G. Chatté, A. Niguès, L. Bocquet, A. Siria, and A. Colin, "Pairwise frictional profile between particles determines discontinuous shear thickening transition in non-colloidal suspensions," *Nature Communication*, 2017.
3. R. Hartkamp, A. L. Biance, L. Fu, J. F. Dufrêche, O. Bonhomme, and L. Joly, "Measuring surface charge: Why experimental characterization and molecular modeling should be coupled," *Curr. Opin. Colloid Interface Sci.*, 2018.
4. D. Lis, E. H. G. Backus, J. Hunger, S. H. Parekh, and M. Bonn, "Liquid flow along a solid surface reversibly alters interfacial chemistry," *Science*, 2014.
5. F. Liu, A. Klaassen, C. Zhao, F. Mugele, and D. Van Den Ende, "Electroviscous Dissipation in Aqueous Electrolyte Films with Overlapping Electric Double Layers," *J. Phys. Chem. B*, 2018.

Illustrations :



TITLE: IONIC TRANSPORT AT SOLID/LIQUID INTERFACES AT THE SINGLE CHARGE SCALE

Topic number : 2021_105

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield: Solid/Liquid Interfaces, Single Molecule Localization Microscopy, 2D materials, Defects

ParisTech School: ESPCI Paris - PSL

Research team: <https://blog.espci.fr/jcomtet/>

Research lab: SIMM - Sciences et ingénierie de la matière molle

Lab location: Paris

Lab website: <https://www.simm.espci.fr/-Home-.html>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Comtet Jean jean.comtet@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD:

Understanding the structure, transport and dynamics of ionic charges at solid-liquid interfaces is relevant to a variety of domains, from energy harvesting or energy storage, to catalysis, nanofiltration or electrochemistry . However, fundamental understanding of these dynamic interfacial processes, related to surface group dissociation and ionic adsorption, remains poor, due the difficulties in obtaining surface-specific information at both high spatial and temporal resolution. In this context, we were recently able to observe the diffusive dynamics of single proton charges at the interface between defected hexagonal boron nitride and aqueous solutions, applying Single Molecule Super-Resolution Microscopy to optically active defects hosted at the surface of the 2D hBN crystal .

Understanding the structure, transport and dynamics of ionic charges at solid-liquid interfaces is relevant to a variety of domains, from energy harvesting or energy storage, to catalysis, nanofiltration or electrochemistry . However, fundamental understanding of these dynamic interfacial processes, related to surface group dissociation and ionic adsorption, remains poor, due the difficulties in obtaining surface-specific information at both high spatial and temporal resolution. In this context,

we were recently able to observe the diffusive dynamics of single proton charges at the interface between defected hexagonal boron nitride and aqueous solutions, applying Single Molecule Super-Resolution Microscopy to optically active defects hosted at the surface of the 2D hBN crystal .

The aim of this PhD is to extend these super-resolution techniques, to access to the nanometric structure and dynamics of charges at the solid/liquid interface. In a first step, we will use the optically active defects present at the hBN surface, to understand how single proton charge transport at the solid/liquid interface can be affected and biased by various out-of-equilibrium forcing applied to the interface, e.g. related to electric fields or liquid flow. In a second step, we will extend these measurements towards other materials. We will here rely on Super-resolved PAINT microscopy (Points Accumulation for Imaging in Nanoscale Topography) to obtain nanometrically resolved spatial maps of electrostatic interactions between charged fluorophores in solutions and materials of interest. Measurements of the transient adsorption and diffusion of individual fluorophores at the solid surface, will provide us with insights on the in-plane distribution and dynamics of charges at the interface. These measurements will be carried out on model substrates, as well as novel 2D-materials such as hexagonal Boron Nitride, Graphene Oxide or MoS₂, which have poorly understood chemical reactivity in water.

Bonn et al., Water at charged interfaces. Nat. Rev. Chem. 5, 466-485 (2021).

Comtet et al. Direct observation of water-mediated single-proton transport between hBN surface defects. Nature Nanotechnology, 15(7), 598-604. (2020).

Comtet et al. Anomalous interfacial dynamics of single proton charges in binary aqueous solutions. Science Advances (2021).

Figure : (A) Detection of the transient adsorption of a positively charged fluorophore on a negatively charged patch at the solid surface. (B) Reconstructed super-resolved image of charged groups on an hBN flake using a cationic dye.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Comtet et al. Direct observation of water-mediated single-proton transport between hBN surface defects. Nature Nanotechnology, 15(7), 598-604. (2020).

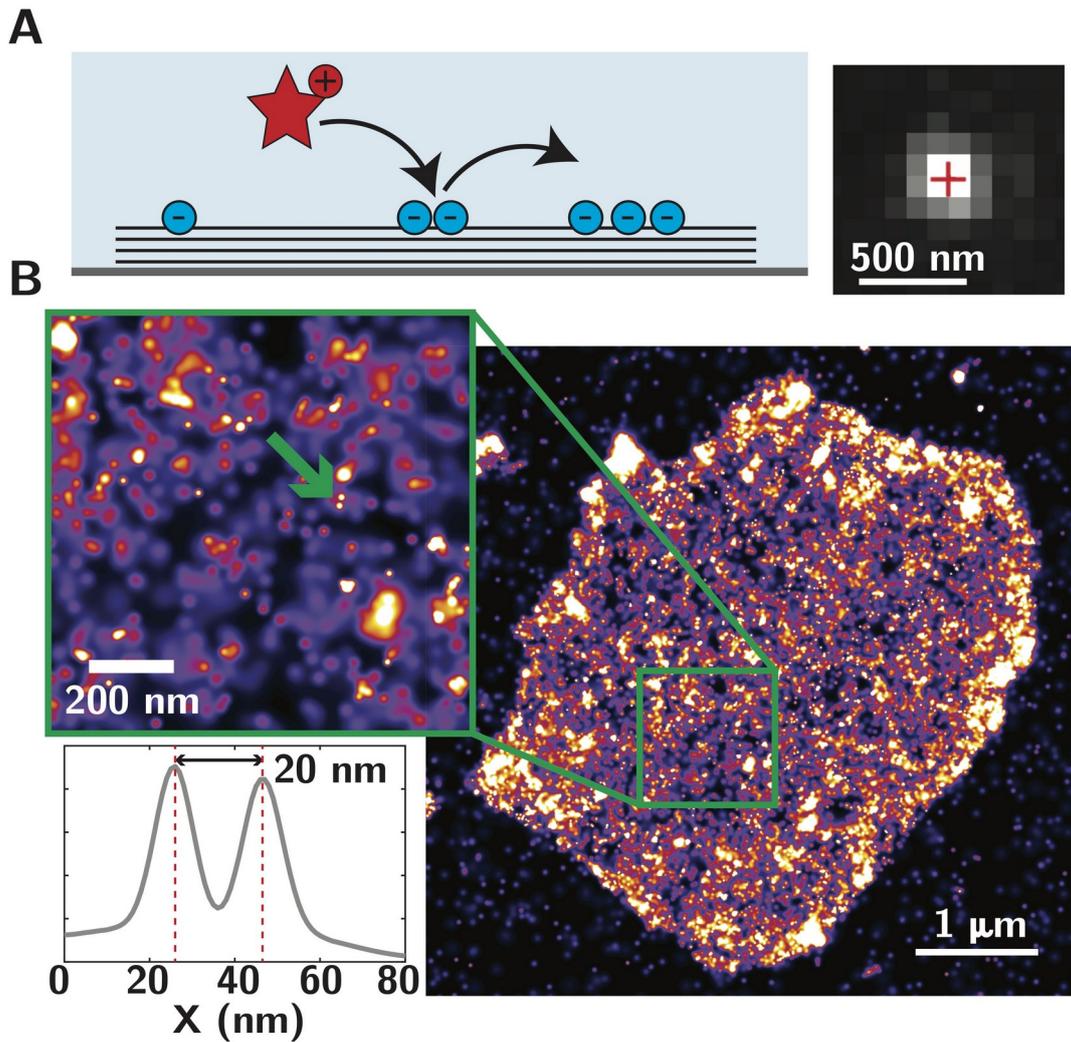
2. Comtet et al. Anomalous interfacial dynamics of single proton charges in binary aqueous solutions. Science Advances (2021).

3. Bonn et al., Water at charged interfaces. Nat. Rev. Chem. 5, 466–485 (2021).

4. Van Roij et al., Flow-induced surface charge heterogeneity in electrokinetics due to Stern-layer conductance coupled to reaction kinetics. Physical review letters, 120(26), 264502 (2018).

5.

Illustrations :



**TITLE: MODELING OF THE WOOD BEHAVIOR UNDER SEVERE LOADING
CONDITIONS: CASE OF THE VENEER CUTTING BY ROTARY PEELING PROCESS**

Topic number : 2021_106

Field : Design, Industrialization, Energy, Processes, Environment
Science and Technology, Sustainable Development, Geosciences, Material
science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: Wood sciences, Wood peeling, wood grading
[http://labomap.ensam.eu/wood-material-and-machining-100680.kjsp?
RH=1415278881726&RF=1415535985117](http://labomap.ensam.eu/wood-material-and-machining-100680.kjsp?RH=1415278881726&RF=1415535985117)

Research lab: LABOMAP - Laboratoire Bourguignon des matériaux et
procédés

Lab location: Cluny

Lab website: <http://labomap.ensam.eu/>

Contact point for this topic: Arts et Métiers

Advisor 1: Denaud Louis louis.denaud@ensam.eu

Advisor 2: Yaich Mariem mariem.yaich@ensam.eu

Advisor 3: Girardon Stéphane stephane.girardon@ensam.eu

Advisor 4:

Short description of possible research topics for a PhD: The wood material presents an interesting alternative to reduce the carbon impact of industry and construction, especially veneer industry according to the huge amount of design possibilities offered by this material. However, its use is still limited in many applications because of its natural high variability. In order to encourage the use of local hardwood and fast-growing species, characterized by a high heterogeneity, the peeling process has been used for many decades for the construction of technical wood products (plywood, LVL, CLT...) with high mechanical properties. Contrary to other manufacturing processes, the guarantee of the good quality of the chip, which is the veneer in our case, is deeply required. This still is difficult to ensure due to either an inadequate definition of the machining conditions or an under comprehension of the material behavior. Despite the continuous efforts to experimentally determine the main reasons of the damage initiation and propagation within the machined veneer, the setting up of a reliable numerical modeling is

deeply required. It aims to allow the access to local and instantaneous information, as well as to determine the effect of material property and process parameter on the veneer quality. This constitutes the main objective of this thesis subject, which will be focused initially on determining the effects of the machining conditions on the peeling process for homogeneous species. Comparisons between different plasticity criteria, rheology and damage models will be set up in the aim to determine the most accurate ones, which are able to adequately reproduce the wood behavior under several loading conditions. The material behavior under sever loading conditions, similar to those reached during the peeling process, will be studied. The thermomechanical contact conditions in the tool-veneer-pressure bare interfaces will be also investigated to study the effects of both hydrothermal wood preparation and cutting conditions. Afterword, more generalized material behavior will be defined to the numerical simulations. The proposed strategy aimed to establish a reliable modeling of peeling process, even in the case a highly heterogeneous material with pronounced variability and coupling material parameters. Comparisons between the computed cutting forces, veneer thickness and the experimental ones obtained from the instrumented industrial peeling line of the LaBoMaP will be performed to validate the numerical simulations. Attention will be paid to the distribution of numerical plastic strain, strain rate, stress and damage parameter in the veneer during and after the peeling process in order to determine the main reasons of the damage initiation and propagation. The main advantageous of the proposed study is summarized on its ability to consider the high variability of the wood and to separately determine the material and process parameters affecting the veneer quality, which remains impossible based only on an experimental approach.

Required background of the student: Mechanical engineering, Programming, Finite element modeling (A good knowledge of the wood material and its manufacturing will be appreciated)

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. R. Duriot, G. Pot, S. Girardon, L. Denaud (2021) New perspectives for LVL manufacturing from wood of heterogeneous quality - Part 2: Modeling and manufacturing of variable stiffness beams. *Forests*, 12 (9): 1275
2. Thibaut, B., and Beauchêne, J. (2004). Links between Wood Machining Phenomena and Wood Mechanical Properties: The Case of 0°/90° Orthogonal Cutting of Green Wood.

3. S. Stefanowski, R. Frayssinhes, G. Pinkowski, L. Denaud (2020). Study on the in-process measurements of the surface roughness of Douglas fir green veneers with the use of laser profilometer. *European Journal of Wood and Wood Products*, 78 (3), 555-564

4. Thibaut, B., Denaud, L., Collet, R., Marchal, R., Beauchêne, J., Mothe, F., Méausoone, P.-J., Martin, P., Larricq, P., and Eyma, F. (2016). Wood machining with a focus on French research in the last 50 years. *Annals of Forest Science* 73, 163-184

5.

Illustrations :

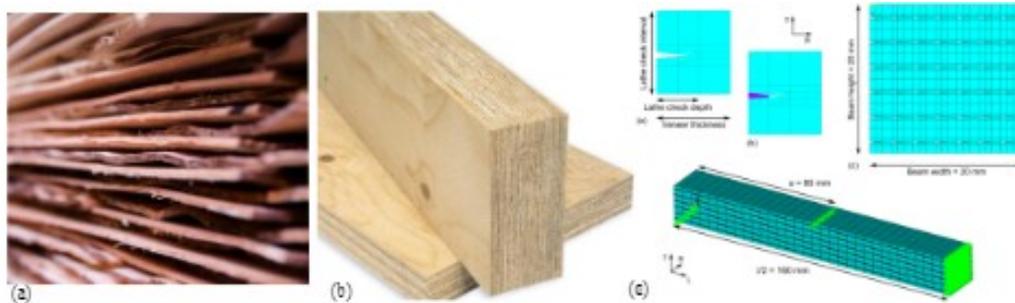


Figure 1 : Examples of (a) veneers, (b) Laminated Veneer Lumber LVL and (c) LVL damage modeling

**TITLE: SINGLE MOLECULE INVESTIGATION OF POLYMER CHAIN DYNAMICS
AT INTERFACES**

Topic number : 2021_107

Field : Material science, Mechanics and Fluids, Physics, Optics

Subfield: Polymer, Interfaces, Single Molecule Techniques

ParisTech School: ESPCI Paris - PSL

Research team: <https://blog.espci.fr/jcomtet/>

Research lab: SIMM - Sciences et ingénierie de la matière molle

Lab location: Paris

Lab website: <https://www.simm.espci.fr/-Home-.html>

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Comtet Jean jean.comtet@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Molecular-scale interactions between polymers in solutions and solid surfaces govern a large number of processes in soft matter, ranging from surface functionalization with adsorbed or self-assembled polymer layers, polymer flow in porous media, lubrication and friction by thin polymer layers, etc... These interfacial processes are typically probed at the ensemble level and described by average phenomenological coefficients (slip length, surface concentration etc...). Going beyond this traditional description and rationalizing these coefficients requires to be able to precisely measure and describe the molecular-scale processes taking place at these interfaces, which remained - until recently - experimentally inaccessible. In the recent years, novel experimental techniques combining Single Molecule Localization Microscopy with fluorescently tagged polymers have demonstrated their potential for direct, in-situ and spatially-resolved study of polymer dynamics at solid/liquid interfaces, revealing in particular heterogeneous diffusion of polymer chains at interfaces, characterized by a succession of transient adsorption events, followed by fast transport through the solvent (see Figure and). The aim of this PhD is to take advantage of these novel Single Molecule techniques developed in the team to probe interfacial polymer dynamics under various out-of-equilibrium situations, related to hydrodynamic flow

of solvent, friction or adhesion. To do so, we will bring and develop these state-of-the-art single molecule microscopy techniques to the field of soft matter, performing direct observations of out-of-equilibrium polymer dynamics at the single-molecule scale. In each out-of-equilibrium situations, we will relate the statistics of the heterogeneous dynamics measured at the molecular scale to the average dynamic response of the interface. Ultimately, this will allow us to move towards a molecular understanding of the averaged phenomenological response of the interface in these various situations (slip length, friction coefficient...).

Comtet, J., Grosjean, B., Glushkov, E., Avsar, A., Watanabe, K., Taniguchi, T., ... & Radenovic, A. (2020). Direct observation of water-mediated single-proton transport between hBN surface defects. *Nature Nanotechnology*, 15(7), 598-604.

Comtet, J., Rayabharam, A., Glushkov, E., Zhang, M., Ahmet, A., Watanabe, K., ... & Radenovic, A. Anomalous interfacial dynamics of single proton charges in binary aqueous solutions. *Science Advances* (2021).

Yu, C., Guan, J., Chen, K., Bae, S. C., & Granick, S. (2013). Single-molecule observation of long jumps in polymer adsorption. *ACS nano*, 7(11), 9735-9742.

Skaug, M. J., Mabry, J. N., & Schwartz, D. K. (2014). Single-molecule tracking of polymer surface diffusion. *Journal of the American Chemical Society*, 136(4), 1327-1332.

Wang, D., & Schwartz, D. K. (2020). Non-Brownian Interfacial Diffusion: Flying, Hopping, and Crawling. *The Journal of Physical Chemistry C*, 124(37), 19880-19891.

Figure : Dynamics of a single PEG chain hopping at a solid/liquid interface.

Required background of the student:

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Comtet, J., Grosjean, B., Glushkov, E., Avsar, A., Watanabe, K., Taniguchi, T., ... & Radenovic, A. (2020). Direct observation of water-mediated single-proton transport between hBN surface defects. *Nature Nanotechnology*, 15(7), 598-604.

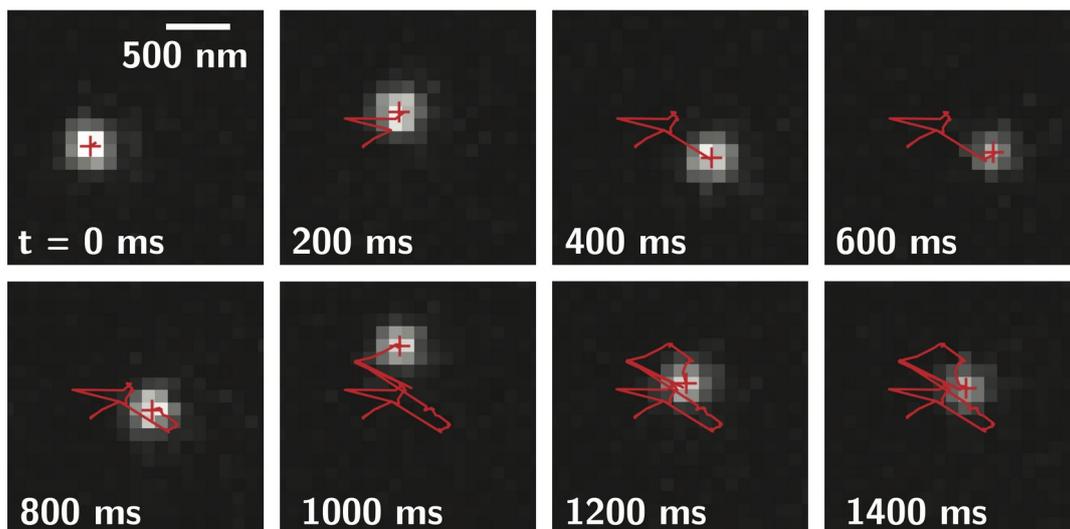
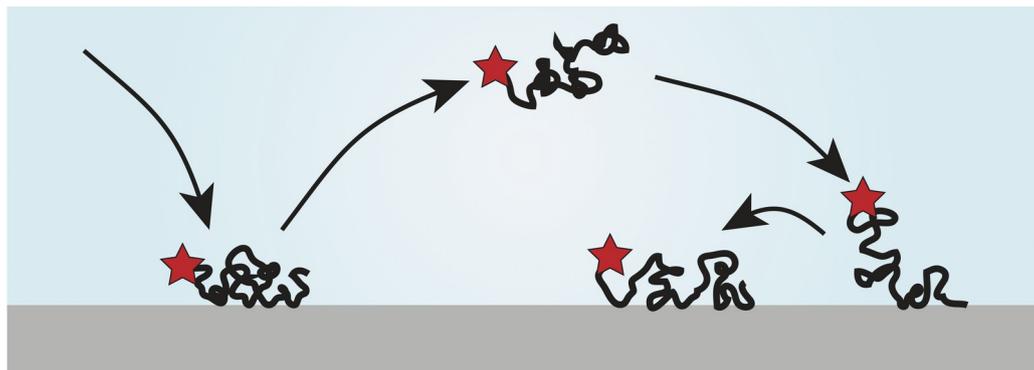
2. Comtet, J., Rayabharam, A., Glushkov, E., Zhang, M., Ahmet, A., Watanabe, K., ... & Radenovic, A. Anomalous interfacial dynamics of single proton charges in binary aqueous solutions. *Science Advances* (2021).

3. Yu, C., Guan, J., Chen, K., Bae, S. C., & Granick, S. (2013). Single-molecule observation of long jumps in polymer adsorption. *ACS nano*, 7(11), 9735-9742.

4. Skaug, M. J., Mabry, J. N., & Schwartz, D. K. (2014). Single-molecule tracking of polymer surface diffusion. *Journal of the American Chemical Society*, 136(4), 1327-1332.

5. Wang, D., & Schwartz, D. K. (2020). Non-Brownian Interfacial Diffusion: Flying, Hopping, and Crawling. *The Journal of Physical Chemistry C*, 124(37), 19880-19891.

Illustrations :



TITLE: SURFACE REACTIVITY OF Mg ANODE IN HIGH-ENERGY DENSITY Mg-AIR BATTERY

Topic number : 2021_108

Field : Chemistry, Physical chemistry and Chemical Engineering, Energy, Processes

Subfield: Surface Science, Material Science, Battery, Energy Storage and Conversion

ParisTech School: Chimie ParisTech - PSL

Research team: PCS Physico-Chimie des Surfaces

<https://www.ircp.cnrs.fr/la-recherche/equipe-pcs/>

Research lab: IRCP - Institut de Recherche de Chimie de Paris

Lab location: Paris

Lab website: <https://www.ircp.cnrs.fr/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Swiatowska Jolanta

jolanta.swiatowska@chimieparistech.psl.eu

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Metal-air batteries are promising candidates to replaced Li batteries in many fields. Among various types of metal-air batteries, Mg-air batteries have been explored much less than lithium, zinc or aluminium-air batteries. Mg-air batteries could be widely used in many fields because of their high theoretical voltage (3.09 V), high specific capacity (2205 mAh/g), high energy (3910 Wh/kg), low cost, abundance and environmental friendliness. However, the main issues of Mg-air batteries are the high polarization, low coulombic efficiency, a high rate of self-discharge, and the battery irreversibility. These problems are related to the side-reaction in the Mg anode, like the corrosion of Mg. The hydrogen evolution reaction (HER) and negative difference effect (NDE) as well as impurities are the main factors for the corrosion of Mg. Therefore, searching for a suitable Mg-based anode or electrolyte in order to form a robust and stable electrode/electrolyte interface are necessary to improve Mg-air battery performance. This PhD project will be focused on characterization of electrode/electrolyte interface and better understanding the surface

reactivity of Mg anode. The ultimate objective will be to optimize the electrochemical and discharge performance of Mg anode and the Mg-air battery. The combined electrochemical, microscopic and surface spectroscopic techniques (XPS, ToF-SIMS) will be used.

Required background of the student: The candidate should have a good background in chemistry, physical chemistry, electrochemistry, batteries and material science (e.g., metals, alloys, metallic oxides). The former experience in battery, metal-air battery, electrochemistry, electrochemical characterization by cyclic voltammetry, impedance spectroscopy and materials characterization (by scanning electron microscopy, transmission electron microscopy, X-ray diffraction or surface sensitive techniques such as X-ray photoelectron spectroscopy) is a plus.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. B. Tian, J. Swiatowska, V. Maurice, S. Zanna, A. Seyeux, P. Marcus, The effect of sulfide additive in alkaline electrolyte on improved performances of Fe-based air batteries, *Electrochim. Acta* 259 (2018) 196-203. DOI: 10.1016/j.electacta.2017.10.136.
2. L. Wang, J. Swiatowska, S. Dai, M. Cao, Z. Zhong, Y. Shen, M. Wang, Promises and challenges of alloy-type and conversion-type anode materials for sodium-ion batteries, *Materials Today Energy* 11 (2019) 46-60. DOI: 10.1016/j.mtener.2018.10.017.
3. S.-J. Zhang, Z.-W. Yin, Z.-Yu Wu, D. Luo, Y.-Y. Hu, J.-H. You, K.-X. Li, X.-R. Yang, J.-W. Yan, X.-D. Zhou, S. Zanna, P. Marcus, J. Swiatowska, S.-G. Sun, Z.-W. Chen, J.-T. Li, Achievement of High-Cyclability and High-Voltage Li-Metal Batteries by Heterogeneous SEI film with Internal Ionic Conductivity/External Electronic Insulativity Hybrid Structure, *Energy Storage Materials* 40 (2021) 337-346. DOI: 10.1016/j.ensm.2021.05.029.
4. Z.-Y. Wu, Y.-Q. Lu, J.-T. Li, S. Zanna, A. Seyeux, L. Huang, S. -G. Sun, P. Marcus, and J. SSwiatowska, Influence of Carbonate Solvents on Solid Electrolyte Interphase Composition over Si Electrodes Monitored by In Situ and Ex Situ Spectroscopies, *ACS Omega* (2021). DOI: 10.1021/acsomega.1c04226
5. C. Pereira-Nabais, J. Swiatowska, A. Chagnes, F. Ozanam, A. Gohier, P. Tran-Van, C.-S. Cojocar, M. Cassir, P. Marcus, Interphase chemistry of

Si electrodes used as anodes in Li-ion batteries, Applied Surface Science, 266 (2013) 5-16. DOI: 10.1016/j.apsusc.2012.10.165.

Illustrations :

TITLE: RECONSTRUCTION OF HETEROGENEOUS SURFACE RESIDUAL-STRESSES IN POLYCRYSTALLINE MATERIALS FROM X-RAY DIFFRACTION MEASUREMENTS

Topic number : 2021_109

Field : Material science, Mechanics and Fluids

Subfield:

ParisTech School: Arts et Métiers

Research team: PIMM - COMET GROUP <https://pimm.artsetmetiers.fr/>

Research lab: PIMM - Laboratoire Procédés et ingénierie en mécanique et matériaux

Lab location: Paris

Lab website: <https://pimm.artsetmetiers.fr/>

Contact point for this topic: Arts et Métiers

Advisor 1: BRAHAM CHEDLY chedly.braham@gmail.com

Advisor 2: MORIN LEO leo.morin@ensam.eu

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Residual stresses have a significant influence on the engineering properties components such as fatigue life. X-ray diffraction (XRD) constitutes a high accuracy and non-destructive way to determine residual stresses with a very good precision and resolution in depth due to the important absorption of X-ray in metallic alloys. Despite its important success and its high precision in-depth, the X-ray diffraction method remains inaccurate in the presence of high surface stress gradients, due to averaging effects over the irradiated area. This has important consequences in processing validation because averaging effects on residual stresses measured by XRD prevent a proper comparison with the local residual stresses determined numerically by finite elements. The main purpose of this PhD is to develop a method to reconstruct heterogeneous residual-stresses at the surface of polycrystalline materials from XRD measurements. 2D maps of residual-stress will be collected on specimens obtained by several processes (such as severe plastic deformation or laser hot peening) using an articulated robot. A deconvolution method will be developed in order to reconstruct the local residual stress field from the average data collected. Finally, finite

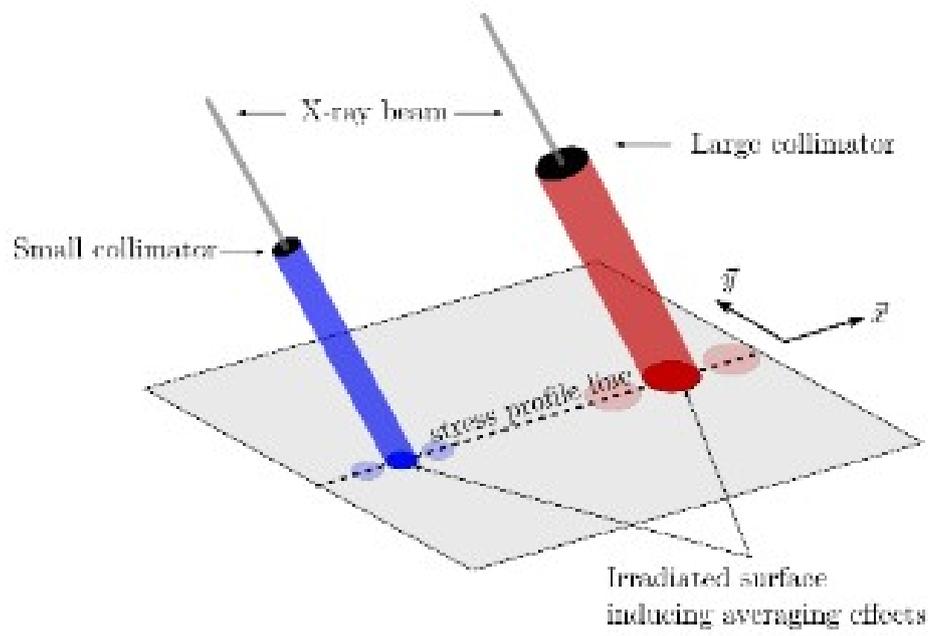
element simulations of the processes considered will be performed to assess the reconstructed residual stress distributions.

Required background of the student: Mechanical engineering, material science

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. 1. Peyre, P., Sollier, A., Chaieb, I., Berthe, L., Bartnicki, E., Braham, C., Fabbro, R., 2003. FEM simulation of residual stresses induced by laser Peening. The European Physical Journal - Applied Physics 23, 83-88.
2. 2. Rhouma, A.B., Sidhom, N., Makhlouf, K., Sidhom, H., Braham, C., Gonzalez, G., 2019. Effect of machining processes on the residual stress distribution heterogeneities and their consequences on the stress corrosion cracking resistance of AISI 316l SS in chloride medium. The International Journal of Advanced Manufacturing Technology 105, 1699-1711.
3. 3. Reyes-Ruiz, C., Figueroa, I.A., Braham, C., Cabrera, J.M., Zanellato, O., Baiz, S., Gonzalez, G., 2016. Residual stress distribution of a 6061-T6 aluminum alloy under shear deformation. Materials Science and Engineering: A 670, 227-232.
4. 4. Ezequiel, M., Figueroa, I.A., Elizalde, S., Cabrera, J.M., Braham, C., Morin, L., Gonzalez, G., 2020. Numerical and experimental study of a 5754-aluminum alloy processed by heterogeneous repetitive corrugation and straightening. Journal of Materials Research and Technology 9, 1941-1947.
5. 5. Morin, L., Braham, C., Tajdary, P., Seddik, R., Gonzalez, G., 2021. Reconstruction of heterogeneous surface residual-stresses in metallic materials from X-ray diffraction measurements. Mechanics of Materials 158, 103882.

Illustrations :



**TITLE:ASYMMETRIC CATALYSIS TOWARD BIORELEVANT ARCHITECTURALLY
NOVEL NATURAL AND UNNATURAL PRODUCTS**

Topic number : 2021_110

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Organic Chemistry, Catalysis

ParisTech School: Chimie ParisTech - PSL

Research team:Catalysis, Synthesis of Biomolecules and Sustainable Development

Research lab: I-CLEHS - Institute of chemistry for life and health

Lab location: Paris

Lab website:<https://iclehs.fr/>

Contact point for this topic: Chimie ParisTech - PSL

Advisor 1: Vidal Virginie virginie.vidal@chimieparistech.psl.eu

Advisor 2: Phansavath Phannarath

phannarath.phansavath@chimieparistech.psl.eu

Advisor 3:

Advisor 4:

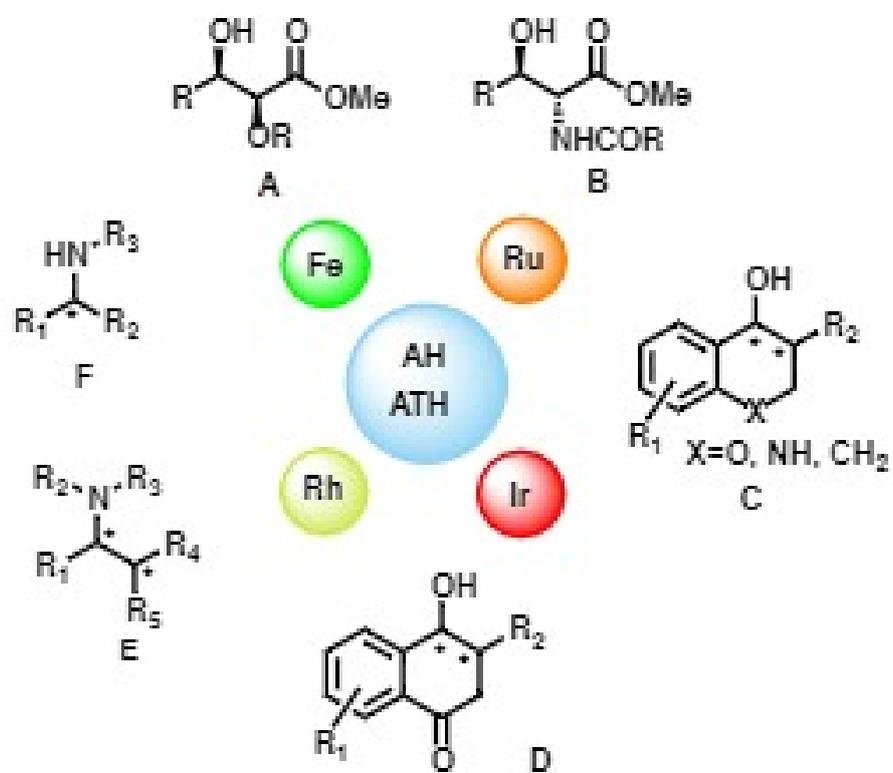
Short description of possible research topics for a PhD: Our group develops new catalytic processes for the synthesis of natural products and targets of biological interest. We have been interested in the development of novel methods for synthetic efficiency and atom and step economical processes using transition metal-catalyzed reactions as they provide a direct and selective way toward the synthesis of highly valuable products. The research program will be dedicated to the development of asymmetric catalytic methods in a context of sustainable development for carbon-carbon and carbon-hydrogen bond forming reactions using asymmetric hydrogenation (AH) or asymmetric hydrogen transfer reactions (ATH) through dynamic kinetic resolution (DKR) to target scaffolds of biorelevant molecules of medicinal. The PhD research program aims at developing new catalytic asymmetric approaches to address long-standing problems in the synthesis of chiral key intermediates such as A-F to access natural products and pharmaceutical drugs.

Required background of the student: Chemistry, Organic Chemistry, Catalysis

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. R. Molina-Betancourt, Echeverria, P.-G.; Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Synthesis* 2021, 53, 30-50
2. He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org. Chem. Front.* 2020, 7, 975
3. He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org Lett* 2020, 21, 3276
4. Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org Lett* 2019, 21, 2998
5. Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. *Chem. Commun.* 2018, 54, 283

Illustrations :



TITLE: INTERACTIONS BETWEEN THE CIRCADIAN AND DOPAMINERGIC SYSTEMS IN PARKINSON DISEASE STUDIED IN DROSOPHILA

Topic number : 2021_111

Field : Biology, Biophysics and Biochemistry, Life and Health Science and Technology

Subfield: Neurosciences, Neuropathology

ParisTech School: ESPCI Paris - PSL

Research team: Genes Circuits Rhythms and Neuropathology

<https://www.bio.espci.fr/-Serge-Birman-Genes-Circuits-29->

Research lab: Plasticité du cerveau

Lab location: Paris

Lab website: <https://www.bio.espci.fr/-Home->

Contact point for this topic: ESPCI Paris - PSL

Advisor 1: Serge Birman serge.birman@espci.fr

Advisor 2:

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: Parkinson's disease (PD) is the most common neurodegenerative movement disorder in humans, characterized by the dysfunction and loss of a significant proportion of midbrain dopaminergic neurons. The primary causes of the pathology remain poorly understood and there is currently no cure for this disease. An increase in oxidative stress, chronic neuroinflammation and the disruption of cellular degradation processes appear to be major determinants of PD pathogenesis. The physiology and behavior of most animals are controlled by internal circadian clocks (period of about 24 hours), synchronized by alternating day and night. The loss or weakening of the circadian clock is a risk factor that can also decrease oxidative stress resistance and contribute to neurodegenerative disease progression. In our laboratory, we use *Drosophila* to study the cellular and molecular mechanisms of PD pathogenesis (1-3). We previously demonstrated that specific circadian genes appear to control locomotor aging, stress resistance and dopaminergic neurodegeneration in this model (4, 5). The aim of this PhD project will be to carry out an in-depth analysis on the function in neurodegenerative processes of a new cycling protein that we have recently identified as being involved in circadian

activity and oxidative stress resistance. A parallel objective will be to identify brain dopaminergic circuits that are involved in this essential physiological pathway.

Required background of the student: Master's degree in Life Sciences (or Agriculture), ideally with previous training in Molecular Biology

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. 1. Riemensperger et al. (2013) A single dopamine pathway underlies progressive locomotor deficits in a *Drosophila* model of Parkinson disease. *Cell Rep* 5:952–960 doi:10.1016/j.celrep.2013.10.032
2. 2. Cassar et al. (2015) A dopamine receptor contributes to paraquat-induced neurotoxicity in *Drosophila*. *Hum. Mol. Genet.* 24(1):197-212 doi:10.1093/hmg/ddu430
3. 3. Issa et al. (2018) The lysosomal membrane protein LAMP2A promotes autophagic flux and prevents SNCA-induced Parkinson disease-like symptoms in the *Drosophila* brain. *Autophagy* 14(11):1898–1910 doi:10.1080/15548627.2018.1491489
4. 4. Vaccaro et al. (2017) *Drosophila* Clock is required in brain pacemaker neurons to prevent premature locomotor aging independently of its circadian function. *PLOS Genet* 13(1):e1006507 doi:10.1371/journal.pgen.1006507
5. 5. Hajji et al. (2019) Neuroprotective effects of PACAP against paraquat-induced oxidative stress in the *Drosophila* central nervous system. *Hum Mol Genet* 28(11):1905-1918 doi:10.1093/hmg/ddz031

Illustrations :

TITLE: FORMULATION OF BIOSYNTHETIC OPALS: HOW TO BETTER IMITATE THE MINERALOGY AND DEVELOP INVENTIVE SYSTEMS

Topic number : 2021_112

Field : Chemistry, Physical chemistry and Chemical Engineering, Material science, Mechanics and Fluids

Subfield:

ParisTech School: MINES ParisTech - PSL

Research team:

Research lab: CEMEF - Centre de mise en forme des matériaux

Lab location: Sophia-Antipolis

Lab website: <https://www.cemef.minesparis.psl.eu/>

Contact point for this topic: MINES ParisTech - PSL

Advisor 1: BOYER SEVERINE A.E. Severine.BOYER@mines-paristech.fr

Advisor 2: BURR Alain Alain.BURR@mines-paristech.fr

Advisor 3:

Advisor 4:

Short description of possible research topics for a PhD: The family of opals presents various sub-varieties, some of which are used in jewelry and classified as semi-precious stones; these varieties are distinguished by their origin, the background color or its nature. Without color schemes it is classified as "common", with color schemes it is classified as "precious" or "noble". Similar to the natural gem-opals, the as-synthesized opals exhibit a beautiful opalescence (Fig. 1 - Ref. 1).

Our study aims to understand in which coupling chemo-thermal conditions new synthetic opals can be created. Dedicated formulations will be developed; chemistry and also stricter selection of SiO₂ spheres will be of concerns as the processes of 'creation' by reverse engineering (Fig. 2 - Ref. 2).

The kinetic of the arrangement of these spheres to a quasi crystalline state requires careful developments to obtain a « crude gem ». Then, micro-structural changes to synthetic opal by heat treatments will be investigated (scanning electron microscopy SEM, X-ray, Fourier transform infrared FTIR, colorimetry). Transformation technics such as supercritical drying (Ref. 3) and/or coupled/decoupled hot isostatic pressure (HIP) will be employed.

From more fundamental skills, phase diagrams will be attempted to be

constructed. Mechanisms of structural evolution will be modeled with comprehensive chemo-physics (Ref. 1). These combinations of concepts will permit to discuss the imitation quality.

To be used in niche applications, proofs of concept implemented in 3D printing (in gel mode) are proposed to be performed (Fig. 3 - Ref. 4). The optical properties and the stability of the 3D shape will be associated with micro-structural achievements carried out in the first part of the work.

Key-words: synthetic blends, crystal of spheres, silica gel, 3D printing, optical rerendering

Required background of the student: Materials, Chemistry-Physics, Modeling

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Ref. 1- A. Arasuna, M. Okuno, H. Okudera, T. Mizukami, S. Arai, S.I. Katayama, M. Koyano, N. Ito. Structural changes of synthetic opal by heat treatment. Phys. Chem. Minerals (2013) 40: 747-755.

Doi: 10.1007/s00269-013-0609-1

2. Ref. 2- P. Ni, P. Dong, B. Cheng, X. Li, D. Zhang. Synthetic SiO₂ opals. Adv. Mater. (2001) 13: 437-441.

Doi: 10.1002/1521-4095(200103)13:6<437::AID-ADMA437>3.0.CO;2-8

3. Ref. 3- A.I. Puzynin. The Application of supercritical drying in the synthesis of silica-based materials. Russ. J. Phys. Chem. B (2014) 8: 944-952.

Doi: 10.1134/S1990793114070112

4. Ref. 4- S.A.E. Boyer, L. Jandet, A. Burr. 3D-Extrusion manufacturing of a kaolinite dough taken in its pristine state. Front. Mater. (2021) 8: 582885 1-12.

Doi: 10.3389/fmats.2021.582885

5.

Illustrations :

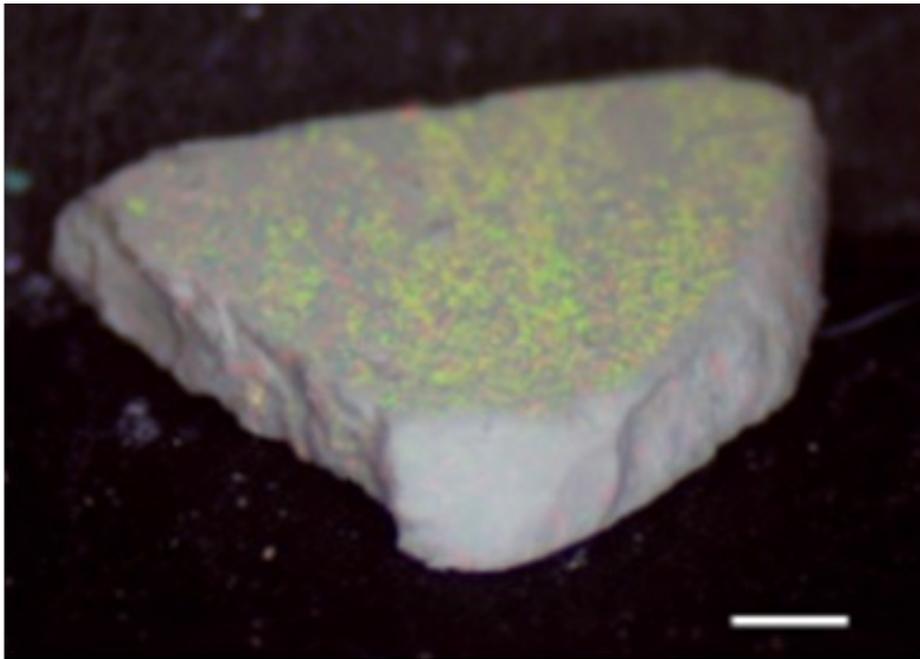


Fig. 1 - Ref. 1- Opalescence of synthetic opal (scale 1 mm).
(*Phys. Chem. Minerals* (2013) 40: 747-755)

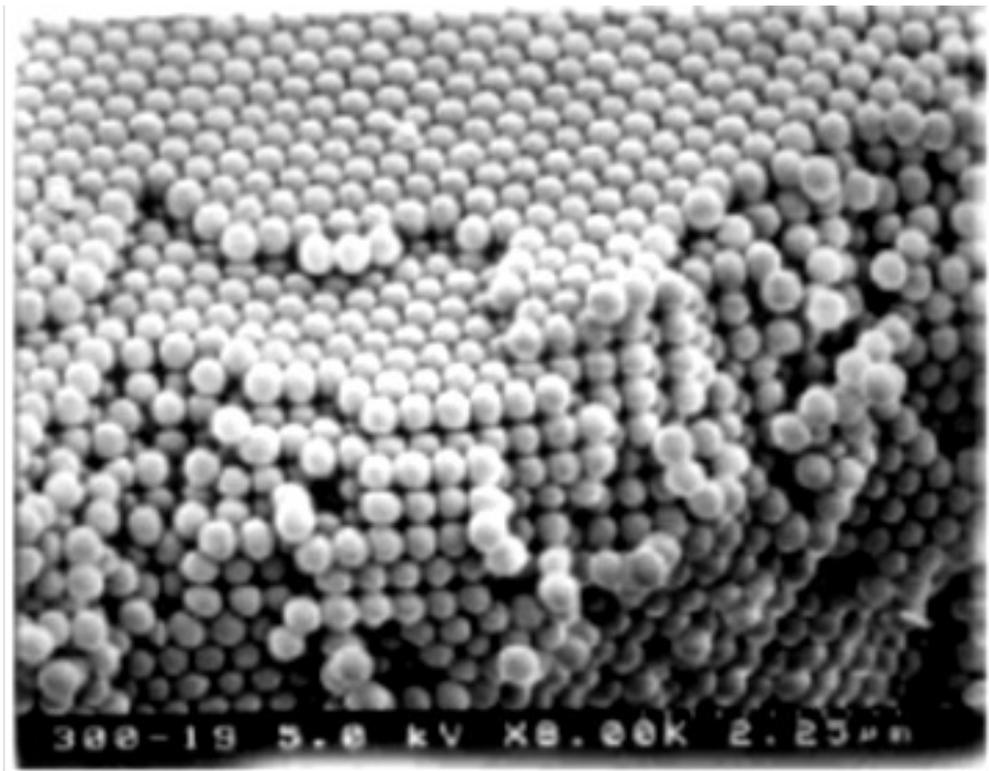


Fig. 2 - Ref. 2- Boundaries of cleaved facets in the SiO_2 opal (SEM).
(*Adv. Mater.* (2001) 13: 437-441)

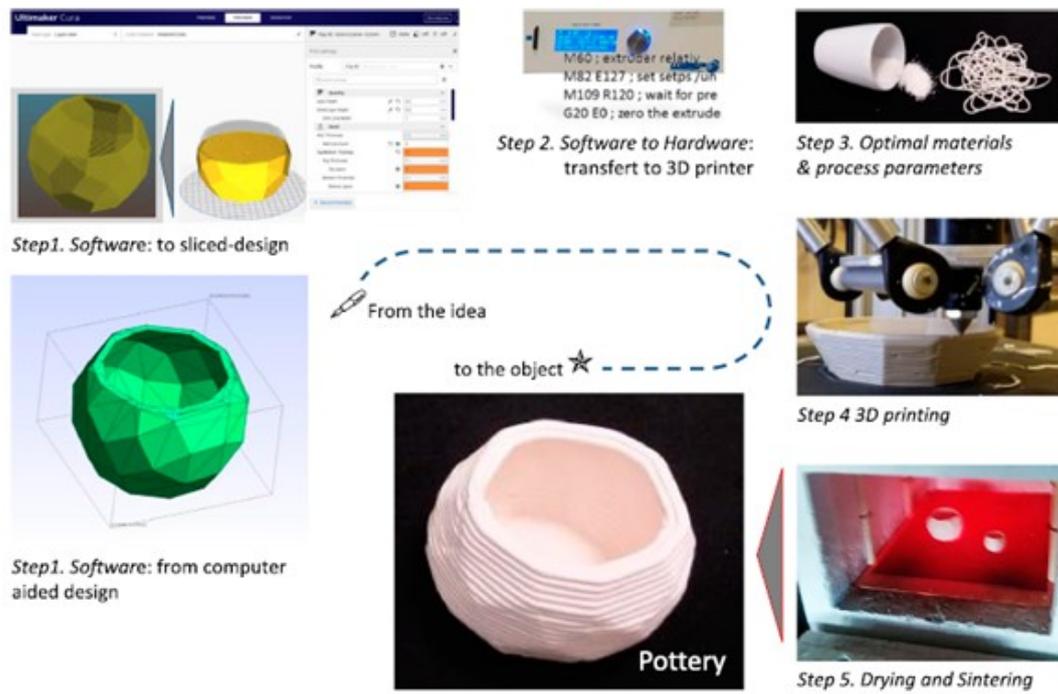


Fig. 3 - Ref. 4- Hydrated kaolinite to build artistic pottery.
 (Front. Mater. (2021) 8: 582885 1-12)