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SCIENTIFIC REPORT 2020

INSTITUT CARNOT
Energies du futur

Directors' foreword

The main event that marked the year 2020 was, without a doubt, the Covid-19 pandemic. The public health and economic crises that ensued are still ongoing today. Research and innovation have emerged from this turbulent context as more necessary than ever in the health sector, obviously, but also in the energy, industrial, and environmental sectors, less-directly affected by the pandemic.

Urban air pollution declined sharply as the economy slowed down during Covid-19 lockdowns around the world. Even this, however, did not curb overall atmospheric CO_2 emissions. Looking ahead, new eco-designed energy systems will ensure a smaller carbon footprint at every stage in the lifecycle. Built on breakthrough technologies, such systems will offer the levels of energy efficiency that will be necessary to achieve carbon neutrality by 2050 and slow global warming.

At CEA-Liten, our research, development, and innovation activities address these challenges. We develop new breakthrough concepts in materials, components, and processes, as well as control and management systems, taking them all the way to the prototype stage to test their potential. Our programs, all of which integrate circular economy concerns, focus on carbon-free energy production, energy storage, energy grids, and energy efficiency.

At the end of 2020, we had 150 PhD students conducting research in our labs. We supported 26 dissertation defenses, earned five new Habilitations (HDR), authored nearly 180 publications in peer-reviewed journals, and filed 210 patents as we continued to cultivate scientific and technological excellence throughout what is now known as "the year of the coronavirus."

Our Carnot label was renewed in 2020 for an additional four-year period. We also ramped up our cooperation with France's national center for scientific research, CNRS, through the joint submission of an ambitious early-stage hydrogen R&D project. This far-reaching project aims at supporting the foundations for a hydrogen industry in France. We also contributed to launching the Solar Academy Graduate School at our site in Le Bourget du Lac.

Inside this year's Annual Scientific Report, you will find a host of exciting scientific and technological advances made as a result of R&D conducted with our partners from academic research and from industry, all with the goal of shaping tomorrow's carbon-free energy landscape.

François Legalland,
CEA-Liten CEO

Florence Lefebvre-Joud,
Deputy Director for Science

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Liten (the Laboratory for Innovation in Technology for Energy and Nanomaterials) is Europe's largest research institute entirely dedicated to the energy transition. It is an institute of the CEA (the French Alternative Energies and Atomic Energy Commission) and a leader of Carnot Énergies du Futur, a consortium dedicated to research partnerships with businesses. Its main facilities are located in Grenoble and Chambéry, France. In just fifteen years, Liten has carved out a position as a leader in technology research for energy and the environment in support of economic growth.

At CEA-Liten, we work on projects at different stages in the lifecycle of a given technology with partners from both academic research and industrial R&D. From research on new materials and components to the development of simulations and models coupled with lab and field testing, we have the capacity to bring a technology from a laboratory prototype up to functional demonstrators at a scale representative of a real life application.

Our experience has led us to the conclusion that the energy transition can only succeed with the convergence of renewable energy, smart grids, and overall energy efficiency. The institute explores various topics such as solar energy, grid management, and energy storage including batteries and hydrogen. Energy efficiency and the circular economy form an integral part of CEA-Liten's research. The developed technologies address several markets, from power generation and distribution to transportation, and from industrial processes to greentech.

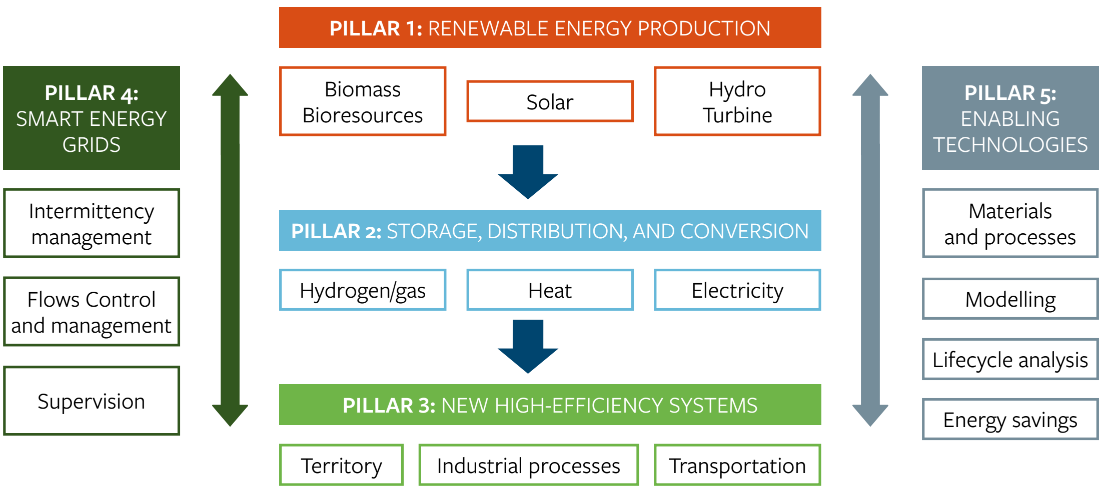
CEA-Liten has leveraged its position within the CEA, one of the world's most innovative government research organizations, to lead the development of complementary, cost-competitive, and more environmental friendly solutions to support an energy strategy built on multiple energy vectors and complementary time and space scales.

This year's Scientific Report is organized around four R&D pillars, namely *Producing decarbonated energy*, *Smart grids & Energy efficiency*, *Energy storage & Flexibility* and *Circular economy & Materials*. You will find selected extended papers and highlights for each of them, underlining some major results obtained in 2020. They will provide deeper understanding of the kinds of scientific and technological advances happening at CEA-Liten.

CEA-LITEN AT THE CENTER OF THE RESEARCH-INNOVATION CONTINUUM THROUGH ITS INVOLVEMENT IN CARNOT *ENERGIES DU FUTUR*

CEA-Liten is a founding partner of the energy research institute Carnot Energies du Futur (Carnot EF), established in 2007. The institute is managed jointly by Grenoble INP and CEA-Liten, which holds the deputy directorship and chief operational management posts.

Carnot EF conducts R&D on low-carbon-footprint energy systems and energy efficiency from two closely intertwined sites in Grenoble and Le Bourget du Lac. Specifically, R&D programs target innovations in the industrial and transportation sectors, and various adjacent markets. This focus aligns closely with CEA-Liten's positioning. Carnot EF is a unique alliance of ten academic research labs and four CEA-Liten departments that, together, deliver a range of R&D services broad enough to address any TRL (Technology Readiness Level) on any topic related to renewable energy deployment.

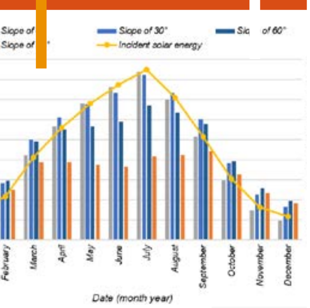


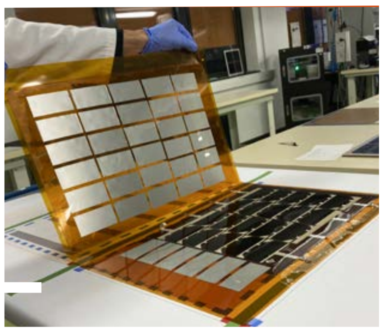
Carnot EF's label was renewed for the first time in 2011, again in 2016, and, most recently, in March 2020. With each renewal, Carnot EF has readjusted its scope and priority research topics to reflect the changing needs of companies and society. For example, Carnot EF included hydrogen and battery research and two additional CEA-Liten departments in 2011. In 2015, the business models research and GAEL lab were integrated into Carnot EF. Finally, in 2019, Carnot EF benefitted from closer cooperation between CEA-Liten and G2ELab, LOCIE, and LEPMI to ramp up its smart, multi-vector energy grid activities and bolster its support of hydrogen deployment across industry, transport, and the public sector.
During the most recent label cycle, Carnot matching funds supported some 20 pump-priming research projects per year, most of the projects being multi-year. Emerging research topics like high-temperature water electrolysis, printed PEMFCs, all-solid-state batteries, and Si/perovskite tandem PV cells have all benefited from these matching funds. In addition to these topics, Carnot EF recently sharpened its focus on multi-vector energy grids and continues to invest in eco-design and additive manufacturing for energy components. Support for these new programs is evidence of Carnot EF's ongoing commitment to driving high-potential innovations for tomorrow's energy systems.

INSTITUT CARNOT Energies du futur

PRODUCING DECARBONATED ENERGY

CEA-LITEN RESEARCH ENCOMPASSES THE ENTIRE SOLAR PHOTOVOLTAIC COMPONENT VALUE CHAIN. THE INSTITUTE LEVERAGES INDUSTRIAL SCALE EQUIPMENT TO PRODUCE MODULES WITH YIELDS OF 25% ON SILICON. THE ULTIMATE GOAL IS TO OBTAIN YIELDS IN EXCESS OF 30% WITH TANDEM TECHNOLOGIES. IN ADDITION TO OUR WORK ON COMPONENTS, WE ALSO DEVELOP INNOVATIVE SYSTEM ARCHITECTURES TO INCREASE THE PRODUCTIVITY OF GROUND-MOUNTED SOLAR POWER PLANTS AND TO INTEGRATE SOLAR PANELS INTO ENVIRONMENTS RANGING FROM BUILDINGS AND INDUSTRIAL PARKS TO RAIL AND ROADWAYS.





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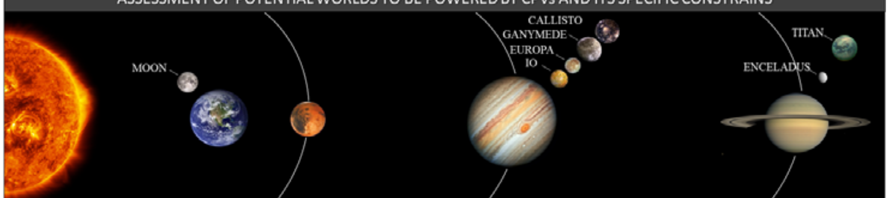
SOLAR ARRAYS FOR SPACE APPLICATIONS

Over the past decades, the space industry has launched a revolution with the emergence of new players and new technologies. For instance, the appearance in 1999 in the USA of so-called Cubesat satellites, based on 10 cm elemental cubes, allowed universities and states to send objects into space, mainly in low orbit (300 - 1200 km), for Internet of Things (IoT) applications. Today more than 1,400 Cubesats have been launched in orbit and this number is expected to double in the coming years. The arrival of the GAFA in the space field also significantly transformed the ecosystem, which was then dominated by national agencies. Constellation projects, such as Oneweb, Kuipert and Starlink, plan to send tens of thousands of satellites to provide Internet globally. For all those missions, as well as for future Lunar and Martian bases, photovoltaic solutions remain the preferred power source. Finally, for the past 10 years, the propulsion systems of telecommunication satellites operating in geostationary orbit have been switched to electric power, giving up the heavy and voluminous chemical systems. Thus, the need for solar generators has considerably evolved over the last decade, from a few tens of kW to several tens of MW. To address this problem, it becomes necessary to review the manufacturing processes, to speed up the production, and to ensure the availability of a number of expensive components such as photovoltaic solar cells. The use of COTS (Commercial Off-The-Shelf) components from terrestrial applications also reduces the needs of scarce materials (such as Germanium) and is therefore an essential lever for cost reduction. Currently, solar generators are rigid assemblies of PVA (PhotoVoltaic Array) themselves formed by SCA (Solar Cell Assembly) glued on a honeycomb structure. A SCA consists of a cover glass of 100 to 150 µm thickness, protecting the device from irradiations, a layer of low outgassing silicone glue providing the connection between the cover glass and the solar cell, interconnectors allowing the serial of the cells, a bypass diode and a photovoltaic cell. The SCA, thanks to its III-V multi-junction cell architecture, has an efficiency > 30 % for an irradiance of 1361 $W.m^{-2}$ with an extra-terrestrial AM0 spectrum. The specific power of standard PVA is around 75 $W.kg^{-1}$ with a compactness of 8 $kW.m^{-3}$.
For more than 20 years, CEA-Liten has been working on terrestrial photovoltaic applications and their associated processes. The objective is to develop and promote photovoltaic technologies, for terrestrial solar power plants but also for innovative applications. Building on this experience, CEA-Liten focuses its research and development effort towards space photovoltaic applications. This article presents four corresponding R&D topics: space concentrator photovoltaic, advanced characterization for space applications, flexible high power photovoltaic arrays and silicon photovoltaic arrays.

SPACE CONCENTRATOR PHOTOVOLTAIC – CPV

Concentrator photovoltaic, which focuses sunlight using optics on high-efficiency photovoltaic cells (multi-junction III-V), allows to reach efficiencies greater than 30% at module level. This solution decreases the prices of PVA by replacing costly surfaces of III-V solar cells by cheaper concentrating optical elements such as mirrors or lenses. For terrestrial applications, micro-concentrator PV modules, with solar cells in the millimeter size range, are more efficient than traditional (larger) concentrators. Studies at CEA were initiated from 2016 to 2018 through an R&D Project led by the CNES [P1], and was

ASSESSMENT OF POTENTIAL WORLDS TO BE POWERED BY CPVs AND ITS SPECIFIC CONSTRAINS



Mean Distance (AU)	~1					1.67	5.5								10			
Solar Flux (W/m²)	1,366					589	51								15			
WORLD	EARTH			MOON		MARS	JUPITER	IO	EUROPA		GANYMEDE		CALLISTO		SATURN	ENCELADUS		TITAN
MISSION / CONDITION	LEO	MEO	GEO	O/F	L/R	O/F	O/F	O/F	O/F	L/R	O/F	L/R	O/F	L/R	O/F	O/F	L/R	O/F
Atomic Oxygen	●	○				○			○		○		○			○	○	
Dust					○													
Extreme Temperatures	○	○	○	○	○	○	●	●	●	●	●	●	●	●	●	●	●	●
Harsh Radiation e- p+	○	●	●				●	●	●	●	●	●	●	●	○	○	○	○
Micrometeoroid	●	○	○	○	○		○								○			
Plasma	○	○	●				●	●							○	○		
Thermal Cycling	●	●	●	●	●	○	○	●	○	○	○	○	○	○	○	○	○	○
UV Radiation	●	●	●	●	●	●	○	○	○	○	○	○	○	○	○	○	○	○

Convention: ● High impact ○ Moderate impact on Concentrator PhotoVoltaics (CPV). AU : Astronomical Unit (~150 $x10^9$m). Low Earth Orbit (LEO), Medium Earth Orbit (MEO), and GEosynchronous Orbit (GEO). O: Orbiter, F: Flyby, L: Lander, R: Rover. e-: electrons, p+: protons.

Figure 1: *Assessment of potential worlds to be powered by CPVs according to their specific constraints* [3].

the first work specifically dedicated to CPV for space. Optical, electrical and thermal characteristics were investigated. The designed system was based on Total Internal Reflection running at a low concentration of 7.6 X in order to achieve an acceptance angle compatible with GEO missions. With linear optics and multi-junctions solar cells (13 x 1.5 mm²), the prototype reaches an efficiency close to 20 % at AM0 with an experimental optical efficiency of 75 %. Specific power of the first system was 20 $W.kg^{-1}$ with a potential of 150 $W.kg^{-1}$.

However, such specific power was not high enough for this disruptive technology in comparison with classical PVA (75 $W.kg^{-1}$) [1]. To get a broader view on the potential of this technology for space, the work was then focused on a review assessing CPV specificities for space. Constraints of various destination and mission types: (e.g. orbiter, flyby, aerial and rover) have been evaluated. More than 30 missions concepts to explore 14 celestial bodies have been identified and summarized, and 4 types of worlds have been sorted: Earth orbits, dusty worlds (Moon and Mars), high temperature (Venus, Mercury and the near-Sun), and low intensity low temperature conditions for gas giants. The results of this work are summarized in Figure 1. This table allows to quickly identify if CPV or even PV can be a solution to power given missions [3]. Thanks to these previous works and the funding from CARNOT [P2], a patent pending solution has been developed [T2, T3]. This solution should be proposed to the space community, and qualified. This innovative and totally integrated solution will allow specific power of more than 200 $W.kg^{-1}$.

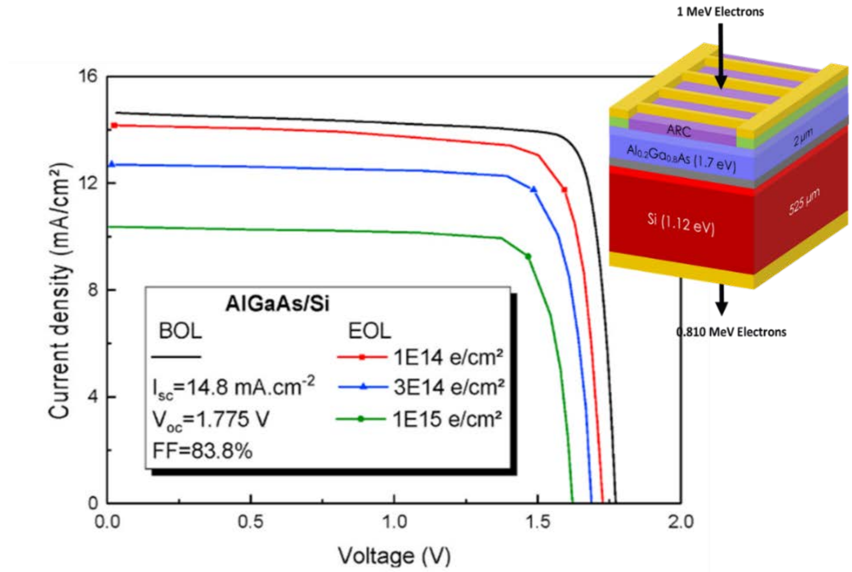


Figure 2: *Schematics of III-V/Silicon tandem solar cell (top-right) and experimental J-V curves under AM0 extra-terrestrial spectrum, before (BOL) and after electrons irradiations at increasing fluences (EOL) [3]*

ADVANCED CHARACTERIZATION FOR SPACE APPLICATIONS

As space missions have various and complex environmental constraints, characterization is often a real challenge to validate materials behavior and electrical performances of PVA; accurate testing is a key point. CEA-Liten has collaborations with the IRAMIS Plateform at CEA Saclay and ONERA at Toulouse to evaluate materials and COTS components under particles irradiations. First irradiations are often performed with 1 MeV electrons at a fluence of 10^{15} $e.cm^{-2}$ (close to GEO equivalent fluence). During a recently defended PhD thesis, a specific work was focused on the behavior of III-V on silicon tandem solar cells under irradiations [T1], a technology that has a high efficiency potential while getting rid of scarce/expensive germanium substrates. Figure 2 presents the experimental J-V curves under AM0 extra-terrestrial spectrum, before (BOL) and after electrons irradiations at increasing fluences (EOL). These key results allow to size the electrical architecture and the mechanical structure of the solar generators following the needs of the bus and the payload. A study has also been conducted with the CNES to evaluate the potential of emerging solar cells technologies for space [P3]. A promising candidate is under investigation at CEA-Liten: perovskite solar cells [T4]. This flexible and lightweight technology currently developed for terrestrial applications attracts more and more attention for space related opportunities.

Advanced characterization can also play a key role in the PVA performance evaluation. Today, the method used in the space solar array industry to detect bubbles at the cell/substrate interface, whose typical order of magnitude is a few millimeters, consists in carrying out thermal vacuum test at panel level during equipped panel acceptance test sequence. These thermal vacuum tests are relatively expensive and time consuming. CEA proposed a new method was based on Transient ElectroLuminescence (TEL), stemming from a project funded by the CNES [5][P4]. As one can see in Figure 3, this non-destructive method localizes voids between the solar cells and the substrate (Kapton here).

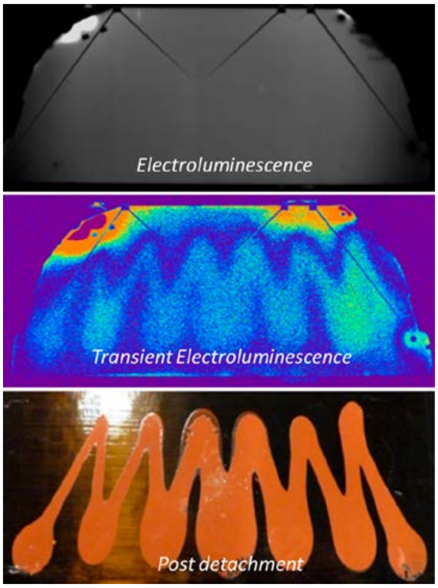
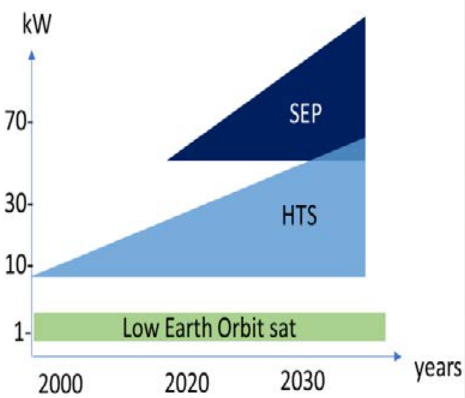


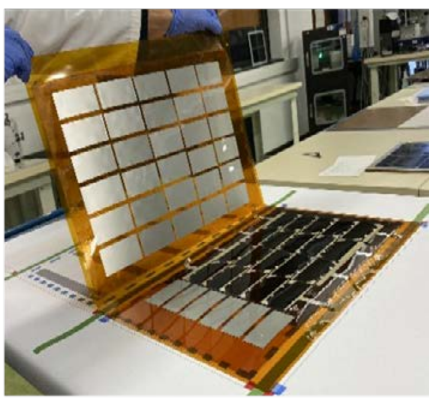
Figure 3: *Steady state (top) & transient (middle) electroluminescence (TEL) pictures of III-V space solar cells; post-detachment pictures (bottom) revealing the glue pattern below the solar cell. The TEL Method allows non-destructive gluing defects detection between cells and module backsheet [5].*

FLEXIBLE HIGH POWER PHOTOVOLTAIC ARRAYS

To answer the growing power demand in space applications, the solution lies neither in stacking more of the existing heavy and rigid space solar arrays, nor by marginal power conversion efficiency improvements on the already performant III-V multi-junction solar cells. An increased surface of solar cells is necessary, in combination with a reduction of solar array stowage volume ($W.m^{-3}$) and increased power/mass ratio ($W.kg^{-1}$). More solar cells per unit of volume are needed; flexible solar arrays are one promising solution for this high-power demand challenge. In the ALFAMA EU H2020 project - Advanced Lightweight and Flexible Array with Mechanical Architecture - a Z folded lightweight solar array (see Figure 4) was developed to face this emerging high power demand. Four innovative axes have been developed:

- Modular mechanical architecture adapted to large PVA (> 70 kW capability)
- Volume gain, by flexible PVA & compact stowed configuration
- System cost reduction, with terrestrial PV inspired fabrication processes
- High power per mass ratio, thanks to high efficient ultra-thin solar cells & PVA.





SILICON PHOTOVOLTAIC ARRAYS

To meet the market demand for lower costs, a promising route is to use terrestrial silicon cells. Figure 5 shows the drop in yields after irradiation of bare cells; it can go up to 50 % for important irradiations fluences, characteristic of geostationary missions for instance. In contrast, for low earth orbits, silicon solar cells have a power loss of only 20-30 %.

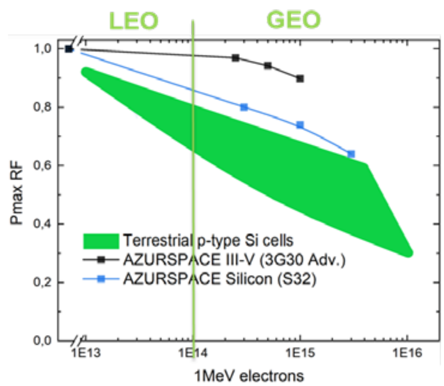


Figure 5: *Remaining factors for the power of Terrestrials p-type Silicon cells versus Silicon S32 and III-V 3G30 from AZURSPACE.*

Thus, CEA-Liten teams are working on silicon cell & module processes and studying the behavior of these PVAs in respect to irradiative, but also thermal and mechanical environmental constraints. In 2020, the laboratory acquired thermal chambers able to achieve cycles between -180°C and +150°C at atmospheric pressure and thermal cycles from -120°C to +120°C under vacuum. The aim is to achieve an industrial transfer. Patents have been filed [6] and studies and developments continue on this highly competitive and promising topic.

Figure 4: *ALFAMA flexible solar array solution: III-V solar cells (& metallic dummies) are laminated on Kapton® foil with printed conductive tracks. The Z-folded approach allows a very compact stowed configuration for launching [5].*

PERSPECTIVES

Important R&D work has been performed on prototyping for concentrators and photovoltaic arrays. Emphasis was also placed on perovskite solar cells development and on innovative characterizations for solar generator performances in combination with various accelerated ageing tests. Both geostationary and constellations applications can benefit from this research. With those developments in hand, CEA-Liten is becoming a major R&D player for space PV market. The next step is to succeed with the industrial transfer of our technologies (silicon array, flexible arrays, etc.) and to pursue R&D on PV arrays to anticipate the next evolutions.

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REFERENCES

Papers / Patents:

[1] P. Voarino et al, “A space self-integrated micro-concentrator design: the SLIT,” 2019 European Space Power Conference (ESPC), Juan-les-Pins, France, 2019, pp. 1-6, doi: 10.1109/ESPC.2019.8932023.
[2] A. Bermudez-Garcia, P. Voarino, O. Raccurt, “Environments, Needs And Opportunities For Future Space Photovoltaic Power Generation: A Review”, Applied Energy journal, 2021, https://doi.org/10.1016/j.apenergy.2021.116757.
[3] K. Medjoubi et al, « Electrons irradiation of III-V//Si solar cells for NIRT conditions », Sol. Energy Mater. Sol. Cells, 223, 110975 (2021).
[4] R. Cariou et al, “Characterization of solar array’s cells to substrate bonding interface,” 2019 European Space Power Conference (ESPC), Juan-les-Pins, France, 2019, pp. 1-5, doi: 10.1109/ESPC.2019.8932090.
[5] T. Guerin et al, “ALFAMA project: Development of a flexible and laminated space photovoltaic array”, 2020 Proceedings of the EUPVSEC 37th European Photovoltaic Solar Energy Conference and Exhibition (EUPVSEC2020) 1261–1263 doi:10.4229/EUPVSEC20202020-5BO.15.1.
[6] V. Maneval, F. Chabuel, Y. Roujol, J. Gaume, « Procédé de fabrication d’un module photovoltaïque avec réticulation partielle et lamination », FR 1914469 (2019) Patent Pending

Defended / on-going thesis:

[T1] K. Medjoubi, “Investigation of the emerging III-V//Si tandem solar cell behavior under irradiation for space applciations”, PhD Thesis, CEA Liten - Grenoble / CEA –Saclay, 2021.
[T2] A. Bermudez-Garcia, “Photovoltaic micro-concentration for space applications”, PhD Thesis, CEA Liten – Grenoble, 2019 - 2022.
[T3] V. Vareilles, “Micro-concentration for Space Applications”, PhD Thesis, CEA Liten – Grenoble, 2020 - 2023.
[T4] C. Costa, “Ageing study of perovskites–based solar cells in space environments: absorber degradation mechanism and devices optimization”, PhD Thesis, CEA Liten - Grenoble / ONERA, 2020 - 2023.

Projects:

[P1] R&T CNES, Concepts de micro-concentration pour générateurs solaires, 2016-2018.
[P2] CARNOT Energies du Futur, MICROFLEX: développement d’architectures de modules innovantes à base de cellules micrométriques et flexibles, 2018-2021.
[P3] R&T CNES, Evaluation de cellules Photovoltaïques émergentes, 2019-2020.
[P4] R&T CNES, Utilisation de la méthode Transient Electroluminescence (ELM) pour vérifier le collage des cellules solaire, 2018-2019.
[P5] ALFAMA: Advanced Lightweight and Flexible Array with Mechanical Architecture - European Union’s Horizon 2020 research and innovation Program - grant N° 821876.

INFLUENCE OF SURFACE DEFECTIVITY ON SI HETEROJUNCTION CELL (SHJ) PERFORMANCE

The handling and transportation steps during the industrial fabrication of SHJ cells induce depassivated regions (the "defectivity") at the silicon (c-Si) surfaces that hinder the cell performances [1]. Thanks to our combined experimental & simulation approach, we propose a quantification and, for the first time, a physical understanding of such effects [2].

APPROACH

Since the characterization of the depassivated regions induced by handling and automatic transportation tools hardly gave information on their geometrical and physical properties, the correlation between the defects properties and the associated performance losses were still missing. To circumvent this limitation, we have developed a simulation code (for TCAD Silvaco software [3]) with the implementation of variable localized depassivated regions. In parallel, we have intentionally generated defects on CEA-Liten cells corresponding to the simulated ones. The comparison between simulations and experimentally measured trends provided a validation of the simulation code. The simulations were then used to study the influence of the defect properties and spatial distribution on their induced losses. For each condition, the simulations allowed to understand the physical mechanisms thanks to the mapping of key physical quantities (see typical map of current densities in the c-Si in Figure 1.).

RESULTS AND PERSPECTIVES

Both simulations and measurements showed that the depassivation as low as 0.2% of the cell surface could lead to 6% power losses, which highlights the detrimental influence of the defectivity. Whether the defectivity is on the front or the backside does not change significantly its effects. In addition, the parametric studies allowed us to understand the influence of the defectivity and to propose ways to mitigate the resulting effects in order to transpose our conclusions to cells produced at CEA-Liten. We highlighted that for a given depassivated surface:

- A single and wide defect is preferred to a distribution of several thin defects.
- If the defects cannot be fully merged into a single defect, their spatial concentration remains an efficient lever to mitigate the losses, provided that the distance between them is smaller than the minority carrier diffusion length.

We have also shown that reducing the c-Si wafer resistivity is beneficial, which can partly explain why low resistivity ranges are currently preferred on the SHJ pilot line.

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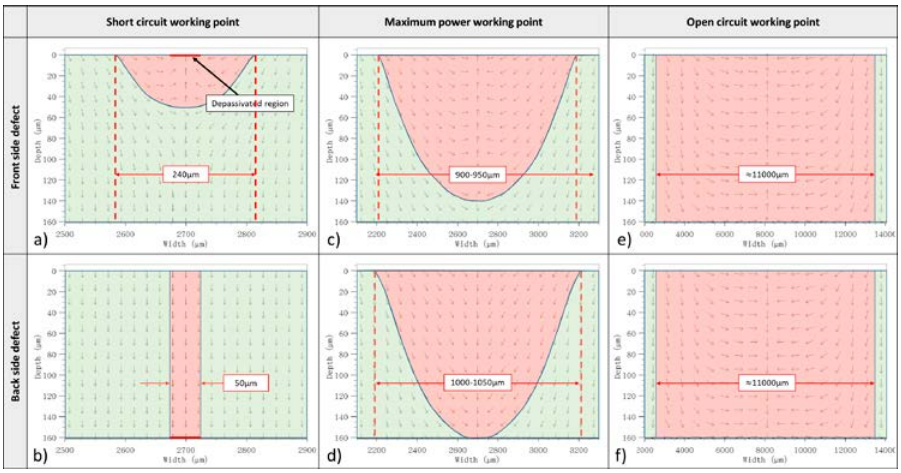

Figure 1: *Hole current density map within the c-Si for a cell with a front side or a back-side depassivated region at the short-circuit, maximum power and open circuit working points. The red zone on each graph illustrates the area impacted by the depassivated region.*

REFERENCES

[1] A. Fischer, IV. Vulcanean, A. Moldovan, J. Rentsch, "Approach to clarify the cause of handling defects in silicon heterojunction cell production through the interplay of different imaging techniques", Proc. 36th Eur. Photovolt. Sol. Energy Conf. Exhib. Marseille, France, 2019: 541-545.

[2] V. Giglia, R. Varache, J. Veirman, E. Fourmond, "Understanding of the influence of localized surface defectivity properties on the performances of silicon heterojunction cells", Prog Photovolt Res Appl. 28 (2020) 1333–1344. https://doi.org/10.1002/pip.3330.

[3] Atlas package from Silvaco. https://www.silvaco.com/products/tcad/device_simulation/atlas/atlas.html

CONSENSUS ON STABILITY ASSESSMENT AND REPORTING FOR PEROVSKITE BASED PHOTOVOLTAICS

The existing characterization procedures to evaluate emerging photovoltaic devices are not appropriate for halide perovskite solar cells, a new generation of solar cells called to overcome the present state-of-the-art technologies. A group of worldwide scientists, including a team from CEA-Liten, have reached a consensus on the suitable procedures and the variables to be reported in stability studies of this kind of solar cells.

APPROACH

In 2010, the organic solar cells community established guidelines for stability testing of thin film solar cell technologies, such as polymer or dye-sensitized solar cells [1]. Such guidelines were called "ISOS procedures". Perovskite photovoltaics emerged in 2009. Since then, power conversion efficiency boomed, reaching up to 25.5 % [2]. Concerning the stability, it quickly appeared that phenomena specific to perovskites must be taken into account such as recovery after stress, particular sensitivity to electrical bias or light. Thus, existing ISOS guidelines needed to be completed in order to describe more accurately the ageing procedures and lifetime reports on perovskite solar cells. In 2018, the group of scientists gathered at the International Summit on Organic and hybrid photovoltaics Stability), led by Prof. Lira-Cantú (ICN2) and Prof. A. Katz (Ben-Gurion University of the Negev), decided to draft an updated version of ISOS procedures.

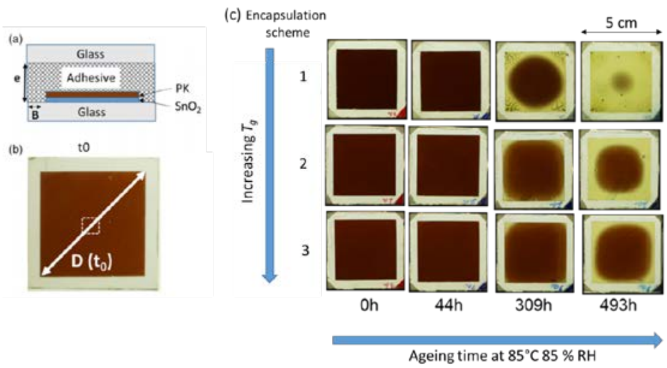

Figure 1: a) Side view of glass encapsulation of a perovskite layer; b) Top view (photograph) of the initial glass encapsulated perovskite layer before ageing (from [6]); c) Overview of ageing at 85°C and 85% relative humidity of a perovskite layer encapsulated with three different encapsulation schemes, having increasing glass transition temperatures (denoted Tg).

REFERENCES

[1] M. O. Reese et al., "Consensus stability testing protocols for organic photovoltaic materials and devices", Sol. Energy Mater. Sol. Cells, Vol. 95, Issue 5 (2011), 1253 - 1267. https://doi.org/10.1016/j.solmat.2011.01.036

[2] M. Green et al., "Solar cell efficiency tables (version 57) ", Prog. Photovolt. Res. Appl., 29 (2021), 3 – 15. https://doi.org/10.1002/pip.3371

[3] M. V. Khenkin et al., "Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures", Nat. Energy 5 (2020), 35 – 49. https://www.nature.com/articles/s41560-019-0529-5

[4] E. Booker et al., "Perovskite Test: A High Throughput Method to Screen Ambient Encapsulation Conditions", Energy Technol., vol. 4, no. 4 (2020), 2000041. https://doi.org/10.1002/ente.202000041

RESULTS AND PERSPECTIVES

This consensus paper was published in Nature Energy in 2020 [3]. The CEA-Liten team was involved in establishing this consensus statement regarding its expertise in perovskite device processing, encapsulation and lifetime assessment, be it intrinsic (stability in inert atmosphere) or extrinsic (stability against moisture and oxygen). The team gave recommendations notably regarding definition of atmosphere, electrical bias, and proper description of encapsulation scheme. Such information is crucial since encapsulation not only delays ambient species ingress, but it also prevents diffusion out of the solar cell of volatile degradation products. The team also highlighted the importance of characterizing the encapsulation scheme itself in order to better understand solar cell stability. With this perspective, it is recommended to assess two aspects of encapsulation : its efficiency and its stability. Efficiency is characterized by gas-barrier measurement of membranes alone and in addition, the team also developed a procedure to determine permeation pathways through the whole encapsulation scheme [4]. Application of ISOS procedures on encapsulation materials is highly recommended.

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A LIGHTWEIGHT TRIANGULAR BUILDING INTEGRATED PHOTOVOLTAIC MODULE

Building integrated photovoltaic modules are essential for Net Zero Energy Buildings. Nevertheless, their installation on complex shape buildings is rare due to fastening issues and important electrical energy losses. CEA-Liten optimized the mounting process and performance of an innovative triangular lightweight photovoltaic prototype suitable for integration into geodesic dome facets.

APPROACH

Building integrated photovoltaic modules (BIPV) combine basic functions of traditional construction elements (sealing, daylighting...) with electrical production, which is compatible with Nearly Zero Energy Buildings requirements. Nevertheless, very few BIPV projects deal with complex shape buildings mainly due to fastening issues (detachment, weight...) and important energy losses (existing multiple shadings and orientations). Thus, we optimized the mounting process and performance of a novel esthetical, lightweight triangular thin film photovoltaic module suitable for integration into geodesic dome polymer cover [1]. We defined first a prototype assembly method and evaluated its relevance. Then, we developed and validated with an outdoor tiltable test bench a dynamic thermal and electrical model of the BIPV system, including dummy parts and a dome cover triangular facet, with nodal approach. Finally, using this model and four slopes, we determined locations on a geodesic dome that optimize a south-oriented BIPV triangle thermal behavior and annual electrical production.

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RESULTS AND PERSPECTIVES

We proposed a gluing process and a simplified method to identify photovoltaic module adhesion issues based on measured thermal gradients between layers. Then, the validation on cold weeks of the numerical model developed was satisfactory, showing slight underestimation of measured data with mean absolute errors between 0.31°C and 1.97°C and mean bias errors between -0.44°C and -0.02°C. The calculated monthly photovoltaic module mean temperature was up to 22°C with a maximum temperature of 58.2°C, considering south-orientation and slopes up to 90° at Lyon. The BIPV triangle provided monthly array energy yields up to 54.8 Wh/Wp, monthly electrical efficiencies between 7.7% and 8.3% and annual energy productions up to 5.9 kWh (see figure 1). These results highlight that slopes between 30° and 60° represent a good trade-off for the system integration at both thermal and electrical levels. On-going works consider the BIPV triangle optimization, varying its orientations, composition, and weather conditions.

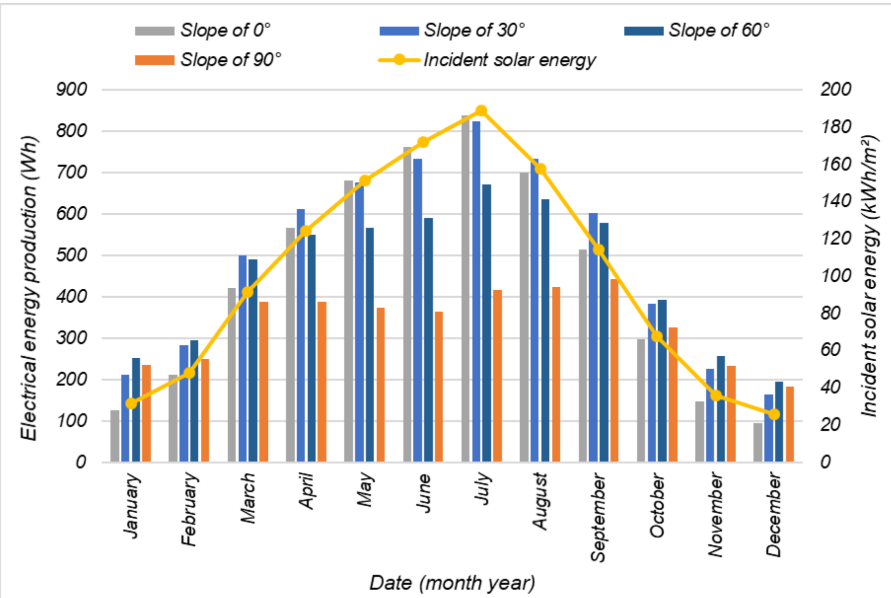


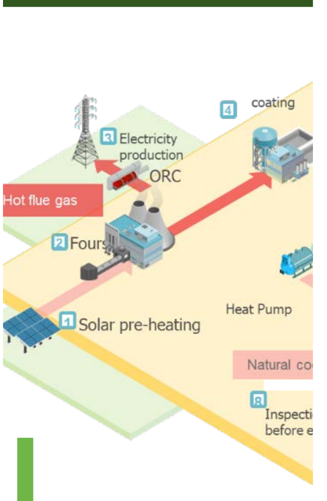
Figure 1: *Calculated monthly cumulated electrical energy production of the south- oriented thin film photovoltaic triangle integrated into a geodesic dome located at Lyon for four slopes (0°; 30°; 60° and 90°) and measured cumulated monthly incident solar energy during a year.*

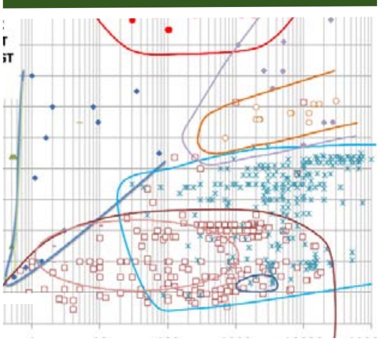
REFERENCE

[1] Y.B. Assoa et al., "A lightweight triangular building integrated photovoltaic module", Applied Energy, vol. 129 (2020), 19 p.

SMART GRIDS & ENERGY EFFICIENCY

NEW SCENARIOS LIKE THE INTRODUCTION OF INTERMITTENTLY-PRODUCED RENEWABLE ENERGY INTO GRIDS; EMERGING MODES OF CONSUMPTION LIKE ELECTRIC VEHICLES, ELECTROLYZERS TO PRODUCE HYDROGEN, AND SELF-CONSUMPTION; AND THE COUPLING OF DIFFERENT ENERGY VECTORS LIKE ELECTRICITY, HEAT, COLD, AND GAS ARE ALL HALLMARKS OF THE ENERGY TRANSITION. CEA-LITEN LEVERAGES MULTI-ENERGY-VECTOR TEST PLATFORMS AND DEEP KNOWLEDGE OF ENABLING TECHNOLOGIES TO DEVELOP ITS OWN SOFTWARE TO OPTIMIZE THE DIMENSIONING AND CONTROL OF ENERGY SYSTEMS AND GRIDS. CEA-LITEN ALSO DEVELOPS ELECTRICAL AND THERMAL ENERGY MANAGEMENT COMPONENTS FOR GENERATION, CONVERSION, AND STORAGE TO MAKE ENERGY SYSTEMS AND GRIDS AS EFFICIENT AS POSSIBLE.





CONTENTS

THERMODYNAMIC SYSTEMS FOR WASTE HEAT VALORIZATION

Industry uses very often energy in the form of heat. Depending on applications, the whole range of temperature levels is present from very high ones, like blast furnaces (>1500°C), down to quite low temperature agro-food industry ovens. This industrial heat is generally produced using fossil resources but other alternatives are now studied to avoid CO_2 emissions, like the use of electricity. However all the processes cannot be transformed in this way. In all cases, the main aspect to consider, to limit CO_2 emissions, is the efficiency of energy consumption. Usually energy needs for the process (temperature level increase, phase change...) are two or three times lower than the actual consumed energy. Therefore, it is important to improve process efficiency, but if it is not possible or too complicated, the main concern is to reuse this rejected heat, generally called waste heat. Recent studies from ADEME in France have pointed out that industry rejects directly in the atmosphere 109 TWh of waste heat, half of it at low temperature. The picture in Figure 1 presents a scheme of an industrial plant dedicated to steel forming, which is particularly of interest because the same material is successively heated and cooled twice. Different technologies for waste heat use are proposed directly in the process, some of them will be developed in this paper. It is also possible to use this heat outside the industrial plant with a connection to a district heating network in the surrounding area.

Two main reasons limit the use of waste heat. The first one at the recovery level, is the difficulty linked with the contents of flue gas or liquids at the exit of an industrial process. The second one is related to the difficulty to find a relevant use of this heat in the same industrial plant or nearby. After a few words about heat transfer in fouling conditions, this paper will focus on heat conversion in another form of energy, locally more convenient, like electricity or cold.

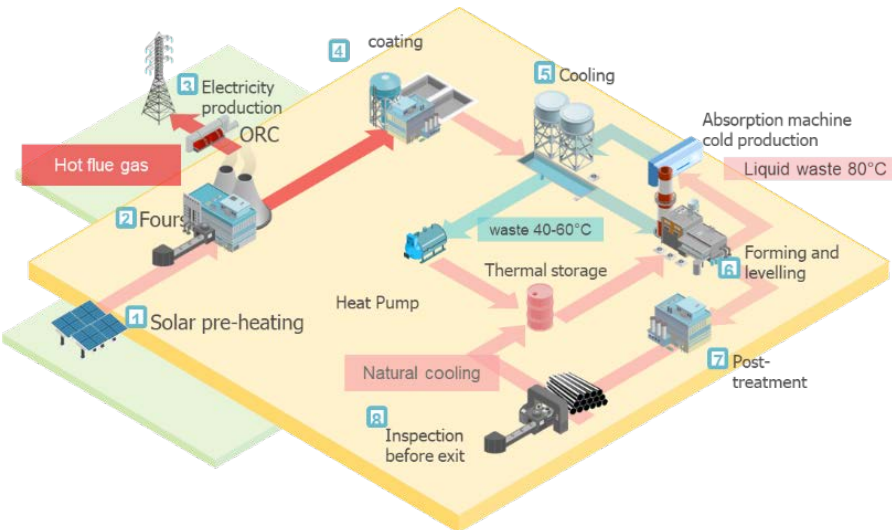


Figure 1: *Scheme of main heat fluxes in an industrial plant dedicated to steel forming*

WASTE HEAT RECOVERY IN FOULING CONDITIONS

In most industrial processes, heat is rejected in the form of hot flue gases containing solid particles or components able to produce acids when condensing. Thus it is not possible to use directly these fluids in another process. The first step is to transfer heat, through a heat exchanger to a "clean" fluid that can be used directly in the same industrial plant or in a thermodynamic system for conversion. To study heat exchangers fouling, the CEA-Liten has developed experimental loops which can reproduce a gas (hot air) containing particles, with a management of quantities and grain sizes. Samples of heat exchangers are tested by measuring the evolution of pressure and heat transfer even up to clogging. This leads to evaluate adequately their performances in real conditions. After a trial, the heat exchanger is observed and characterized, with special attention to the localization of particles accumulation, to help for the choice of the most suitable geometry. The evolution of heat transfer resistance can also be followed to evaluate the behavior of heat exchangers. In some cases heat transfer reaches an asymptotic value, which means that it could be used in fouling conditions, or the resistance increases continuously up to clogging. Phenomenological analysis of the fouling in such laboratory conditions can also be used to establish behavior correlations, depending on main parameters like local wall shear stress. This can help to manage real waste heat recovery and heat exchanger cleaning phases.

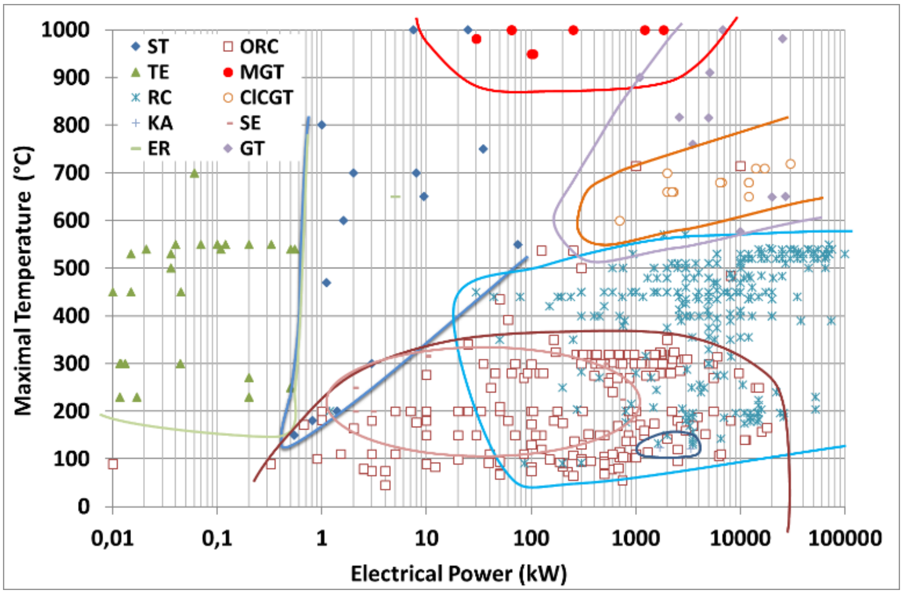


Figure 2: *map of maximum temperature versus power technologies* [1]

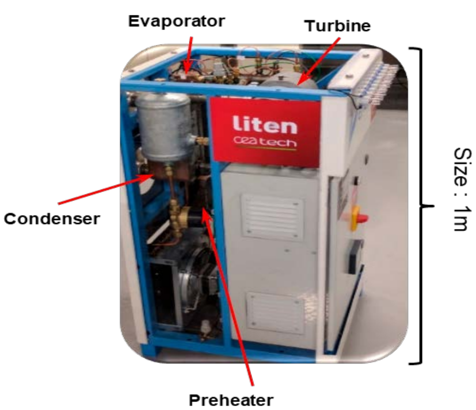
WASTE HEAT TO POWER CONVERSION TECHNOLOGIES

The conversion of (waste) heat into electricity includes a wide set of technologies: a database of more than 1100 references has been built since years. It illustrates the range and applicability of each technology (Figure 2, with the corresponding nomenclature: Rankine cycle plant (RC), Steam engine (SE), Organic Rankine Cycle plant (ORC), Kalina cycle plant (KA), Gas turbine plant (GT) and Micro gas turbine (MGT), Closed cycle gas turbine plant (ClCGT), Ericsson engine (ER), Stirling engine (ST), Thermogenerator (TE), Thermoacoustic generator (TA), Combined cycle plant (CCGT)).

Different cycles are possible: Brayton, Rankine and Stirling are the most well-known. However Brayton and Stirling cycles are suited for very high temperature heat sources (generally > 500°C) which is commonly not the case for waste heat configurations. Steam Rankine cycles are practically adapted for large power plants (generally > 3-5 MWe). Thus Organic Rankine cycle (ORC) with power production levels range from 1 kW to 50 MW for heat sources between 100°C and 300°C is generally the most adapted to waste heat conversion. Efficiency (= work production / energy source) depends on both temperature and size. Typical value ranges from 5% to 25%.

ORGANIC RANKINE CYCLE (ORC)

Contrary to traditional steam Rankine cycle, Organic Rankine Cycle can use an organic medium as a working fluid. ORC system can be described as follows: the working fluid, in its liquid state, is pressurized thanks to a pump, and then heated, evaporated and possibly superheated in contact with the hot source through a heat exchanger. Organic vapor is expanded, producing mechanical work; at expander exit, then the fluid is cooled, condensed and sub-cooled by the cold source within the condenser, and pumped again.



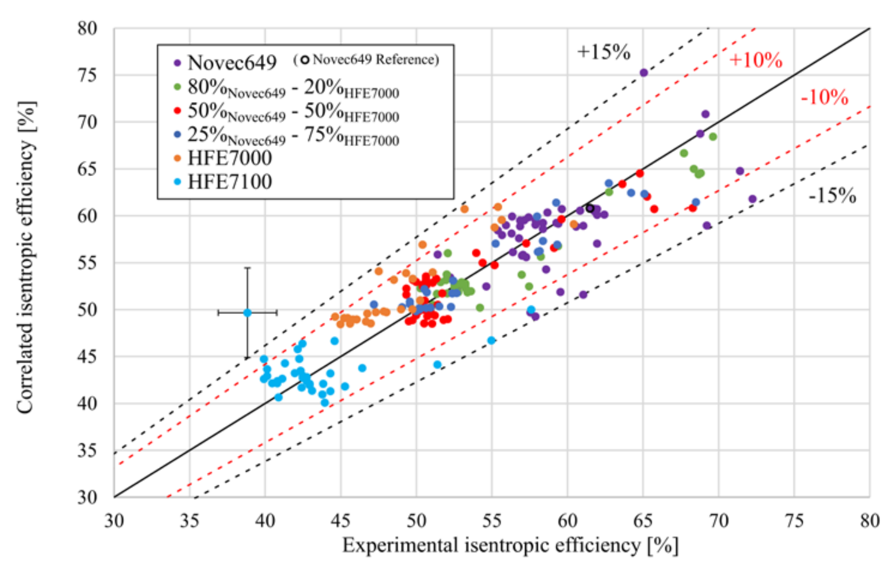


Figure 3: *1 kWe - ORC device (left); generalized model of turbine efficiency – usable for all tested HFE fluids and mixtures (right)* [T1]

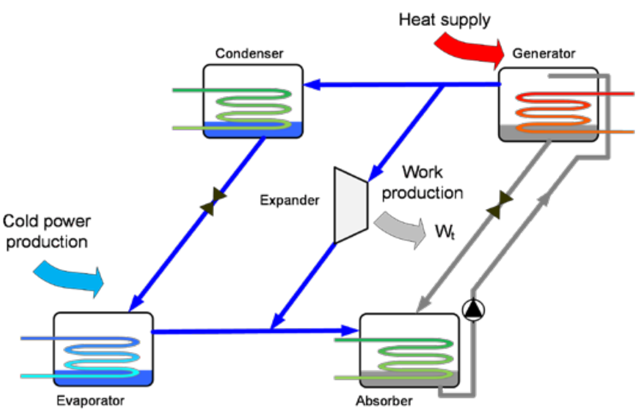
In a specific project, a compact experimental ORC installation ($0.25m^3$) has been studied in order to valorize a low temperature heat source (Fig. 3 – left). The working fluid is a mixture of new generation fluids (i.e. composed of Novec649, HFE7000 and HFE7100 in different mass compositions) and is expected to be a potential candidate to substitute the traditionally used fluids in ORC which can have a high global warming potential [2]. Analyses based on a massive experimental investigation highlight that the expansion element, an axial micro-turbine in the study, behaves properly with alternative fluids in various conditions. Secondly, the right part of Fig. 3 presents a comparison between a prediction model and experimental measurements to evaluate expander efficiency. It shows a very good agreement for both mixtures and pure fluids. Thirdly, it has been shown that the use of a zeotropic mixture as a working fluid combined with a specific ORC architecture [3] can be a high performance low power installation, compared to other reported low temperature heat recovery systems [T2]. This work opens the way to other mixtures such as natural refrigerants which could be used in transcritical Rankine cycles [4].

AMMONIA-WATER ABSORPTION CYCLE

Another way to use waste heat is to transform heat to a useful energetic function, i.e. refrigeration. Direct thermal conversion of heat to refrigeration is only possible if mechanical energy is provided. Complex tri-thermal thermodynamic cycles were conceived to overcome this difficulty thanks to a thermal compression (instead of an electro-mechanical process in a conventional refrigeration machine). Based on these results, a 10-year development performed at CEA-Liten (initially for solar applications) has led to various prototypes such as a 100 kWth refrigeration machine. The thermal compression relies on absorption properties of some fluids and the absorption refrigerator prototype uses ammonia and water. As in a common refrigeration cycle, evaporative cooling is used. When the working fluid evaporates, it takes some heat away with it, providing the cooling effect. Typical COP (coefficient of performance = cooling energy / energy source) can be as high as 60% and can typically use waste heat at 70-180°C and produce refrigeration at 20°C down to -15°C. This kind of cycle is also able to be used in a heat-pump mode to convert waste heat to a high and more useful temperature heat [5].

HYBRID CYCLE FOR POWER PRODUCTION AND REFRIGERATION

In the context of massive development of intermittent energy sources and needs, a specific cycle to simultaneously produce electricity, heat and refrigeration from a (waste) heat source was developed. This trigeneration cycle is shown in Figure 4 (left). It consists of a water-ammonia absorption cycle (abso NH_3/H_2O) generating cold power in parallel to an ORC system that employs part of the desorbed ammonia as a working fluid, and an expander for work production (W_t). A prototype is currently being developed to assess the performance and to evaluate the dynamic capacity of simultaneous co-production and instant optimization [T3; T4]. Fig. 4 (right part) illustrates the typical response of the power and refrigeration productions to a typical regulation from a co-production mode to a pure power production mode. The unsteady behavior was calculated through dynamic simulations performed with DYMOLA software and shows an effective regulation scheme and a short time response (150 s) [6].



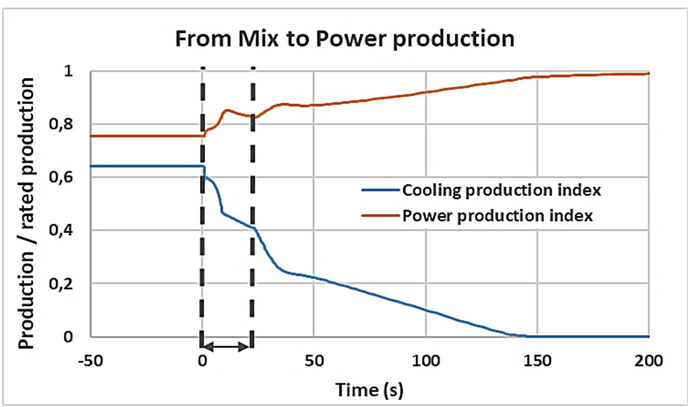


Figure 4: *Scheme of the hybrid cycle (left); transient numerical simulation of co-production (right). To match the behavior of classic automated valves, the valve switching time was set to 20 seconds*

A main challenge for refrigeration machines is the difficulty to maintain high values of COP (coefficient of performance) when the desired refrigeration temperature is low (typically -20°C) or when the waste (intermittent) heat is not available. A specific configuration of the aforementioned hybrid architecture (Fig. 4) could bring a solution. It consists in using both an expander and an electric generator in reverse mode (inverse rotation) to act as a compression assisted absorption cycle. In this configuration W_t becomes negative [7]. The preliminary results show that COP in compression assisted mode (1 kWe added to 15 kW provided by a waste heat supply) offers better COP (= 45%) compared to non-assistance mode (COP = 8%) at low evaporation temperatures [8].

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REFERENCES

Papers / Patents

[1] A. Landelle, N. Tauveron, P. Haberschill, R. Revellin, S. Colasson, "ORC design and performance comparison based on experimental database", Applied Energy, 2017.

[2] Blondel, Q., Tauveron, N., Caney, N., Voeltzel, N., "Experimental study and optimization of the Organic Rankine Cycle with pure NovecTM649 and zeotropic mixture NovecTM649/HFE7000 as working fluid", (2019) Applied Sciences, 9 (9), art. no. 1865.

[3] Blondel, Q., Tauveron, N., Caney, "Cogeneration system of electrical energy and thermal energy by a Rankine cycle module", patent application EP3670854, 2019-12-19.

[4] F. Ayachi, N. Tauveron, T. Tartière, S. Colasson, D. Nguyen, "Thermo-Electric Energy Storage involving CO_2 transcritical cycles and ground heat storage", Applied Thermal Engineering, 108, 2016, pp. 1418-1428.

[5] N. Voeltzel, H.T. Phan, N. Tauveron, "System for co-producing electrical energy and hot and cold thermal energy and associated method", patent application EP3748274, 2020-06-05.

[6] N. Voeltzel, H.T. Phan, Q. Blondel, B. Gonzalez, "Steady and dynamical analysis of a combined cooling and power cycle", Thermal Science and Engineering Progress, 19, 2020, 100650.

[7] N. Voeltzel, H.T. Phan, N. Tauveron, "System for co-producing electrical energy and cold thermal energy and associated method", patent application EP3748137, 2020-06-05.

[8] N. Tauveron, N. Voeltzel, H.T. Phan, B. Gonzalez, "Focus on ammonia expander in a hybrid cycle for power production and cooling", Refrigeration Science and Technology, 2020, pp. 240-248.

Theses

[T1] Q. Blondel, "Study and energetic optimization of zeotropic mixtures for Rankine cycles", PhD thesis, Grenoble, 2021.

[T2] A. Landelle, "Experimental and numerical study of transcritical Organic Rankine Cycles for low-grade heat conversion into electricity from various sources", PhD thesis, Grenoble, 2017.

[T3] S. Braccio, "Experimental study & numerical simulation of a combined cycle producing cold and electricity", PhD thesis, Savoie-Mont Blanc, ongoing.

[T4] M. Wirtz, "Experimentation and modeling of a combined plate generator for NH3-H2O absorption machine", PhD thesis, Savoie-Mont Blanc, ongoing.

Projects

[P1] SELECO2 project, ANR project (2014-2018).

[P2] TRICYCLE project, Carnot project (2017-2020).

[P3] SURORC project, Carnot project (2013-2014).

[P4] POCPACABSO project, POC project (2020-2021).

[P5] ABSONANO project, BU project (2020-2021).

INNOVATIVE POWER-TO-POWER STORAGE SYSTEM INCLUDING THERMAL ENERGY STORAGE

The continued increase of the part of electricity from renewable energies requires massive electricity storage solutions to overcome the gap between the production and the use of electricity. This work defines a new thermodynamic system architecture including high temperature thermal storage (900 °C to 1200 °C). This solution is efficient in terms of energy and economics compared to other technologies such as PSP (pump storage plant), CAES (compressed air energy storage), battery or hydrogen.

APPROACH

The spreading of renewable energies will depend on the accessibility and efficiency of solutions for massive storage. Among existing solutions, thermal storage via a power-to-heat-to-power type system is interesting. In this study, we investigated the interest of high temperature thermal storage based on air as a coolant. Air has many advantages: available and free, non-toxic, possibility of high thermal / electrical conversion efficiency and high energy storage density. However, its use at high temperature leads to technological challenges. Furthermore, we had to define the best thermodynamic systems for both performance and cost. We have developed a model of unsteady thermodynamic systems to study the reciprocal constraints between the storage and the system during the charging and discharging phases. In addition, the investment and operating costs have been studied for each system.

RESULTS AND PERSPECTIVES

Among the studied sytems (combined cycle without combustion, combined cycle with combustion at 1200 °C or 1400 °C, gas cycle with combustion at 1200 °C), we have shown that the system with a simple cycle with gas combustion at 1200°C presents the best efficiency / cost trade-off. Furthermore, for this type of intermittent operating system (only a few hours per day), the combined cycle does not accumulate enough running hours to counterbalance its high investment cost. The solution is a bit more expensive than PSP or CAES, but these solutions can only be built at very specific locations. Batteries also offer this possibility, while their cost are higher than our solution. The forthcoming study will consist in developing a prototype to validate the technological choices for thermal storage at high temperature.

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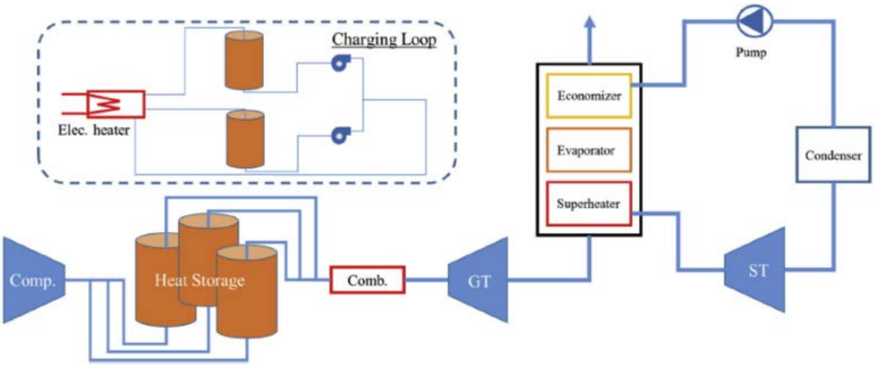

The four studied cases and their LCOE result.

Design parameters	Base Case	Case 2	Case 3	Case 4
Type of cycle	Combined	Combined	Combined	Brayton
Combustion	No	Yes	Yes	Yes
W_{net}	60 MWe	60 MWe	60 MWe	60 MWe
$Q_{storage}$	409 MWh_{th}	205 MWh_{th}	148 MWh_{th}	302 MWh_{th}
$T_{in,GT}$	900 °C	1200 °C	1400 °C	1200 °C
PR	10	14	15	15
LCOE	213 $/MWh	252 $/MWh	253 $/MWh	186 $/MWh

Figure 1: *CAES: Compressed Air Energy Storage, PSP: Pump Storage Plant (use of hydraulic dam)*

REFERENCE

[1] K. Attonaty et al., "Thermodynamic and economic evaluation of an innovative electricity storage system based on thermal energy storage", Renewable Energy, vol. 150 (2020) 1030-1036.

THE ROLE OF ENERGY STORAGE TO COPE WITH INTERMITTENT SUPPLY IN THE FRENCH ELECTRICITY SYSTEM

The rising share of Variable Renewable Electricity Sources, and the shrinking share of dispatchable production (nuclear in France) lead to new challenges in balancing production and consumption at all times. The present work provides new insights on how energy storage could handle this variability, focusing on different time scales, and including both electricity storage and thermal storage.

APPROACH

We have highlighted how wavelet decomposition of the production and consumption signals allow to understand that necessary storage size increases very sharply with the time scale, in the absence of dispatchable production [1]. Batteries are shown to be relevant for daily storage, hydrogen in steel bottles for weeks, but mature technologies are still lacking for longer times. Using a Mixed Integer Linear Programming optimization, we analyzed for realistic time series how the various technologies can interact together, and with production oversizing when several times scales are present at the same time [2]. Oversizing consists in installing more renewable sources than necessary to fulfill consumption, in order to reduce the need for storage. We focused on the seasonal timescale which is the most difficult point to address with electricity storage, and which inherently comes from the high demand for heating in winter. We studied the contribution of large scale thermal storage, coupled with district heating, to the flexibility of the electricity system. Thermal and electrical energy systems can possibly be coupled via heat pumps.

RESULTS AND PERSPECTIVES

We demonstrated that a low storage cost is of utmost importance for long time scales, while a high efficiency is preferred for short time scales. At seasonal scale, storage is too expensive and production oversizing is usually preferred, except for very strong intermittencies. Indeed, the production being sometimes close to zero, oversizing is very ineffective. Using real world time series, the optimal solution involves a mix with a significant oversizing of production, while both long term and short term storages cooperate to smooth the intermittency. Including also the coupling to the thermal vector to study the seasonal time scale leads to several domains of operation depending on electricity and gas prices, as shown in Figure 1. These simplified parametric studies are very useful to understand the behavior of the system and the effect of the main parameters. Future work will analyze in depth the links between electric and thermal storages but also gas energy systems using real time series. The complementarity between storage and dispatchable production will also be studied. This is today the cheapest way to bring flexibility to the electricity system.

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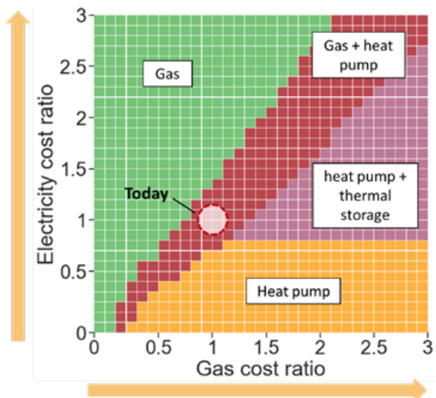

Figure 1: *Diagram showing how a coupled electric/thermal energy system provides seasonal flexibility. A high gas cost (or a CO_2 tax) favors heat pump over gas heating. Then there is a tradeoff between production oversizing (for low electricity cost), or large seasonal thermal storage and district heating (for higher electricity cost).*

REFERENCES

[1] A.Clerjon, F. Perdu, “Matching intermittency and electricity storage characteristics through time scale analysis: an energy return on investment comparison”, Energy and Environmental Science, vol. 12 (2019) 693-705.

[2] A. Clerjon, “Analysis and modeling of the impacts of the development of intermittent renewable energies on the French electricity system: Study of the potential of electricity storage and the complementarity with heat”, PhD thesis, Grenoble, 2021

PROSPECTIVE DEVELOPMENT OF THE EUROPEAN GRID BY 2050

To face the large-scale development of VRES (Variable Renewable Energy Sources), the power system needs to add more flexibility such as demand side management, storage technologies and VRES curtailment. To analyze these impacts and evaluate new solutions, a coupling of the long-term energy model POLES (Prospective Outlook on Longterm Energy Systems) and the EUTGRID module (European Transmission Grid Investment and Dispatch) is proposed.

APPROACH

In order to study the interrelated impacts of climate energy policies and the transmission grid architecture evolution as well as the interactions with other flexibility options, an approach is proposed and based on coupling POLES and the EUTGRID module. This methodology permits to assess the climate energy policies using POLES and to quantify the transmission grid requirements both in time and regionally. It also gives access to analysis of interactions with other flexibility options. The EUTGRID model contains in fact an optimal power flow simplified as a DC load flow for the transmission system. The linear equations representing the AC load flow are implemented in GAMS using the solver CPLEX.

RESULTS AND PERSPECTIVES

The results show that, for high share of VRES (above 60%) reinforcement is the preferred solution for the three considered distribution grids. For lower VRES penetration rates, the curtailment of VRES production or installation of storage capacities can be cheaper. A combination of the presented flexibility solutions might be more realistic, but the results indicate already the interest of including the distribution grids models in the European power system prospective study when facing issues with the large-scale integration of VRES. An exploratory work has been carried out with the introduction of generic distribution grids (urban, semi-urban and rural) in EUTGRID. The results have shown that the reinforcements can be slightly delayed with a greater use of back-up technologies and an increase of total CO_2 emissions.

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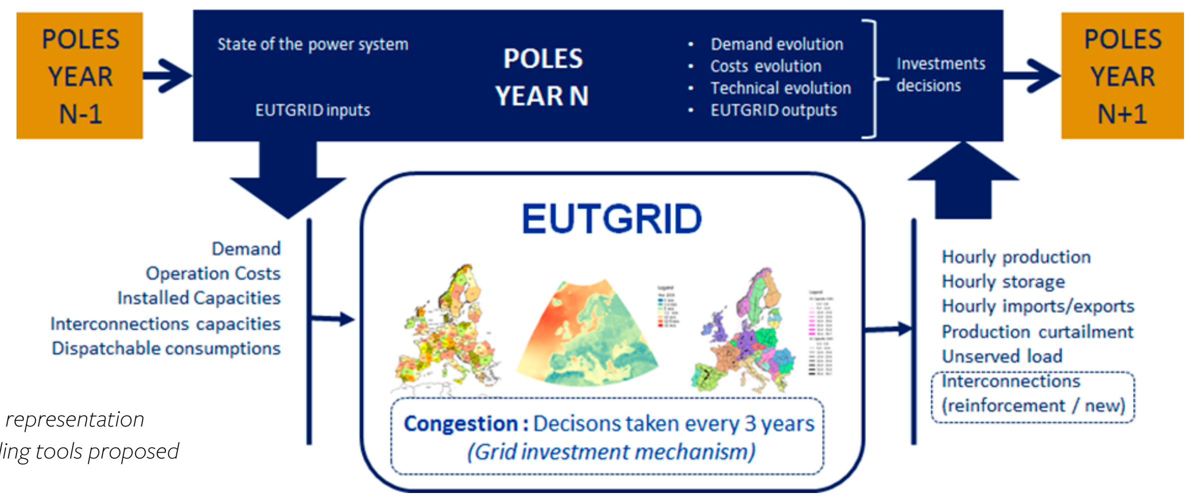


Figure 1: *Recursive representation of the set of modeling tools proposed*

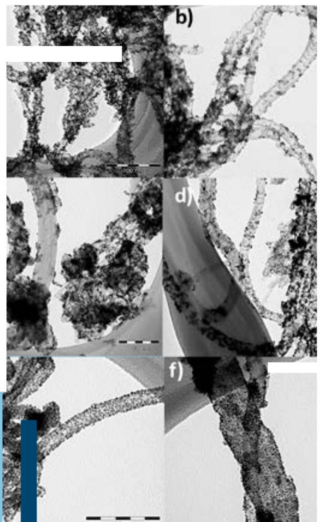
REFERENCES

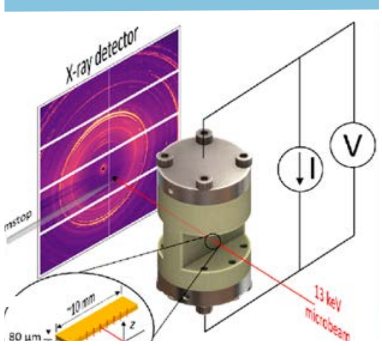
[1] S. Allard, S. Mima, V. Debusschere, T. Tran Quoc, P. Criqui, N. Hadjsaid, "European transmission grid expansion as a flexibility option in a scenario of large scale variable renewable energies integration", Energy Economics, Volume 87, March 2020, 104733; 28); https://doi.org/10.1016/j.eneco.2020.104733

[2] S. Allard, V. Debusschere, S. Mima, T. Tran Quoc, N. Hadjsaid, P. Criqui, "Considering distribution grids and local flexibilities in the prospective development of the European power system by 2050", Applied Energy, Elsevier, vol. 270, July 2020; https://doi.org/10.1016/j.apenergy.2020.114958

ENERGY STORAGE & FLEXIBILITY

ENERGY STORAGE WILL BE CRUCIAL TO THE DEVELOPMENT OF INTERMITTENTLY-PRODUCED RENEWABLE ENERGY AND TO ACHIEVING A CARBON-FREE TRANSPORTATION SECTOR. CEA-LITEN IS WORKING ON TWO MAIN SOLUTIONS: BATTERIES AND HYDROGEN. OUR BATTERY R&D FOCUSES ON INCREASING ENERGY DENSITIES WITHOUT SACRIFICING SAFETY OR RELIABILITY. OUR APPROACH TO HYDROGEN IS COMPREHENSIVE, WITH RESEARCH ON PRODUCTION (USING HIGH-TEMPERATURE ELECTROLYSIS), STORAGE, TRANSPORTATION, AND CONVERSION (BY FUEL CELLS).





CONTENTS

PROGRESS IN PEMFC DEVELOPMENT: FROM INNOVATIVE MATERIALS TO EFFICIENT AND DURABLE SYSTEMS

Since two decades, CEA-Liten has been involved in the development of Proton Exchange Membrane Fuel Cells (PEMFC) from the research on new materials to the development of innovative systems. These research activities are strongly linked to the two main bottlenecks limiting PEMFC deployments. Firstly, to reduce the fuel cell cost CEA-Liten has focused research activities on new catalyst development, in order to lower the use of Platinum Groups Metals (PGM) and to increase the stack performances at constant PGM loading. This is realized through the decrease of the quantity of materials and components needed to reach the targeted power. Secondly, in order to increase the system fuel cell lifetime, an intensive activity has been performed to better understand the phenomena occurring within the fuel cell and the link between these phenomena and the operating conditions. Finally, more stable materials and fuel cell management system have been developed to mitigate degradations occurring in real life operation. In the future, these research topics, carried out in close collaboration with our academic and industrial partners, will contribute to increase the viability of fuel cell systems in various applications.

COST DECREASE OF FUEL CELL CORE

Development of new catalyst materials is a major key point to decrease the cost of a fuel cell stack and to develop a cheaper fuel cell system for a wide range of applications. Because of its very good activity for oxygen reduction and hydrogen oxidation, platinum remains the most used material to manufacture PEMFC. Current loadings for the automotive market are in the range of 0.3 to 0.5 mg_{Pt} / cm^2 of active surface which makes a total of 30 to 50 g_{Pt} for of a 100 kW stack (at 1 W/cm^2) while catalytic converters for combustion engine exhaust contain about 5 grams of noble metals. This use of platinum raises an issue regarding the cost and the possible dependence to raw materials suppliers. To be competitive with ICE, the target of 10 g_{Pt} for a 100 kW stack is therefore generally set, i.e. 0.1 g/kW.

One way to manage this issue is the development of innovative catalysts and the optimisation of the associated active layers. In collaboration with the CNRS (LCC Toulouse), a series of catalyst for ORR based on platinum-cobalt or platinum-nickel nanoparticles has been developed. In order to mitigate the impact of carbon corrosion on the catalyst layer lifetime, carbon nanotubes were used as carbon support. Carbon nanotubes, and more especially thermally treated nanotubes, are known to exhibit more graphitic domains than commonly used carbon blacks such as Vulcan. First, sulfur and nitrogen doped carbon nanotube (S-NTC, N-NTC) have been prepared [1]. Then, to allow a good dispersion of small metal particles (mean diameter: 2 nm) it has been demonstrated that, due to the metal-carbon interaction, the choice of both the nanotube structure and the non-noble metal is of importance [T1]. Finally, catalysts with higher mass activity and better tolerance towards degradation (single cell test, AST for carbon corrosion) than commercial reference were synthesized [2] as shown in Figure 1.

Nevertheless, even if the use of carbon nanotubes as catalyst support leads to a decrease of the degradation kinetics of supported Pt based catalyst, it also has drawbacks which must be tackled. Indeed, the integration of such material in active layers is not straightforward because this kind of material tends to form aggregates or very compact catalyst layers with bad diffusion properties. This has been solved by mixing an optimized ratio of Pt deposited on N-CNT and Pt deposited on few graphene layer (FGL) as catalyst support. In a rotating disk electrode set up, this mixture showed better resistance towards degradation compared to Pt on carbon black (Vulcan like). Finally, the know-how developed to synthesized catalyst nanoparticles homogenously dispersed on graphitized carbon nanotube can be easily transferred on other graphitized and structured carbon based supports to enhance catalyst stability and decrease Pt content in PEMFC stack.

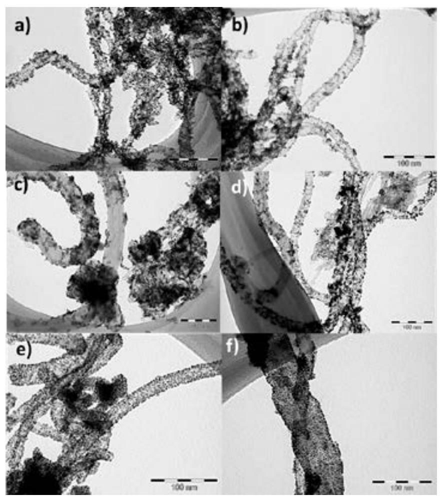


Figure 1: *TEM micrographs of: a) Pt_3Co/N-CNT; b) Pt_3Co/N-CNT_{HT}; c) Pt_3Co/S-CNT; d) Pt_3Ni/N-CNT; e) Pt_3Ni/N-CNT_{HT}, and f) Pt_3Ni/S-CNT. Scale bar = 100 nm*

The second way to decrease the catalyst cost is the development and the integration of critical raw material (CRM) free catalysts. In the frame of the H2020 PEGASUS project, CEA-Liten is working on the fine characterization and integration of platinum-free catalysts. The objective is to define the best active layer structure integrating these materials, thanks to a coupling with modelling developments. Using SECM (Scanning ElectroChemical Microscopy,) developed with CEA-Iramis, it has been possible to disregard the structure of the active layer in order to define the relationship U = f (I). This relationship has been integrated into the active layer models developed by CEA-Liten. In parallel, a benchmark of the different techniques used to fabricate PMG free-based MEA (Membrane Electrode Assembly) has shown that CCM (Catalyst-Coated Membrane) methods whose cathode was previously printed using a Teflon sheet before decal could be the best way to manufacture high performance MEA. CEA-Liten also works on the synthesis of PGM free catalysts for ORR [T2]. These catalysts are based on carbon, nitrogen and iron. The developed manufacture processes are compatible with large-scale production, with attention to limit the use of solvents or aggressive materials, and finally to limit the number of required steps. The synthetic routes allow a fine control of the 3D structure of the catalyst.

Even if important progresses have been made to manufacture non PGM catalyst layers during the last years, the current performances remain lower when compared to common platinum made electrodes. This is mainly ascribed to a lower active site activity and a shelf-aging mechanism. Reaching the cost target still needs important efforts to develop platinum-based catalysts however promising routes are being explored actively.

OPTIMISATION OF THE ELECTROCHEMICAL PERFORMANCES OF STACKS AND SYSTEMS TO REDUCE THE MANUFACTURING COST.

Even if the catalyst optimization remains an important way to decrease the cost of the fuel cell technology, it is not the only improvement able to decrease it. Indeed, stack optimization induces also a decrease of the manufacturing cost by decreasing the need of components to reach a targeted stack power. To optimise the stack performances it is necessary to understand how stack design modifies the local electrochemical performances of the MEA. CEA-Liten has developed a strong knowledge in locally resolved characterization using an electrochemical methodology [3], magnetic measurements [4,5], and neutron probes[6,7]. Recently, neutron imaging has been used to understand the water distribution within real stacks in operation [8]. These measurements shown in Figure 1 have been obtained in close collaboration with NCNR-NIST. Theyprovide very useful information to improve the ability of our model to take into account liquid water in a wide range of operation[8,9]. A comparison between experimental and simulated water content in a given stack region is depicted in Figure 2 [9].

INCREASE OF THE FUEL CELL STACKS DURABILITY IN REAL OPERATION.

System sustainability is an other key point to ensure massive deployment of the PEMFC technology. Whereas lasting target is around 8,000 hours for automotive applications and higher for duty vehicles (30,000 hours) and stationary applications, the real lifetime of fuel cell systems remains too low to completely fulfil the requirements. To increase the system robustness it is necessary to reach a complete understanding of the phenomena occurring in a fuel cell stack during operation. This will allow to manage these phenomena by the increasing of materials robustness and by optimization of the fuel cell management system to avoid harsh operating conditions. The activities at CEA-Liten cover the two aforementioned key points.

Start and stop behavior is one of the most degrading operating conditions occurring during fuel cell operation. To manage this step, it is necessary to understand which phenomena occur and what are the key parameters to mitigate this degradation. A homemade model developed for years has been used to simulate transient local conditions inducing fuel starvation, and as a consequence degradation [T3]. Using this approach, predict

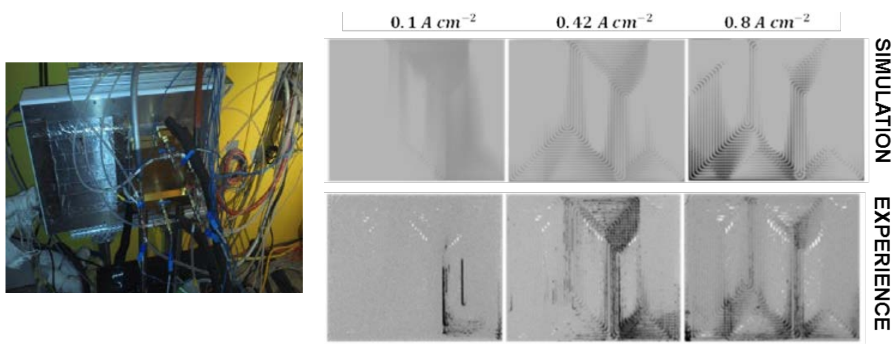


Figure 2: (*left*) *stack, designed for neutron imaging experiment, installed at NIST. Water distribution at different operating current densities measured using neutron imaging* (*bottom right*) *and simulated using Muses model* (*Top right*)

carbon corrosion at the entire surface of the MEA has been possible as well as simulated mitigation strategies [10]. A thesis work dedicated to experimentally characterize these mitigation strategies is in progress [T4].

Fuel cell management system plays also an important role to reach durability targets, as the degradation is strongly dependent on the internal conditions during operation. Recently, CEA-Liten has developed diagnostic tools for fuel cell stack using physical simulations [T5]. This strategy has been chosen because it allows an increase of the methodology robustness, while taking into account potential degradations. [11]. The use of a meta-model and the choice of only two measurements (voltage and high frequency resistance) to diagnose stacks has permitted the creation of a simple plug-in tool [T5]. Using the same approach, prognosis algorithm has been developed using Kalman filter approach, to calculate on board the remaining lifetime of a fuel cell stack [T6]. It takes into account degradation phenomena linked to platinum dissolution to estimate the fuel cell stack degradation in operation, and then the evolution of the stack performances. In the future, the two different approaches will be combined in an innovative fuel cell management system and will be used to optimise system durability during its lifetime.

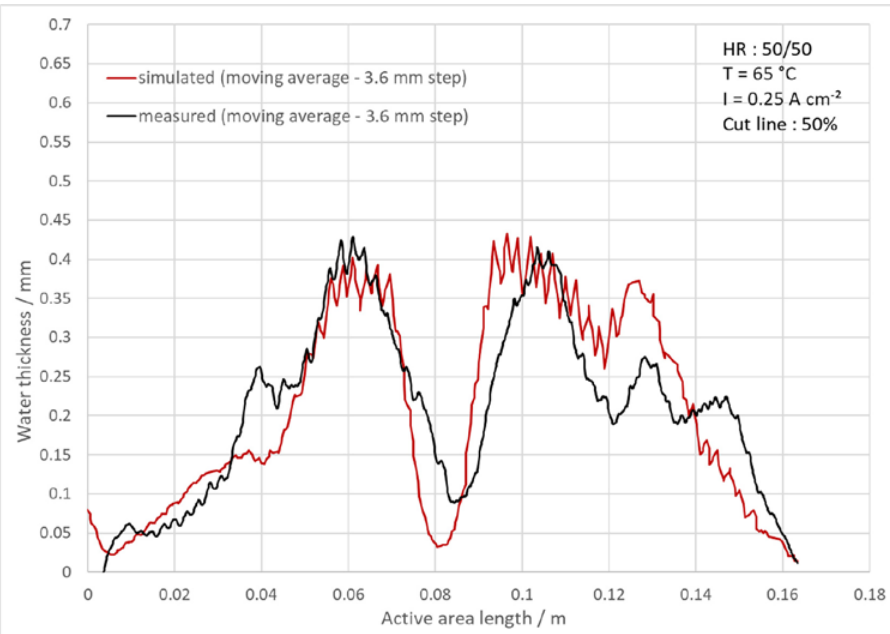


Figure 3: *Water thickness measured (black line) and simulated (red line) at a specific region of the stack (1.5 bar, Hydrogen/Air Stoichiometry coefficient: 1.5/2; gases Relative humidity: 50%) for a current density of 0.25 A cm^{-2}.*

DEVELOPMENT OF AN INNOVATIVE SYSTEM AND ANALYSIS FEEDBACK TO INCREASE PEMFC COMPETITIVENESS

In addition to stack optimisation, system development and deployment are important to prove the viability of fuel cells system and to collect knowledge in real life operation. CEA is involved in system deployment since 2006; initially with the industrial PSA group and more recently with the famous project “Energy Observer”. The feedback resulting from this experimentation showed that the hydrogen production and storage efficiency is close to 41% in real operation and the fuel cell system efficiency is in the same order of magnitude. Even if these efficiencies remain quite low compared to battery storage system, the energy density and the robustness of the hydrogen chain proved satisfactory to fulfil targets of this particular application. In addition to these deployment activities, CEA-Liten researches have been focused on the development of innovative means to build a more efficient and cheaper fuel cell system. As an example a new architecture described in a dedicated highlight has been recently proposed to reach the target system [12].

PERSPECTIVES

CEA-Liten has been involved for many years in the development of Proton Exchange Membrane Fuel Cells from the research on new materials to the development of innovative systems. These developments have been strongly linked to cost and durability of fuel cell systems and fuel cell stacks. To address these two bottlenecks, a particular attention has been paid to non-PGM catalysts development and optimization of platinum based catalysts. Meanwhile, the links between stack fluidics properties and electrochemical performances have been intensively studied using coupled characterization and modelling approaches. These activities have brought a better understanding of phenomena driving the stack performances, an increased knowledge and know-how for a large set of applications and consequently a decrease of stack cost. Finally, more stable materials and fuel cell management optimization have been developed to mitigate degradation in operation conditions.

For the future, these improvements will be used to develop a cheaper and a more efficient PEMFC system. The non PGM catalysts will be integrated in an active layer with performances close to Platinum electrodes using a tailored MEA manufacturing processes. In parallel, the knowledge obtained in stack design will be used to manufacture high performances fuel cells taking into account the non-homogeneous operating conditions within the active surface. Specific designs to adapt fluidic and thermic properties all along the fuel cell stack will be studied and used to manufacture more efficient and cheaper fuel cell systems having long lasting lifetime.

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REFERENCES

[1] S. Louisia, R.C. Contreras, M. Heitzmann, M. Rosa Axet, P.-A. Jacques, P. Serp, Sequential catalytic growth of sulfur-doped carbon nanotubes and their use as catalyst support, Catal. Commun. 109 (2018) 65–70.

[2] S. Louisia, Y.R.J. Thomas, P. Lecante, M. Heitzmann, M.R. Axet, P.-A. Jacques, P. Serp, Alloyed Pt3M (M = Co, Ni) nanoparticles supported on S- and N-doped carbon nanotubes for the oxygen reduction reaction, Beilstein J. Nanotechnol. 10 (2019) 1251–1269.

[3] P. Piela, J. Mitzel, S. Rosini, W. Tokarz, F. Valle, A. Pilenga, T. Malkow, G. Tsotridis, Looking Inside Polymer Electrolyte Membrane Fuel Cell Stack Using Tailored Electrochemical Methods, J. Electrochem. Energy Convers. Storage. 17 (2020).

[4] L. Ifrek, O. Chadebec, S. Rosini, G. Cauffet, Y. Bultel, B. Bannwarth, Fault Identification on a Fuel Cell by 3-D Current Density Reconstruction from External Magnetic Field Measurements, IEEE Trans. Magn. 55 (2019).

[5] L. Ifrek, S. Rosini, G. Cauffet, O. Chadebec, L. Rouveyre, Y. Bultel, Local faults identification on a PEMFC by external magnetic field, in: 8th Int. Conf. Fundam. Dev. Fuel Cells FDFC2019, Nantes, France, 2019.

[6] N. Martinez, L. Porcar, S. Escribano, F. Micoud, S. Rosini, A. Tengattini, D. Atkins, G. Gebel, S. Lyonnard, A. Morin, Combined Operando High Resolution SANS and Neutron Imaging Reveals in-Situ Local Water Distribution in an Operating Fuel Cell, ACS Appl. Energy Mater. 2 (2019) 8425–8433.

[7] J. Lee, S. Escribano, F. Micoud, G. Gebel, S. Lyonnard, L. Porcar, N. Martinez, A. Morin, In Situ Measurement of Ionomer Water Content and Liquid Water Saturation in Fuel Cell Catalyst Layers by High-Resolution Small-Angle Neutron Scattering, ACS Appl. Energy Mater. 3 (2020) 8393–8401.

[8] F. Nandjou, J.-P. Poirot-Crouvezier, M. Chandesris, S. Rosini, D.S. Hussey, D.L. Jacobson, J.M. LaManna, A. Morin, Y. Bultel, A pseudo-3D model to investigate heat and water transport in large area PEM fuel cells - Part 2: Application on an automotive driving cycle, Int. J. Hydrog. Energy. 41 (2016) 15573–15584.

[9] E. Tardy, F. Courtois, M. Chandesris, J.-P. Poirot-Crouvezier, A. Morin, Y. Bultel, Investigation of liquid water heterogeneities in large area PEM fuel cells using a pseudo-3D multiphysics model, Int. J. Heat Mass Transf. 145 (2019) 118720.

[10] B. Randrianarizafy, P. Schott, M. Gerard, Y. Bultel, Modelling Carbon Corrosion during a PEMFC Startup: Simulation of Mitigation Strategies, ENERGIES. 13 (2020).

[11] G. Jullian, C. Cadet, S. Rosini, M. Gerard, V. Heiries, C. Berenguer, Fault Detection and Isolation for Proton Exchange Membrane Fuel Cell Using Impedance Measurements and Multiphysics Modeling, Fuel Cells. 20 (2020) 558–569.

[12] S. Rodosik, J.-P. Poirot-Crouvezier, Y. Bultel, Simplified anode architecture for PEMFC systems based on alternative fuel feeding: Experimental characterization and optimization for automotive applications, Int. J. Hydrog. Energy. 45 (2020) 19720–19732.

[T1] S. Louisia, Synthèse de catalyseurs bimétalliques supportés sur nanotubes de carbone dopés pour pile à combustible PEM, INPT, 2017.

[T2] C. Roiron, catalyseur sans Platine avec une structuration 3D pour PEMFC, These en préparation, Université Grenoble Alpes, 2018.

[T3] B. Randrianarizafy, Multi-physics modeling of startup and shutdown of a PEM fuel cell and study of the carbon support degradation : mitigation strategies and design optimization, Université Grenoble Alpes, 2018.

[T4] T. Drugeot, Quantification et optimisation de l'efficacité de stratégies et d'architectures de systèmes PEMFC pour minimiser les dégradations lors des phases d'arrêt/démarrage, Thèse en préparation, Université Grenoble Alpes, 2019.

[T5] G. Jullian, Diagnostic robuste de pile à combustible PEM par modélisation physique et mesures d'impédance: prise en compte de conditions dynamiques et du vieillissement, Université Grenoble Alpes, 2019.

[T6] A. Jacome, Estimation précise et robuste de l'état de vieillissement de piles PEMFC par observateurs bayésiens dans le cadre d'une approche basée modèle, Thèse en préparation, Bourgogne Franche-Comté, 2018.

A NEW ANODE ARCHITECTURE FOR PEMFC SYSTEM COST REDUCTION

Demanding applications, such as transportation, require a drastic reduction of the cost and system complexity for the integration of PEMFC. A new simplified architecture of the anode circuit has been developed and characterized. Cost reduction could reach from 6% to 57% compared to various common architectures, with similar performances.

APPROACH

Recirculation of hydrogen from the stack outlet to the inlet is commonly used at the anode of PEMFC systems, in order to evacuate liquid water from the stack, to supply water vapor at the stack inlet, and to mix undesired species, like nitrogen, with fresh hydrogen. It is more efficient than the Dead-End Anode (DEA) architecture, where the anode circuit consists simply of one inlet valve for hydrogen supply and one draining valve for water and nitrogen periodic rejection. However, it is also more complex and expensive due to the need of additional devices, such as pumps or ejectors.

In the new anode architecture proposed by CEA-Liten [1], the stack is split into several interconnected groups of cells, which are fed alternately with fuel (represented with two groups on Fig. 1). This process enhances water transport and gas mixing, without the use of complex device or control strategy.

RESULTS AND PERSPECTIVES

The characterization of the Alternative Fuel Feeding (AFF) strategy has been conducted with a 5-kW stack integrated into a dedicated PEMFC system test station. The stack is composed of two groups of 35 cells connected in series, assembled on both sides of a central distribution plate and fed alternatively with hydrogen with two inlet valves.

The specific operating parameters of this strategy, such as the "AFF frequency", namely the switching valve frequency at the hydrogen inlet, have been studied experimentally. The test results allowed us to identify the optimal AFF parameters depending on general stack operating conditions, like temperature, current and gas pressure. A simple model has been proposed to predict the optimal AFF parameters [2].

After a first implementation of this technique in the 10-kW system and the analysis of its impact on PEMFC durability [T1], AFF appears as a promising way to reduce PEMFC system weight and cost.

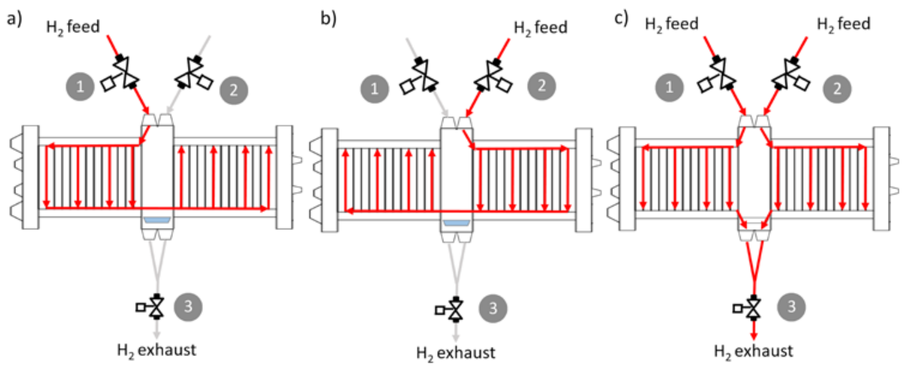

Figure 1: *Alternating Fuel Feeding operation with two groups of cells assembled on a central plate consists in a frequent switch between left group feeding and right group feeding, respectively during step a) and b), interrupted periodically by a brief opening of all the valves, inducing a purge of the circuit during step c). Both groups of cells share a common manifold going through the central plate, where liquid water can be collected between two purges.*

REFERENCES

[1] J.-P. Poirot-Crouvezier, "Multiple Injection Fuel Cell and Operating Method Thereof", patent application EP2707921, 05/09/2021.

[2] S. Rodosik, J.-P. Poirot-Crouvezier, Y. Bultel, "Simplified anode architecture for PEMFC systems based on alternative fuel feeding: Experimental characterization and optimization for automotive applications", Int. J. of Hydrogen Energy, vol. 45(38), 2020, pp. 19720-19732.

[T1] S. Rodosik, "Study of the Impact of Innovative Fluidic Architectures on the Management, Performance and Sustainability of PEMFC Fuel Cell Systems for Transportation", PhD thesis, Grenoble, 2019.

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DURABILITY OF NANOSTRUCTURED $LaPrNiO_{4+\delta}$ ELECTRODE FOR SOLID OXIDE CELLS APPLICATION

The electrochemical behavior of nanostructured $LaPrNiO_{4+\delta}$ used as oxygen electrode in solid oxide cells has been studied. It has been shown that the electrode exhibits high performance but is not stable in operation. Nevertheless, the products of the $LaPrNiO_{4+\delta}$ decomposition are still active and could be used as innovative materials.

APPROACH

Solid Oxide Cell (SOC) is an energy conversion system working at high temperatures (750-850°C). This technology has attracted attention in recent years thanks to its high electrical efficiency and its good reversibility in fuel cell and electrolysis modes. To support its current industrialization, the performances and durability of SOC still need to be improved. For this purpose, a strategy consists of reducing the operating temperatures while keeping high performances (650-750°C). However, in these conditions, the commonly used material used for the oxygen electrode is not well adapted and must be replaced. The lanthanum-praseodymium nickelates are considered as one of the most promising candidates due to their high electrocatalytic activity at intermediate temperatures [1]. Nevertheless, the stability of these materials in operation still needs to be verified. To address this problem, in collaboration with the LEPMI lab, the durability of $LaPrNiO_{4+\delta}$ (LPNO) has been investigated using nanostructured electrodes prepared by electrostatic spray deposition (ESD).

RESULTS AND PERSPECTIVES

Thanks to the nanoscale structuration of the ESD layer, high electrode performances were obtained even at low temperatures [2]. Long-term experiments were then conducted in both fuel cell and electrolysis modes at 700°C for »1000 h [3]. The performances were found to be stable for the electrodes operated under electrolysis current whereas a significant degradation was observed in fuel cell mode. Tomographic reconstructions have shown that the fine microstructure of the ESD layer was not changed after the operation, whereas severe electrode delamination was detected for the cells tested in fuel cell mode. Moreover, synchrotron X-ray characterizations (Fig.1) have shown that the decomposition of the LPNO phase into secondary phases is strongly accelerated under current. Based on these results, the mechanisms for electrode degradation have been discussed. Moreover, it has been stated that the products of LPNO decomposition are electrochemically active and could be used as innovative materials [4].

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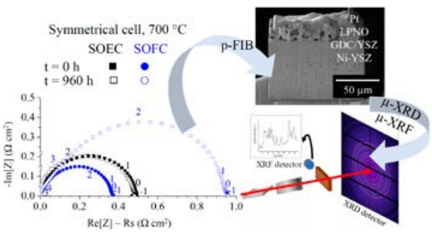

Figure 1: *Electrochemical impedance spectra of $LaPrNiO_{4+\delta}$ electrodes measured before and after operation in electrolysis (SOEC) and fuel cell (SOFC) modes. Thin lamellae were extracted from the tested electrodes by plasma Focused Ion Beam. The samples were then characterized by synchrotron X-ray µ-diffraction and µ-fluorescence at the Paul Scherrer Institute [3]. It can be noticed that the polarization resistance is not changed after operation in SOEC mode but it is increased by more than a factor of two in SOFC mode.*

REFERENCES

[1] J.C. Grenier, J.M. Bassat, F. Mauvy, J.A. Kilner, S.J. Skinner, S.J.C. Irvine, P.P. Edwards (Eds.), "Novel Cathodes for Solid Oxide Fuel Cells, Functional Materials for Sustainable Energy Applications", vol 35, Woodhead Publishing Series in Energy, 2012, pp. 402–444.

[2] N.I. Khamidy, J. Laurencin, E. Djurado, "Improving the electrochemical performance of $LaPrNiO_{4+\delta}$ as an oxygen electrode for intermediate temperature solid oxide cells by varying the architectural design", Journal of Electroanalytical Chemistry, 849 (2019) 113373.

[3] N. I. Khamidy, J. Laurencin, D. Ferreira-Sanchez, F. Monaco, F. Charlot, and E. Djurado, "Durability of nanostructured $LaPrNiO_{4+\delta}$ electrode for solid oxide cells: electrochemical, microstructural, and structural investigation", Journal of Power Sources 450 (2020) 227724.

[4] R.K. Sharma, N.I. Khamidy, L. Rapenne, F. Charlot, H. Moussaoui, J. Laurencin, E. Djurado, "Highly efficient architectured Pr6O11 oxygen electrode for solid oxide fuel cell", Journal of Power Sources 419 (2019) 171–180.

OPERANDO CHARACTERIZATION OF Li-ION BATTERIES

The booming of electric vehicles market is strongly supported by the increase in energy density of the Li-ion batteries. For the last ten years, this density has been almost tripled thanks to design and processing improvements but also thanks to the development of new electrode materials. The latter heavily relies on the deep understanding of the lithiation and degradation mechanisms associated to these materials in order to stabilize their performance and ensure a safe usage. Since the end of the 70s, *in situ* characterisations have proven to be a tool of choice to retrieve such information. However, *in situ* analyses are not sufficient to study dynamic phenomena, as they require stopping the electrochemical processes during the characterisation. During this break time, the system is not completely frozen and concentration gradient relaxation or parasitic reactions may occur. In these cases, being able to characterize the system *operando*, meaning during its operation, is key to getting valuable information. During this last decade, an increasing number of *operando* techniques have emerged for the study of Li-ion batteries. This development depends highly on the design of *ad hoc* cells that should achieve the difficult compromise between the needed conditions to get a representative electrochemical behaviour and the experimental constraints of the chosen analysis techniques. This paper presents several *operando* characterizations for batteries developed at CEA-Liten and their contribution to the understanding of these systems at various scales.

ACTIVE MATERIAL SCALE

X-Ray Diffraction (XRD) gives insight into both the lithiation and the ageing mechanisms of a material. Thus it has been one of the first technique to be adapted for *operando* measurements.

At CEA-Liten, soft pouch cells are used to carry out this characterization at the synchrotron facility, offering both high quality data and high time resolution. The example of the study of the Li/S system illustrates very well the contribution of the *operando* analyses. In this complex system, the sulfur electrode undergoes several solid-liquid reactions upon lithiation, with the sulfur turning into soluble Li_2S_n (n=8, 6, 4 and finally 2) polysulfides that will finally form solid Li_2S. Several *ex situ* and *in situ* studies were reported before our work. The results presented significant discrepancies, for example on the actual presence of Li_2S at the end of the discharge. These discrepancies could be attributed to the presence of several equilibria between the polysulfides in the liquid and the solid phases. These equilibria continue to evolve when the cell is under relaxation for the data acquisition, leading to inaccurate results. This modification depends on the peculiar relaxation protocol and the duration. Using *operando* X-Ray diffraction at the SOLEIL synchrotron with a 3 min time resolution, we were able to capture the dynamics of the system and also to observe, for the first time, that sulfur reprecipitates under a metastable form, namely the β-sulfur isotrope (Figure 1) [1], [2],[T1].

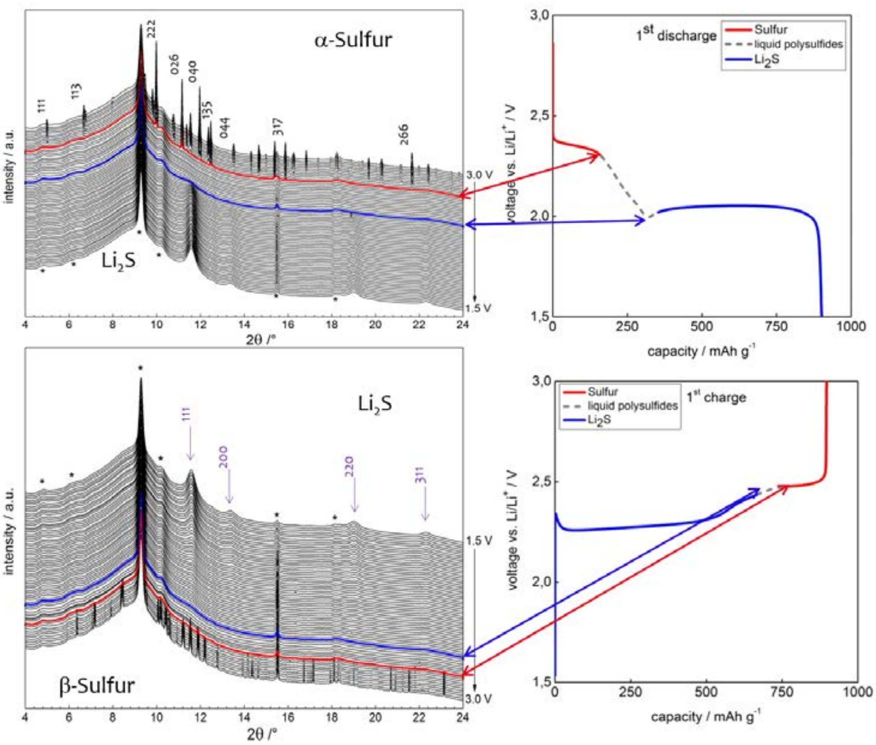

Figure 1: *Evolution of the X-Ray diffractogram of the S electrode and corresponding electrochemical curves*

INTERFACES

Recently, a renewed effort has been directed at understanding the mechanisms involving lithium plating and stripping at the interface between the lithium and the electrolytic medium, to bring optimal solutions with higher safety, coulombic efficiency, and durability. The coupling protocols combining X-ray photoemission spectroscopy (XPS) and electrochemical characterization, carried out in post-mortem conditions, paved the way to considerable progress in this field. However, the progress of *operando* XPS (OXPS) analyses faces complex technological limitations to design functional *operando* electrochemical cells such as the ultra high vacuum, the XPS depth analyses (~ 5 nm), as well as the X-ray beam size dimension (~ 10 µm) to name but a few. At CEA-Liten, we have developed a new *operando* cell and an associated protocol to perform OXPS at the electrode/electrolyte interface during electrochemical processes. To illustrate its performance, the crucial issues associated with the lithium metal/electrolyte interface have been scrutinized using two types of ionic liquids based electrolytes, laden with LiTFSI (lithium bis(trifluoromethanesulfonyl) imide) salt. [3] Figure 2-a and 2b display a symmetrical *operando* Li/Li cell encapsulated and filled with electrolyte and mounted on the developed four contacts sample holder. Figure 2c shows the evolution of XPS core level spectra during voltage profile change under galvanostatic polarization in Li/C_1C_6ImTFSI-LiTFSI/Li operando cell. This original work opens new perspectives to investigate the surface reactivity of the electrodes towards solid electrolytes both at the OCV (Open Circuit Voltage) and under polarization conditions.

ELECTRODE SCALE

A common way to increase the energy density of a cell without changing its chemistry is to increase the thickness of the electrode. Thanks to an adapted formulation, very good performances can be obtained at reasonable rates of charge or discharge. However at high rates, heterogeneities appear and degrade the performances and/or safety of the cell. To better understand this phenomenon in graphite electrodes, CEA-Liten has developed a model that predicts that a maximum of heterogeneity should be observed for each phase transition C→LiC_1→LiC_{12}→LiC_6 [3]. To validate the model, we have built, in collaboration with CEA-IRIG, a cell dedicated to *operando* micro-diffraction analysis of thick graphite electrode. It allowed us to retrieve the in-depth repartition of the different lithiated phases during cycling. The cell presented in Figure 2, is designed for a use on the ID13 beamline of the ESRF synchrotron facility (Grenoble).

On this beamline, the beam can be focused down to a 1µm*1µm size, we could thus probe a grid consisting of 51 points along the thickness of the electrode and 8 points along its length. The acquisition of each of the 408 diffractograms was realised in only 110s granting a sufficient time resolution even

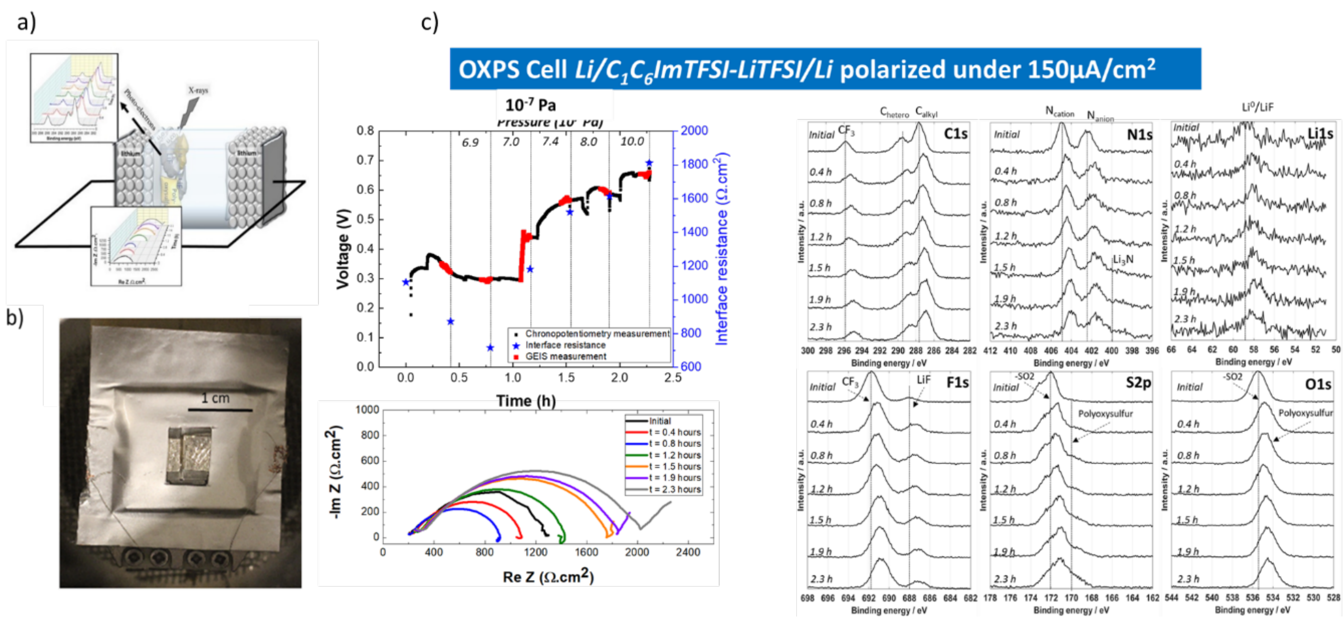

Figure 2: (*a and b*) *symmetrical lithium/lithium OXPS planar cell encapsulated and filled with electrolyte and connected to the four electrical contact sample holder,* (*c*) *XPS core level recorded at the interface Li/electrolyte during galvanostatic polarization. The GEIS measurements were recorded during polarization.* [3]

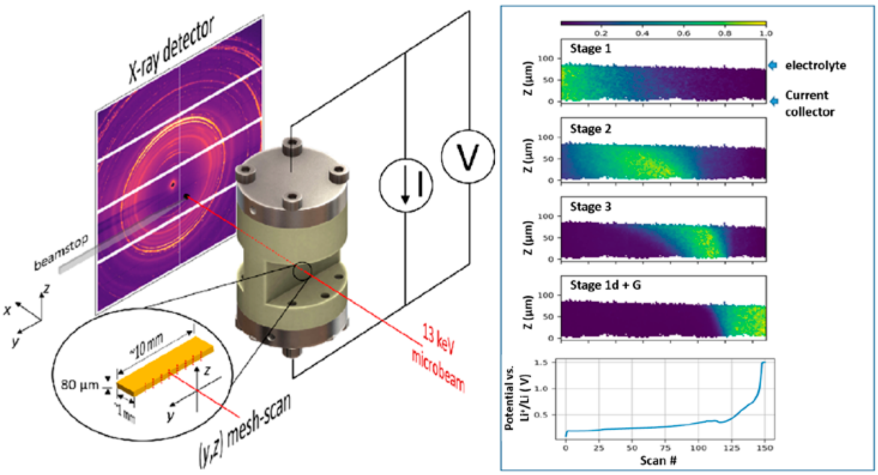

Figure 3. *a) Operando cell for micro-diffraction analysis on ID13 (ESRF) b) Evolution of the phase repartition in the graphite electrode thickness during discharge [4]*

at high C-rates. As expected, during the first two transition steps from LiC_6 (stage 1) to LiC_{12} (stage 2) and from LiC_{12} to LiC_{18} (stage 3), heterogeneities were observed between the surface of the electrode and the collector side. However, no such heterogeneity was detected during the last transition from stage 3 to graphite. This evidenced that the model was not capturing all the important physical processes and still need to be improved.

MULTI-SCALE

Lately, we have also developed a cell dedicated to coupling between tomography and X-Ray Diffraction Computed Tomography [T2]. As for any tomography technique, it allows the reconstruction of 3D volumes and thus gives access to morphological evolutions. But it also enables the collection of a diffraction pattern for each voxel, providing a spatially resolved structural information that can be directly coupled with the morphological one. We used this cell on the ID15 beamline of ESRF to study the Li/S system[5]. Figure 4 a) presents the evolution of the tomograph of the cell during the first charge. At the initial state, the different components of the cell can be clearly identified and delimited. The sulfur electrode is composed of sulfur and carbon fibers, during the discharge the micrometric sulfur particles disappear and smaller Li_2S particles are observed at the end of discharge. Thanks to the spatially resolved diffraction results, it is possible to follow the evolution of the sulfur and Li_2S contents at different depth in the electrode (Figure 4b) to check both the kinetics and the homogeneity of the deposition. Such information is highly valuable to optimise the architecture of this porous electrode to favor an efficient redeposition process. The Li electrode could also be studied at the same time, and an inhomogenous stripping of the Li was observed with the formation of pits that influence the subsequent plating.

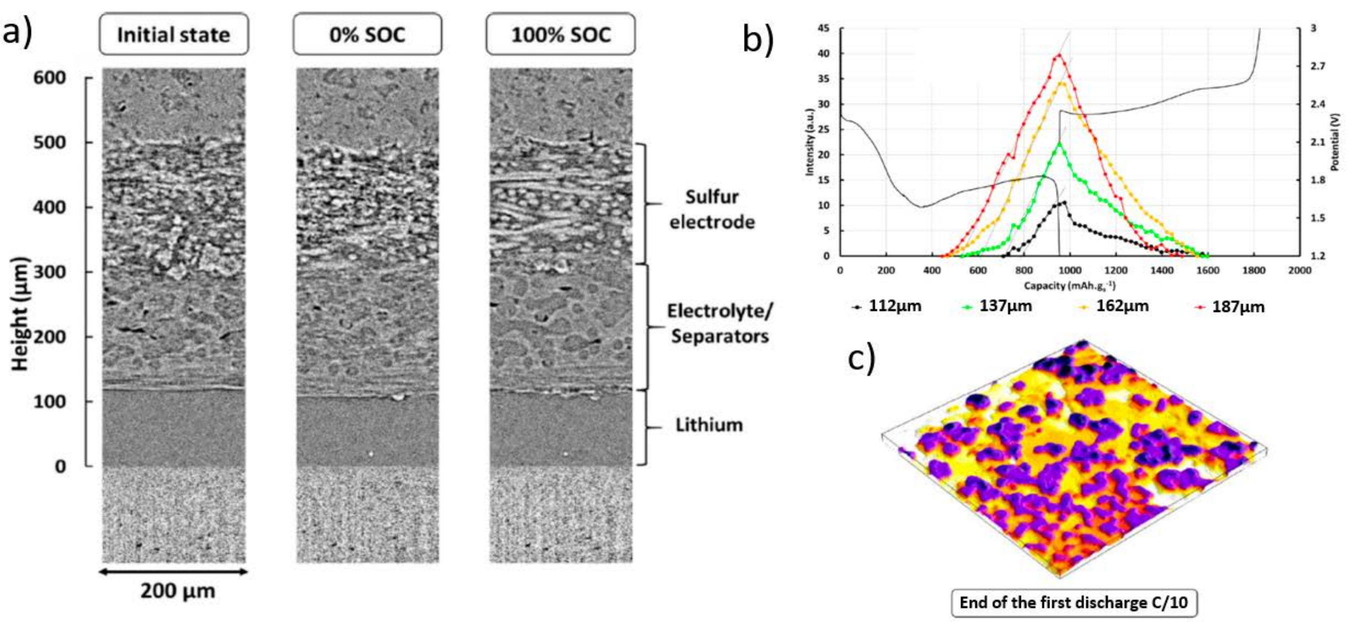

Figure 4: *a) Evolution of the tomographs of a Li/S cell during charge(SOC= State of Charge), b) evolution of the Li_2S content at different depth in the S electrode during cycling, c) Surface state of the Li electrode after the first discharge at C/10*

PERSPECTIVES

Several *operando* tools have been developed at CEA-Liten to collect information at different scales of the system, granting a much more complete view of the studied cells. The results are excellent and provide a real advance in the field of battery characterization, and they bring some light on the remaining challenges. The first one will be to adapt these tools to study the new generation of solid state batteries which will require different assembling processes. Also with this new type of batteries, the study of interfaces will certainly become more important compared to liquid electrolyte-based cells. Interfaces are especially hard to characterize. This requires a very high spatial resolution over a large volume of observation. Studies are ongoing to tackle this issue through the combination of the recent ESRF upgrade and the development of new specific cells.

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REFERENCES

Papers

[1] S. Waluś *et al.*, « New insight into the working mechanism of lithium–sulfur batteries: in situ and operando X-ray diffraction characterization », *Chem. Commun.*, vol. 49, n° 72 (2013) p. 7899-7901

[2] S. Waluś *et al.*, « Lithium/Sulfur Batteries Upon Cycling: Structural Modifications and Species Quantification by In Situ and Operando X-Ray Diffraction Spectroscopy », *Adv. Energy Mater.*, vol. 5, n° 16 (2015)

[3] A. Benayad et al., « Operando XPS: A Novel Approach for Probing the Lithium/Electrolyte Interphase Dynamic Evolution», J. Phys. Chem . A, 125 (2021) 4, 1069–1081

[4] N. Dufour *et al.*, « Lithiation heterogeneities of graphite according to C-rate and mass-loading: A model study », *Electrochimica Acta*, vol. 272 (2018) p. 97-107

[5] S. Tardif *et al.*, « Combining operando X-ray experiments and modelling to understand the heterogeneous lithiation of graphite electrodes », *J. Mater. Chem. A*, vol. 9, n° 7 (2021) p. 4281-4290

[6] G. Tonin *et al.,* « Operando investigation of the lithium/sulfur battery system by coupled X-ray absorption tomography and X-ray diffraction computed tomography », *J. Power Sources*, vol. 468 (2020) p. 228287

Theses

[T1] S. Walus, « Accumulateur lithium/soufre: développement et compréhension des mécanismes électrochimiques », PhD Thesis, Grenoble (2015)

[T2] G. Tonin, « Caractérisation operando des accumulateurs Li/S par tomographie d'absorption et diffraction des rayons X, vers une meilleure compréhension des mécanismes électrochimiques », PhD Thesis, Grenoble (2019)

TOWARDS DIRECT SPECIATION OF LITHIUM POLYSULFIDES BY X-RAY ABSORPTION SPECTROSCOPY

Lithium/sulfur batteries are very attractive thanks to their high energy density and the low cost of sulfur. The electrochemical activity of sulfur involves different lithium polysulfide intermediate species (Li_2S_x, 2 ≤ x ≤ 8), with a complex discharge mechanism, still subject to debate. To better understand this mechanism, a new analytical technique based on High-Energy Resolution Fluorescence Detected X-ray absorption spectroscopy is presented here.

APPROACH

The measurements were performed on different Li_2S_x standard solutions that were introduced in a coin cell designed for XAS (X-ray absorption spectroscopy) experiments, and High-Energy Resolution Fluorescence Detected X-ray absorption spectroscopy (HERFD-XAS) measurements were performed at the European Synchrotron Radiation Facility (ESRF-ID26). Compared to standard XAS, the increased resolution of HERFD-XAS spectra allows the pre-edge peak attributed to terminal atoms of lithium polysulfides to be clearly resolved from the main peak (~2471 eV) generally attributed to elemental sulfur (see figure 1). Consequently, a quantitative analysis could be performed by determining the area of the pre-edge peak relative to that of the main one, to better differentiate the Li_2S_x species.

RESULTS AND PERSPECTIVES

Figure 1 shows that the relative area of the pre-edge peak increases while the polysulfide chain length decreases. A linear relationship between the normalized peak areas of the two main absorption features and the polysulfides chain length was found, which is in agreement with theoretical study of Pascal et al. [3] based on molecular dynamics calculations. Their calculations attribute the two main absorption features to differently coordinated sulfur atoms in the polysulfide. Consequently, the increase in resolution obtained using HERFD-XAS allows the clear separation and the quantitative evaluation of lithium polysulfides. In the future, Operando HERFD-XAS will be used to determine and quantify the soluble intermediate species formed in the battery. This will complement the X-ray diffraction technique which is principally used to quantify the solids formed during the electrochemical process of Li/S batteries [4].

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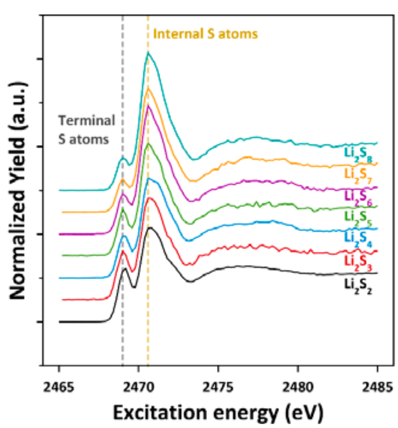


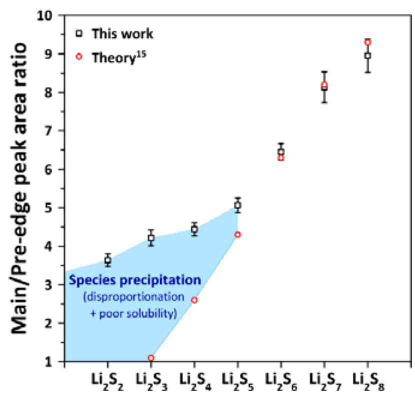


Figure 1: *left: HERFD sulfur K-edge absorption spectra recorded for different lithium PS standard solutions Li_2S_x (x = 2…8); right: Experimental area ratios for the two absorption peaks compared to theoretical values.*

REFERENCES

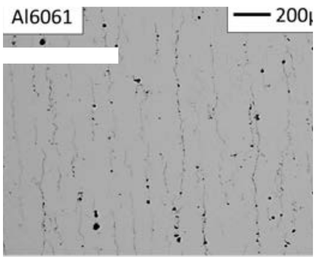
[1] A. Robba, C. Barchasz, K. Bučar, M. Petric, M. Žitnik, K. Kvashnina, G. Vaughan, R. Bouchet, F. Alloin, M. Kavčič, « Fingerprinting Mean Composition of Lithium Polysulfide Standard Solutions by Applying High-Energy Resolution Fluorescence Detected X-ray Absorption Spectroscopy », J. Phys. Chem. Lett., vol. 11 (2020) 5446–5450

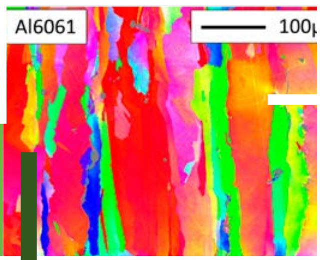
[3] T. A. Pascal, K. H. Wujcik, J. Velasco-Velez, C. Wu, A. A. Teran, M. Kapilashrami, J. Cabana, J. Guo, M. Salmeron, N. Balsara, D. Prendergast, « X-ray Absorption Spectra of Dissolved Polysulfides in Lithium-Sulfur Batteries from First-Principles », J. Phys. Chem. Lett., vol. 5 (2014) 1547–1551.

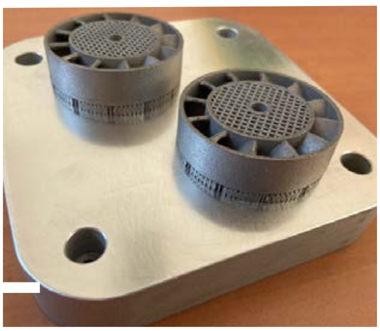
[4] 18. G. Tonin, G. Vaughan, R. Bouchet, F. Alloin, M. Di Michiel, C. Barchasz, « Operando investigation of the lithium/sulfur battery system by coupled X-ray absorption tomography and X-ray diffraction computed tomography », J. Power Sources, vol. 468 (2020) 228287

CIRCULAR ECONOMY & MATERIALS

CIRCULAR ECONOMY CONSIDERATIONS WILL NEED TO BE A MAJOR FACTOR IN TECHNOLOGICAL INNOVATION IF THE IMPACT OF THE ENERGY TRANSITION ON RAW MATERIALS CONSUMPTION IS TO BE LIMITED. CEA-LITEN RESEARCH BRINGS THE CIRCULAR ECONOMY PRINCIPLES OF REDUCE, REUSE, RECYCLE INTO THE ECO-DESIGN AND RECYCLING OF NEW ENERGY TECHNOLOGIES. NEAR-NET-SHAPE MANUFACTURING PROCESSES (LIKE 3D PRINTING) AND STRUCTURAL ELECTRONICS ARE TWO EXAMPLES OF HOW CEA-LITEN DEVELOPMENTS ARE MAKING MORE ECONOMICAL USE OF MATERIALS. THE INSTITUTE ALSO DEVELOPS MATERIALS, PROCESSES, AND SYSTEMS FOR THE CIRCULAR CARBON ECONOMY, I.E. THE CONVERSION OF CARBON-CONTAINING RESOURCES INTO MOLECULES OF INTEREST FOR ENERGY OR CHEMISTRY.







CONTENTS

THE CIRCULAR ECONOMY, A WELL-ESTABLISHED VISION AT CEA-LITEN

Aiming a climate-neutral EU economy by 2050 as set in the European Green Deal [1] will require profound transformations in all sectors, in particular in energy and mobility. The consumption of raw materials [2] is expected to increase drastically in the coming decades to manufacture low-carbon energy production (wind turbines, photovoltaic modules), storage (batteries, hydrogen and fuel cells) and distribution systems (infrastructures for massive electrification). The traditional linear system is unable to sustain such massive growth in material needs. The potential of circular economy [3] to contribute to climate change mitigation has been illustrated [4] [5] to change the way we make, use and manage waste. The European Commission has launched a new Circular Economy Action Plan [6] (CEAP) in order to foster and incentivise economic activities with a low carbon and material footprint. The CEAP is highlighting "*circularity as a prerequisite for climate neutrality*". It also tackles the challenge of strengthening EU's sovereignty regarding its access to sustainable resources, clean energy and its control on strategic value chains. CEA-Liten has the ambition to cover circularity all along product lifecycles as described in Figure 1: from 1) reduction of raw materials consumption, 2) products reutilization to 3) waste recycling [7]. Table 1 gives an overview of the coverage of circular economy at CEA-Liten throughout the difference technological programs. The rest of the section highlights some focusses with key scientific results.

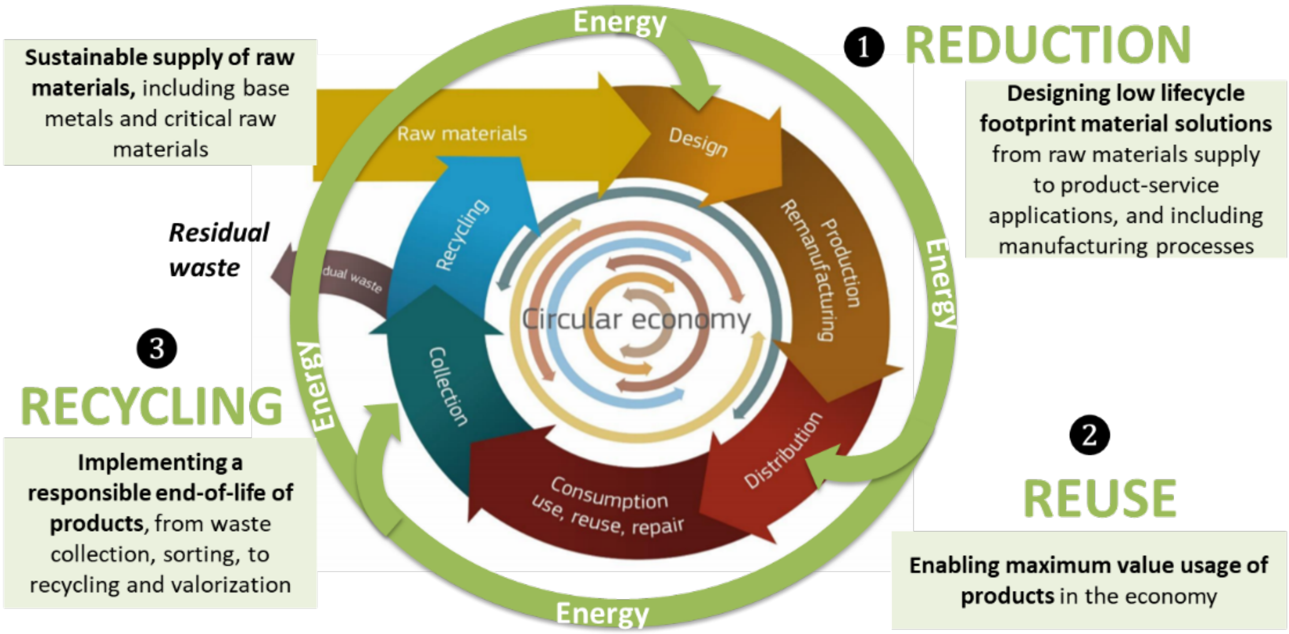


Figure 1: *Scheme of the circular economy principle*

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	REDUCTION	REUSE	RECYCLING
SOLAR PV	Si Kerf recovery Pb reduction in PK	Modules second-life	Ag, Si, In, Cu, Ga recovery Pb recovery in PK
BATTERIES	Ni-rich NMC	Second-life	Ni, Co, Mn recovery
FUEL CELLS	Pt reduction and cells durability	Remanufacturing	Pt recovery
MAGNETS	REE (Nd, Pr, Dy, Tb) substitution	-	REE recovery
BIO-RESOURCES	-	-	High-value molecules from organic waste
POWER ELECTRONICS	Mo, Be, W substitution	-	Precious metals (Au, Si) recovery
FUNCTIONAL ELECTRONICS	Components durability Predictive maintenance	-	-

Table.1: *Overview of main CEA-Liten activities contributing to a circular economy*

RAW MATERIALS CONSUMPTION REDUCTION

One illustration of a circular approach to reduce raw materials consumption is the substitution of an element by another that is less critical. The challenge is to preserve performances with substitutes at the closest level than with the initial composition.

Substitution of Nd by Ce in permanent magnets

Critical rare earth elements Nd and Pr required for permanent magnets are extracted from geological deposits that contain large amount of Ce and La. Due to the growing demand of magnets and the subsequent mining of raw materials, Ce and La are currently overproduced and stored, hence have a lower level of criticality. The substitution of Nd by the unused Ce element would allow sustainable magnet production via a more balanced sourcing of rare earths. However, (Nd,Ce)FeB alloys exhibit lower magnetic properties than their non-substituted counterparts. This is due to the mixed valence of Ce atoms (Ce^{4+} is nonmagnetic) and the formation of the deleterious $CeFe_2$ phase. The implementation of Ce-magnets in electrical motors inevitably requires a machine redesign. Complex shaped magnets could rise the motor performances but the conventional machining of sintered parts is not efficient: more than 30% of the magnet material is lost which cancels the benefit of the Nd substitution. The EIT-Raw Materials project LOWREEMOTORS aims at manufacturing net-shape Ce-magnets with the power injection molding process. Magnets with 20% of Nd atoms substituted by Ce have already been produced by the conventional sintering process on the CEA-Liten pilot line. The characteristics comply with the specification for an electrical machine (remanence = 1.2 T, coercivity = 1100 kA/m) developed by a large OEM, partner of the project. Feedstocks suited for the injection of jet-milled power have been formulated and tested with encouraging results [1]. However, the oxygen pick-up occurring during the mixing of powder and binders, then the carbon contamination upon debinding, have been found to be higher than the specification for magnets (2500 ppm O_2, 800 ppm C). The reactivity between polymers and powder and the microstructural aspects of the debinding step [2] will be more deeply investigated for reducing this degradation.

Substitution of Be, Co, Mo, W by metal matrix composites in power electronics packaging

Power electronics legacy technology uses Cu-W, Cu-Mo, Fe-Ni-Co (Kovar®), Al-Be, Be, Be-BeO alloys, all with suitable Coefficient of Thermal Expansion (CTE) range, but they are heavy, difficult to handle and contain critical raw materials (W, Co, Be) or toxic (Mo, Be) elements. For stringent reliability reasons, due to the CTE of the most demanding semiconductor chips (4 to 6 ppm) or the ceramic (6 to 8 ppm), pure usual electronics metals, such as Cu or Al, cannot be used as thermal management materials in current generation of SiC or GaN chips. MMC (Metal Matrix Composites) with aluminum matrix and several form of carbon reinforcement (fiber, flakes, diamond powder etc.) were successfully designed and fabricated in the EIT-Raw Materials project CRUCIAL with thermal and thermomechanical properties suitable with microelectronics. CRUCIAL aims at scaling up the production of Al/Carbon composite powder and extend the production method to near net shape parts with architectured thermal properties (heat sink and heat spreader function). Along with the production of near net shape parts that are fully recyclable (Al melting and C burning), post processing methods are developed to allow selective deposition of gold and nickel plating, saving raw materials. In CRUCIAL powder mixing process of Al/C MMC were scale up and homogeneous batches of powder were produced that led after optimized sintering to adjustable thermomechanical properties (along with C content and type) suitable for legacy alloys replacement (thermal conductivity beyond state-of-art, i.e. 340 – 460 W/(m.K) and CTE compatible with GaN and SiC chips. The next step will consist in the setting-up of an industrial pilot line for the production of Al/C MMC with a French SME partner.

Sustainable powder metallurgy processes optimization

Another illustration of the reduction of raw materials consumption is to optimize processes for a set of defined materials and production routes throughout the value chain. Powder metallurgy encompasses two main processes families: Near-Net Shape (NNS) and Additive Manufacturing (AM). Among NNS processes, Metal Injection Moulding (MIM) generates roughly 5% of scraps during the injection phase. During the debinding phase, MIM uses feedstocks mostly containing polyacetal-based polymers which produce residues. In H2020 SUPREME project, it was demonstrated [3] that up to 50% of scraps can be reintroduced in a pristine feedstock to produce new MIM parts without altering their properties and without decreasing the process yield. Among the AM processes, Laser Powder Bed Fusion (LPBF) enables to recycle in theory entirely the non-fused powder. However, physical changes of the powder after several recycling are not well quantified. The evolution of a 316L GA stainless steel powder after up to 8 cycles was correlated with the physical and mechanical characteristics of printed parts [4]. A recovery rate of about 70 % was demonstrated. A protocol without neat powder addition, was followed which means that a process allowing the addition of powders would also allow more reuse. Recycling powder did not cause any significant changes in its characteristics since only the chemical composition varies slightly (mainly the O content) and the particle size tends to increase with no impact on other characteristics. Density and mechanical properties of printed parts remain also stable until the last iteration. Key Process Indicators (KPIs), were monitored to demonstrate processes optimization in terms of raw material resources reduction, energy efficiency, yield improvement and reduction of carbon dioxide emissions. These KPIs were calculated thanks to the realization of Life Cycle Assessment (LCA) methodology on these PM processes [5]. A sensitivity analysis on LPBF LCA results has been performed to determine the influence of powder bed recovery on the environmental performance of the process. It has been demonstrated that with a powder bed recovery rate up to 80%, a reduction of 77% of the CO_2 emissions linked to the manufacturing of one part could be obtained (Figure 2). The same trend was observed for resource and energy depletion indicators.

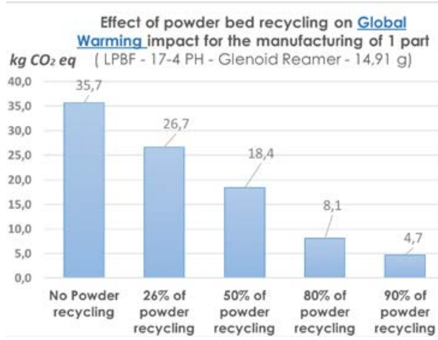

Figure 2: *Sensitivity Analysis results on LPBF powder bed recovery and influence on the CO_2 emissions for the manufacturing of one part*

LCA allowed the identification of potential improvements in terms of energy efficiency, resource consumption and CO_2 emissions: the environmental data collected in SUPREME will be used for further optimization on LPBF and MIM processes.

PRODUCTS REUSE

The waste hierarchy [/1] indicates that before a product reach end-of-life, it is worth identifying if it can be re-introduced in the economy for a second-use. It is very important to distinguish reuse (or second-use) and recycling as they correspond to completely different regulations, value chains and operations.

Second-life of batteries

When batteries retire from electric vehicles, they often still have 70-80% of their initial capacity left. They can target a wide range of stationary applications both in domestic and industrial markets. However, these batteries have very diverse designs, technologies and remaining performance. Depending on the specifications of the targeted application and on the heterogeneity of cells' ageing within the battery pack, it may be used entirely

1 / According to the European Commission's Waste Framework Directive (Directive 2008/98/EC, Article 4), the waste hierarchy is applied as a priority order in waste prevention and management legislation and policy: (a) prevention; (b) preparing for re-use; (c) recycling; (d) other recovery, e.g. energy recovery; and (e) disposal.

or partly dismantled and reconditioned. Developing methods to characterize the battery's performance in this context is a real challenge, which is addressed in the H2020 CIRCUSOL project where CEA-Liten is working on robust diagnosis protocols taking into account the diversity of battery pack design (cells arrangement, Battery Management System, communication protocol) [6]. Safety assessment is also challenging, since the usual methods are often destructive and are thus not applicable for second life, since each battery is virtually unique due to its first life use conditions. Furthermore repurposing is a new end-of-life strategy, designers need guidance to integrate it during the upstream stages of the design process. CEA-Liten has participated in the modification of three usual design tools to facilitate design steps in a repurposing perspective [7]. These results will be used as an input to the ongoing development of international standards, via the participation of CEA-Liten in the IEC TC21 committee.

Second-life of PV modules

The cumulative PV waste is expected to reach up to 8Mt by 2030[2]. Reported field experiences show that the majority of PV modules with diagnosed/classified failures that are decommissioned enter the waste stream and are either disposed as waste (in their majority) or – at best case – recycled, with the latter option representing today a clear minority of less than 10%. However, experts from the IEA PVPS and H2020 CIRCUSOL project (in both of which CEA is major partner) estimate that 45%-65% of them can be actually diverted from the disposal/recycling path, towards repair and second-life PV (re-use) or revamping. In order to ensure the technical-economical bankability of PV re-use, it is important to [8]: (i) identify the addressable "target volume", i.e. the failed PV modules (or strings), the repair of which is technically feasible, and the occurrence or distribution of such failures ; (ii) determine the post-repair efficiency and/or post-revamping reliability of these modules; (iii) integrate optimal reuse and repair in the current PV O&M value chain. CEA-Liten has presented early results [9] of the suitability of advanced PV modelling and diagnostics that can be leveraged for fast on-site and accurate classification of failed/decommissioned PV modules for repair, requalification and reuse/second-life. Further developments are also expected to be linked with the ongoing H2020 SERENDI-PV project.

WASTE RECYCLING

After a second-use (or third or more when relevant), the product becomes a waste and must as much as possible follow a recycling path[3]. It encompasses a set of activities, including separation, and processing, by which products or other materials are recovered from the solid waste stream for use in the form of raw materials in the manufacture of new products (other than fuel for producing heat or power by combustion).

Recovery of Si, In, Ag from end-of-life PV modules

A PV module can be assimilated to a sandwich, generally surrounded by an aluminum frame, made of different layers: a glass front-sheet, a solar cells' layer and a polymer or glass back-sheet, sealed by an encapsulating polymer. This configuration renders very difficult the recovering of valuable materials that are encapsulated in the multi-layered PV sandwich. The main challenge is then to separate properly the components to avoid mixing materials and to be able to recover the embodied materials such as precious and scarce metals with a purity close to the primary resources. The current recycling practices are mainly based on crushing/shredding processes for which the mixed fractions are mostly either landfilled or eventually re-directed to very low-value applications: implying an irreversible loss of valuable and critical resources. CEA-Liten is working on the disassembling of external components (frame, electrical cables), the delamination of the multi-layer sandwich and the extraction of the metals from the solar cells. A completely new approach based on diamond wire cutting will enable the separation on PV multi-layers sandwich without mixing materials. The technology patented by CEA-Liten [10] demonstrates the mechanical separation of the glass sheet from solar cells and the separation of the polymer back-sheet. The direct re-use of the glass sheet on a new PV module has been demonstrated with similar performances compared to a benchmark module. CEA-Liten has established a pioneering iono-metallurgical route to recover Ag without using concentrated mineral acids [11]. Selective and efficient Ag extraction (ratio >95%) from solid waste has been demonstrated with a dissolution rate comparable and higher than the state of art. After dissolution, electrodeposition has been successfully performed to recover Ag under metallic form. This groundbreaking solution will enable high-ratio and high-purity metal recovery using a green solvent recyclable in the loop of the treatment cycle. CEA-Liten is working on new adapted metal ex-

2 / End-of-life management: Solar Photovoltaic Panels. Report IRENA & IEA-PVPS T12-06:2016 © IRENA and © IEA-PVPS

3 / "*all products will eventually reach a point at which they no longer qualify for arranging direct reuse, repair, refurbishment or remanufacturing – either because of the associated cost, or because their implicit quality and utility potential has been degraded. At that point, there is still an essential need for efficient and effective recycling systems to recover the value of the materials contained within the product, and to recirculate those materials back into circular materials economy*", Redefining value- The manufacturing revolution, UN Environment International Resource Panel report (2018).

traction routes for second PV generation, especially concerning the indium recovery in heterojunction solar cells.

Recovery of Co, Li, Ni, Mn from end-of-life batteries

Hydrometallurgy is the most developed process to recover the critical metals as precursors to reintroduce metals in a close loop of LIBs manufacturing. The vast majority of approaches aim at a complete and rapid dissolution of the waste, followed by separation steps of manganese, cobalt, nickel and lithium. The dissolution of active materials and the subsequent separation requires many and complex steps with harsh conditions of treatment. CEA-Liten has recently established the complete dissolution mechanism for NMC-type materials that can be generalized to other electrode materials [12, 13, 14]. The dissolution mechanism is described in two distinct steps that are advantageously used to define a sustainable process. The first step is characterized by the extraction of lithium, which is the initiation step for the release of electrons required for the reduction of oxides. The first phase of dissolution is «self-regulating «, allowing to reduce the amount of reagent. As the reaction progresses, the delithiation weakens and the internal potential of the material increases, reducing the driving force of the reaction until the dissolution is stopped (Figure 2). The second step induces an enrichment in manganese at the particles surface to form a well-defined core-shell structure by manganese oxidation. When the condition of treatment are adjusted, it allows simultaneously complete dissolution of the metals and separation of the manganese as an oxide form. It is highly desirable for both economical and environmental considerations in reducing the number of steps, the amount of reagents, and to facilitate the downstream stages of the treatment process. CEA-Liten is currently developing with ORANO partner the process at an industrial level for all lithium-ion battery chemistries.

CONCLUSION

As circular economy is growing, CEA-Liten already applies the principles and methodologies to the development of the low-carbon technologies. Thus, it not only contributes to the energy transition toward climate-neutrality, but also to more resilient and sustainable industries and societies.

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REFERENCES

[1] T. Bioud et al., "Net-shape NdFeB magnets made by Powder Injection Moulding (PIM): lowering the organic contaminations", oral accepted for EPMA seminar "Functional Materials for Energy" on 1-2 June 2021

[2] S. Rolère et al., "New insights on the porous network created during solvent debinding of powder injection-molded (PIM) parts, and its influence on the thermal debinding", J. Mater. Process. Technol. 295 (2021) 117163

[3] D.Vincent et al., Recyclability of MIM feedstocks using 17-4PH powders produced by Gas or Water Atomization, Proceedings of EuroPM2020 conference, EPMA, Oct.2020

[4] G. Gaillard et al., Impact of powders reuse in LPBF processes on the powder characteristics and samples mechanical properties, Proceedings of EuroPM2020 conference, EPMA, Oct.2020

[5] E.Cor et al., Environmental analysis of the powder metallurgy value chain: a methodology for comparison with conventional manufacturing, Proceedings of EuroPM2020 conference, EPMA, Oct.2020

[6] B. Crouzevialle, "Method for determining the state of health of the cells of a battery", Patent application WO2020120911 A1, 18/06/2020

[7] T. Bauer, T., Mandil, G., Monnier, É., & Zwolinski, P. (2021). Design for cascading applications reuse – understandings of an emerging end-of-use strategy and propositions for its implementation. Journal of Engineering Design, 32(3), 140-163. https://doi.org/10.1080/09544828.2020.1871470

[8] J.A. Tsanakas, et al., "Towards a circular supply chain for PV modules: Review of today's challenges in PV recycling, refurbishment and re-certification", Prog Photovolt Res Appl. 2019;1–11.

[9] J.A. Tsanakas, D-L. Ha, F. Al Shakarchi. Early Casualties in Five PV Plants in France: A Sustainability Perspective on Complete PV Fault Diagnostics for Revamping, in Proc. 37th EU-PVSEC, 2020.

[10] Patent: FR1758013, FR1758010

[11] Patents EP3388554 A1, EP3388556 A1

[12] Billy, E.; Joulié, M.; Laucournet, R.; Boulineau, A.; De Vito, E.; Meyer, D. Dissolution mechanisms of $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ positive electrode material from lithium-ion batteries in acid solution. ACS Applied Materials & Interfaces 2018

[13] E. Billy Academic Innovation Award of FEDEREC 05-04-2019 - https://federec.com/fr/federec-actualites-detail/messages/4-projets-innovants-recompenses/)

[14] Patent FR3034104 A1

CLOSING THE LOOP: LIFE CYCLE ASSESSMENT AND OPTIMIZATION OF A PEMFC PLATINUM-BASED CATALYST RECYCLING PROCESS

The fuel cell is already a promising power source for transportation (automotive and aeronautics) based on the conversion of the chemical energy of hydrogen into electricity. Nevertheless, to reach sufficient energy densities this reaction must be catalyzed by noble metals like platinum. This study demonstrates that it is possible to recycle the platinum in a closed loop using an environmentally friendly recycling method.

APPROACH

This study focused on the development of new processes for the closed loop reuse of platinum and cobalt used as catalysts in fuel cells. Two chemical processes based either on ion exchange resins or on solvent extraction have been developed and compared. Then, in order to demonstrate the closed loop recycling potential, alkaline platinum solutions were treated to synthesize new catalysts for the proton exchange membrane fuel cell (PEMFC) cathode via the polyol method. Finally, a life cycle assessment (LCA) methodology study was carried out in order to identify the solution with the lowest environmental impact, taking into account the the entire PEMFC life cycle.

RESULTS AND PERSPECTIVES

High recycling rates of Pt were reported. The Pt initially contained in PEMFC can was recycled into Pt/C catalysts with yields of 83% and 77% respectively for the solvent based and resin alternatives. The life cycle assessment (LCA) of the two recycling alternatives were compared. Similar impacts have been found for both alternatives from the point of view of the entire PEMFC life cycle. Finally, the recovered platinum alkaline solutions have been further used for Pt/C particles synthesis via a modified polyol method. It was shown that the catalyst prepared via the resins based alternative displayed satisfactory morphological features (around 2.5nm). The electrochemical properties for the oxygen reduction reaction (ORR) with such recycled material performed similarly to a commercial state-of-art Pt/C catalyst. Despite a slightly lower experimental recovery yield, it was demonstrated that the ion exchange resin is the most promising way to recycle Pt and separate Pt and Co. It provides an easy route to synthesize again the Pt/C catalyst with excellent catalytic activity, thus demonstrating the feasibility of a closed loop recycling process [1].

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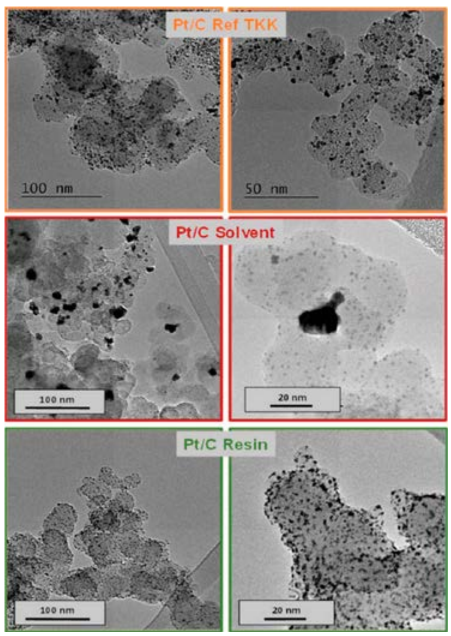

Figure 1: *Transmission electronic microscope images of Pt/C synthesized from solvent regeneration (middle) and resin desorption (bottom) solution using the polyol process compared to the commercial TKK catalyst (top).*

REFERENCE

[1] L.Duclos, R.Chattot, L.Dubau, P-X.Thivel, G.Mandil, V.Laforest, M.Bolloli, R.Vincent, L.Svecova, "Closing the loop: life cycle assessment and optimization of a PEMFC platinum-based catalyst recycling process", Green Chemistry, vol 22 (2020), 1919-1933.

A SOLUTION TO THE HOT CRACKING PROBLEM FOR ALUMINIUM ALLOYS MANUFACTURED BY LASER BEAM MELTING

Laser Powder Bed Fusion (L-PBF) has focused the interest of the scientific and industrial communities over the past few years. Indeed, 3D printed alloys display many specific characteristics. Among all aluminium alloys, some of them, mainly structural grades, are suffering from the hot cracking problem during L-PBF processing. As part of a thesis work, we developed a general methodology to solve this issue [1]focused here on the 6061 alloy. 6061 is a precipitation-hardened aluminium alloy, containing magnesium and silicon as its major alloying elements. This alloy, commonly used in the aeronautic and automotive industries, thanks to its excellent weight to strength ratio and high thermal conductivity, is particularly prone to hot cracking, in particular during LBM processing. The solution to remove cracks proposed in the present paper is to induce grain refinement to avoid the development of large columnar structures. To this end, various quantities of Yttrium Stabilized Zirconia (YSZ).

APPROACH

Severe thermal conditions associated with the L-PBF process often induce columnar grain growth during the transition from liquid to solid state. Unfortunately, this grain structure is particularly prone to hot cracking phenomena. Consequently, cracks are propagating along these columnar grains during process. High strength aluminium alloys are very sensitive to this hot cracking phenomenon due to low melting points elements. Cracks are clearly a non-acceptable issue for mechanical applications. We therefore focus our research efforts on the grain structure downsizing, trying to promote small equiaxed grains. To this end, an Al6061 alloy powder commonly used in the aeronautic and automotive industries is coated with YSZ (Yttria Stabilised Zirconia, containing mainly Zr element) particles through a dry mixing process. This approach targets a slight chemical modification to enhance equiaxed structure during L-PBF printing and as a result get rid of the hot cracking problem.

RESULTS AND PERSPECTIVES

Experiments highlight that the addition of 2 vol% of YSZ allows to fully avoid cracks thanks to a conventionally called duplex microstructure (Figure 1). The Zr liberated after YSZ dissolution combines with Al during cooling to form a nucleant phase for the aluminium grains, allowing the grain structure refinement. A continuous band of small equiaxed grains decorates each melt pool boundaries, and so avoid massive columnar grain growth. This shield prevents cracks from initiating and propagating (Figure 1). Inside each melt pool, coarser elongated grains are observed. Based on theoretical considerations, we recently shed light on the bimodal microstructure formation of Zr-containing Al alloys [2], which has been observed by many authors. In addition, we demonstrated the excellent mechanical response of the new alloy (Al6061+2%vol YSZ). Finally, the feasibility on complex concrete parts has been proved (Figure 2). The proposed solution provides many benefits. First, the increase of cost per kg of powder is quite insignificant (less than 5%). Second, a dry mixing technique is used, which is relatively easy to implement and is very scalable. Last but not least, the method has been transferred to another hot cracking sensitive aluminium grade (7075 alloy), with promising results.

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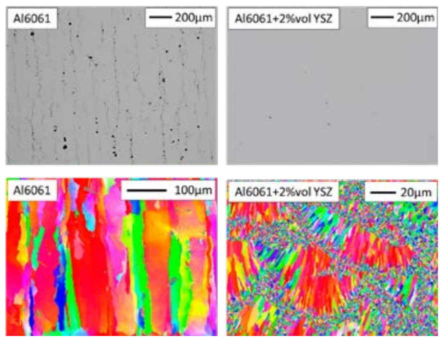

Figure 1: *Optical micrographs and EBSD images showing the cracks removing and the grain structure refinement after the addition of 2 volumetric % of YSZ to Al6061 powder.*

REFERENCES

[1] M. Opprecht et al., “A solution to the hot cracking problem for aluminium alloys manufactured by laser beam melting”, Acta Materialia, vol. 197, p. 40-53, sept. 2020.

[2] M. Opprecht et al., “An understanding of duplex microstructures encountered during high strength aluminium alloy Laser Beam Melting processing”, Acta Materialia, in press (2021) doi.org/10.1016/j.actamat.2021.117024.

CATALYTIC CO_2 VALORIZATION INTO FUELS AND CHEMICALS IN A POWER-TO-LIQUID PROCESS

The Carbon Capture and Utilization (CCU) concept for the synthesis of various products is gaining a lot of interest. The direct combination of CO_2 with low carbon H_2 towards liquid hydrocarbons as fuels and chemicals (Power-to-Liquid (PtL)) is considered as a promising solution to decarbonize both industry and transports, especially for the heavy-duty trucks, marine and air transport, while benefiting from existing infrastructures.

APPROACH

Different routes are reported in the literature to produce liquid fuels from CO_2 hydrogenation. Indirect pathways, including a step of CO_2 conversion into CO are high TRL processes. Direct pathways offering a better energy integration still require investigations and process optimization.

The present project focuses on the direct CO_2 hydrogenation into hydrocarbons via the so-called Fischer-Tropsch pathway illustrated by the equation below: $nCO_2+3nH_2 \leftrightarrow (-CH_2-)_n+2nH_2O (\Delta H_r^{298K}=-125 kJ/mol)$

This exothermal catalytic reaction produces a mixture of paraffins, olefins and oxygenates compounds, depending on the catalysts and on the operating conditions. Research is mostly dedicated to the improvement of catalysts activity and selectivity, while further investigation is needed about detailed kinetics, reaction mechanism, reaction modelling and global process design. [1]

In our work, this CO_2 hydrogenation process is investigated with the aim to understand kinetics, to model and design an efficient heat-exchanger reactor and to assess the global efficiency of the process.

RESULTS AND PERSPECTIVES

A supported potassium-promoted iron catalyst has been selected and synthetized in order to assess the impact of operating conditions on the conversion rate and selectivity. Two approaches have been followed for the development of a kinetic model. Firstly, a macro-kinetic approach, consisting in an improvement of the work proposed on the state of the art in order to take into account the formation of the different products. Then, a micro-kinetic approach, based on the hypothesis of a reaction mechanism, making the assumption that oxygenates, olefins and paraffins are formed on different types of active sites. The obtained experimental results have been used to optimize the kinetic parameters of these kinetic models and to determine the best model among those proposed. Then, the macrokinetic model has been implemented in a heterogeneous reactor model in order to predict the reactor performances and propose an optimized upscaled reactor design. The next step will focus on the whole process scale, evaluating its overall efficiency including the valorization of the obtained products and comparing the potential of this process with the indirect pathways. Moreover, the positive results obtained in the frame of Carlotta Panzone PhD laid the basis of using this technology as a way to reduce CO_2 footprint of biofuels by coupling biomass gasification, electrolysis and both CO_2 and CO hydrogenations into valuable hydrocarbons.

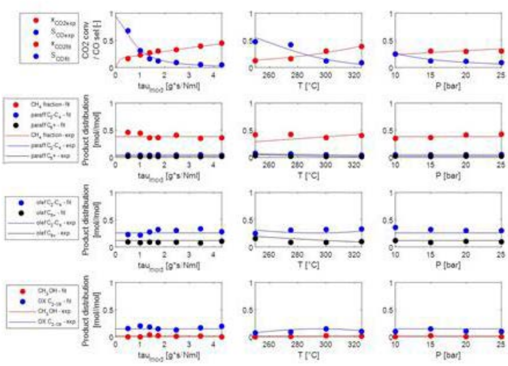

Figure 1: *Reaction behavior: experimental (points) and predicted by the macrokinetic model (lines) – Olef : Olefins / Paraff : paraffins / OX : Oxygenates*

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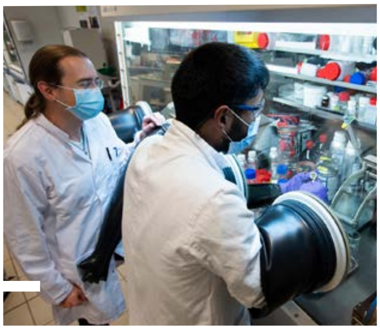
REFERENCE

[1] C. Panzone *et al.*, "Power-to-Liquid catalytic CO_2 valorization into fuels and chemicals: focus on the Fischer-Tropsch route", J. CO_2 Util., vol. 38 (2020) 314-347

SCIENTIFIC OUTPUTS

THE QUALITY OF SCIENTIFIC AND TECHNOLOGICAL SUCCESSES CAN BE ASSESSED IN THE LIGHT OF A WIDE SET OF METRICS. AT CEA-LITEN, WE VALUE OUR RESULTS THROUGH DEMONSTRATORS, PATENTS, INDUSTRIAL ACHIEVEMENTS, BUT ALSO SCIENTIFIC INDICATORS SUCH AS NEW HABILITATIONS (HDR), PHD DEFENSES AND PUBLICATIONS. A DETAILED DESCRIPTION OF THESE THREE KEY ELEMENTS IS PRESENTED IN THE FOLLOWING PAGES.



CONTENTS

2020 HDR DEFENSES AT LITEN

In 2020, five Liten researchers obtained habilitation to supervise PhD students from the French Ministry of Higher Education and Research. They spoke with us about what motivates them and how they approach supervising junior scientists.

Why is it so important to pass the Habilitation to supervise PhD students at Liten ?

Mikaël: If you want to supervise PhD research projects, the habilitation is a must. It is also a form of official recognition for the supervision many of us are already doing every day.

Cédric: The overriding objective is to share our knowledge with students and to lead them effectively in our work environment so that they can acquire the best possible research skills.

Caroline: The accreditation also raises your profile both within and outside of our organization.

Mikaël: If you are accredited, you can sit on thesis defense juries, which creates even more potential connections with the scientific community.

Jean-François: If you work on a lot of industrial R&D projects, the HDR allows you to keep "doing science" every day!

What made you decide to apply for habilitation

Caroline: Writing the required manuscript provided a great opportunity to review my many years of experience in materials science and to see the bigger picture in terms of my career.

Jean-François: Supervising PhD research is an important part of my work. I wanted to be able to do it independently.

Anass: Writing the manuscript of my research helped me consolidate my past experiences and orient my future work toward operando research.

What will you bring to the PhD candidates you supervise?

Cédric: As the official PhD supervisor, your role is to make sure the student's research is conducted properly in scientific terms; this is different from day-to-day supervision of experiments. You have to look at the student's approach from a broader and deeper perspective.

Jean-François: My goal is to help the students I work with stay curious. I also want to give them freedom and autonomy under my supervision.

Mikaël: The high-level supervision and day-to-day guidance both appeal to me. I plan to bring rigorous scientific research methods to my students' process in both cases.

Caroline: I want to help my students see their work within a broader context and to see the big picture in terms of the choices they have to make. I also want to help them publish their work.

Anass: For me, today's PhD students are tomorrow's colleagues! I want to share my professional network with my students so that they can build their own networks going forward.

Where do you see yourself in five years?

Cédric: I have been developing vacuum deposition processes for a number of years, and I am now shifting to plastronics processes. So, this is a crossroads for me professionally. I want to be able to share what I have learned with my new team and my new PhD students.

Mikaël: As a thesis supervisor you can guide and inspire. You can also help your students choose a course and stay on it amid the many opportunities they will be presented with. I hope that the maturity and insights I have gained through my own research will allow me to help my students choose their own path as early on as possible. The three years go by all too fast!

Jean-François: I have fifteen years of experience with lithium batteries. I want to share my knowledge with my students and be exposed to their new ideas, as well!

Any last words?

Mikaël: The HDR is also a commitment to Liten, as it gives the institute the ability to supervise PhD research independently. For the researcher, it takes real motivation. A lot of personal investment goes in to applying for the habilitation.

Cédric: The process has been very rewarding. Having the HDR will also create new opportunities, as part of the dissertations we supervise, to work with scientists outside the CEA and to get their insights on emerging breakthroughs.

Anass: We have to maintain this level of motivation as we pursue our work. We also have to keep working closely with our academic research partners.

Cédric Ducros

"The overriding objective is to share our knowledge with students and to lead them effectively in our work environment so that they can acquire the best possible research skills."

Anass Benayad

"Writing the review of my HDR manuscript helped me consolidate my past experiences and orient my future work toward operando research."

Jean-François Colin

"My goal is to help the students I work with stay curious. I also want to give them freedom and autonomy under my supervision."

Caroline Celle

"I want to help my students see their work within a broader context and to see the big picture in terms of the choices they have to make. I also want to help them publish their work."

Mikaël Cugnet

"I hope that the maturity and insights I have gained through my own research will allow me to help my students choose their own path as early on as possible. The three years go by all too fast!"

2020 PhD DEFENSES AT LITEN

PRODUCING DECARBONATED ENERGY

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12. **Contactless measurement of sheet resistance and mobility of inversion charge carriers on photovoltaic wafers**
    Korsos, F et al., Solar Energy Materials And Solar Cells, 10.1016/j.solmat.2020.110766
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    Becker, M et al., Solar Energy Materials And Solar Cells, 10.1016/j.solmat.2020.110817
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    Khenkin, MV et al., Nature Energy, 10.1038/s41560-019-0529-5
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Grenet, L et al., ACS Applied Energy Materials, 10.1021/acsaem.9b02329
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Le Baron, E et al., AIP Conference Proceedings, 10.1063/5.0028806
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Bourdon, D et al., AIP Conference Proceedings, 10.1063/5.0029639

SYSTEMS, GRIDS & ENERGY EFFICIENCY

32. **Experimental analysis of the hygrothermal performance of new aerogel-based insulating building materials in real weather conditions: Full-scale application study**
Béjat, T et al., Smart Innovation, Systems and Technologies, 10.1007/978-981-32-9868-2_57
33. **An efficient sensitivity analysis for energy performance of building envelope: A continuous derivative based approach**
Jumabekova, A et al., Building Simulation, 10.1007/s12273-020-0712-4
34. **Considering distribution grids and local flexibilities in the prospective development of the European power system by 2050**
Allard, S et al., Applied Energy, 10.1016/j.apenergy.2020.114958
35. **Natural ventilation potential from weather analyses and building simulation**
Sakiyama, NRM et al., Energy and Buildings, 10.1016/j.enbuild.2020.110596
36. **European transmission grid expansion as a flexibility option in a scenario of large scale variable renewable energies integration**
Allard, S et al., Energy Economics, 10.1016/j.eneco.2020.104733
37. **A multi-level Demand-Side Management algorithm for offgrid multi-source systems**
Roy, A et al., Energy, 10.1016/j.energy.2019.116536
38. **A multi-objective approach to the prospective development of the European power system by 2050**
Louis, JN et al., Energy, 10.1016/j.energy.2019.116539
39. **General form of consensus optimization for distributed OPF in HVAC-VSC-HVDC systems**
Aragues-Penalba, M et al., International Journal Of Electrical Power & Energy Systems, 10.1016/j.ijepes.2020.106049
40. **Searching an optimal experiment observation sequence to estimate the thermal properties of a multilayer wall under real climate conditions**
Jumabekova, A et al., International Journal Of Heat And Mass Transfer, 10.1016/j.ijheatmasstransfer.2020.119810
41. **Effect of moisture buffering on surface temperature variation: study of different indoor cladding materials**
Legros, C et al., 12th Nordic Symposium On Building Physics (NSB 2020), 10.1051/e3sconf/202017206002
42. **Experimental study of the combination of a positive input ventilation and active air vents on the air change rates of a house**
Leconte, A et al., International Journal of Ventilation, 10.1080/14733315.2020.1777017
43. **Controlling consumption to reduce stress on grid infrastructure while enhancing PV penetration**
Lucas, C et al., 6th IEEE International Energy Conference, ENERGYCon 2020, 10.1109/ENERGYCon48941.2020.9236567
44. **Robust hybrid control of parallel inverters for accurate power-sharing in microgrid**
Razi, R et al., Proceedings of the IEEE International Conference on Industrial Technology, 10.1109/ICIT45562.2020.9067116
45. **Power management in multi-microgrid system based on energy routers**
Pham, MC et al., Proceedings of the IEEE International Conference on Industrial Technology, 10.1109/ICIT45562.2020.9067200

46. **A co-simulation approach for validating agent-based distributed algorithms in smart grid**
Le, MT et al., 20th IEEE Mediterranean Electrotechnical Conference, MELECON 2020 - Proceedings, 10.1109/MELECON48756.2020.9140496

47. **Integration of SCADA Services and Power-Hardware-in-the-Loop Technique in Cross-Infrastructure Holistic Tests of Cyber-Physical Energy Systems**
Nguyen, VH et al., IEEE Transactions On Industry Applications, 10.1109/TIA.2020.3021365

48. **Real-Time Minimization Power Losses by Driven Primary Regulation in Islanded Microgrids**
Tran, QTT et al., Energies, 10.3390/en13020451

49. **Models for Short-Term Wind Power Forecasting Based on Improved Artificial Neural Network Using Particle Swarm Optimization and Genetic Algorithms**
Viet, DT et al., Energies, 10.3390/en13112873

50. **Stepwise Solar Methane Reforming and Water-Splitting via Lattice Oxygen Transfer in Iron and Cerium Oxides**
Chuayboon, S et al., Energy Technology, 10.1002/ente.201900415

51. **A numerical investigation of some key factors for the simulation of convection-dominated melting**
Beust, C et al., International Journal of Thermal Sciences, 10.1016/j.ijthermalsci.2020.106687

52. **Modeling of a cold thermal energy storage for the flexibility of thermal power plants coupled to Brayton cycles**
Mauger, G et al., Nuclear Engineering and Design, 10.1016/j.nucengdes.2020.110950

53. **Thermodynamic and economic evaluation of an innovative electricity storage system based on thermal energy storage**
Attonaty, K et al., Renewable Energy, 10.1016/j.renene.2019.11.087

54. **Predictive approach of heat transfer for the modelling of large-scale latent heat storages**
Beust, C et al., Renewable Energy, 10.1016/j.renene.2020.04.135

55. **Fault detection and diagnosis for large solar thermal systems: A review of fault types and applicable methods**
Faure, G et al., Solar Energy, 10.1016/j.solener.2020.01.027

56. **Steady and dynamical analysis of a combined cooling and power cycle**
Voeltzel, N et al., Thermal Science and Engineering Progress, 10.1016/j.tsep.2020.100650

57. **Multi-scale modelling of a large scale shell-and-tube latent heat storage system for direct steam generation power plants**
Beust, C et al., AIP Conference Proceedings, 10.1063/5.0028816

58. **Industrial scale CTES cold thermal energy storage: Demonstrator in La Africana CSP power plant and evaluation of benefits - Solwaris project**
Bruch, A et al., AIP Conference Proceedings, 10.1063/5.0028926

59. **Cold thermal energy storage (CTES) for water consumption reduction and performances increase of condenser cooling - WASCOP project**
Bruch, A et al., AIP Conference Proceedings, 10.1063/5.0028928

60. **Shell-and-Tube Heat Exchanger Geometry Modification: An Efficient Way to Mitigate Fouling**
Chambon, A et al., Heat Transfer Engineering, 10.1080/01457632.2018.1522093

61. **RBF-based mesh morphing improvement using Schur complement applied to rib shape optimization**
Mastrippolito, F et al., International Journal Of Numerical Methods For Heat & Fluid Flow, 10.1108/HFF-06-2018-0309

62. **Numerical studies of a hybrid cycle for power production and cooling**
Voeltzel, N et al., Proceedings of the ISES Solar World Congress 2019 and IEA SHC International Conference on Solar Heating and Cooling for Buildings and Industry 2019, 10.18086/swc.2019.55.11

63. **Basic Analysis of Uncertainty Sources in the CFD Simulation of a Shell-and-Tube Latent Thermal Energy Storage Unit**
Konig-Haagen, A et al., Applied Sciences-Basel, 10.3390/app10196723

ENERGY STORAGE & FLEXIBILITY SOLUTIONS

64. **Towards a circular supply chain for PV modules: Review of today's challenges in PV recycling, refurbishment and re-certification**
Tsanakas, JA et al., Progress In Photovoltaics, 10.1002/pip.3193

65. **Techno-economic planning of local energy systems through optimization models: a survey of current methods**
Cuisinier, E et al., International Journal of Energy Research, 10.1002/er.6208

66. **Probabilistic deconvolution of solid oxide fuel cell impedance spectra**
Dolenc, B et al., Lecture Notes in Electrical Engineering, 10.1007/978-3-030-56970-9_3

67. **Coupling electrochemical impedance spectroscopy and model-based aging estimation for solid oxide fuel cell stacks lifetime prediction**
Gallo, M et al., Applied Energy, 10.1016/j.apenergy.2020.115718

68. **Accounting for techno-economic parameters uncertainties for robust design of remote microgrid**
Nadal, A et al., International Journal Of Electrical Power & Energy Systems, 10.1016/j.ijepes.2019.105531

69. **Durability of nanostructured LaPrNiO4+delta electrode for solid oxide cells: Electrochemical, microstructural, and structural investigation**
Khamidy, NI et al., Journal Of Power Sources, 10.1016/j.jpowsour.2020.227724

70. **Particle-based model for functional and diffusion layers of solid oxide cells electrodes**
Moussaoui, H et al., Powder Technology, 10.1016/j.powtec.2020.03.040

71. **A New Conducting Copolymer Bearing Electro-Active Nitroxide Groups as Organic Electrode Materials for Batteries**
Assumma, L et al., Chemsuschem, 10.1002/cssc.201903313

72. **Pairing Cross-Linked Polyviologen with Aromatic Amine Host Structure for Anion Shuttle Rechargeable Batteries**
Cadiou, V et al., Chemsuschem, 10.1002/cssc.201903578

73. **Organic Liquid Crystals as Single-Ion Li(+)Conductors**
Bresser, D et al., Chemsuschem, 10.1002/cssc.202001995

74. **Fault Detection and Isolation for Proton Exchange Membrane Fuel Cell Using Impedance Measurements and Multiphysics Modeling**
Jullian, G et al., Fuel Cells, 10.1002/fuce.202000022

75. **Ante-mortem analysis, electrical, thermal, and ageing testing of state-of-the-art cylindrical lithium-ion cells**
Popp, H et al., Elektrotechnik und Informationstechnik, 10.1007/s00502-020-00814-9

76. **Electrochemical impedance spectroscopy study of lithium–sulfur batteries: Useful technique to reveal the Li/S electrochemical mechanism**
Waluś, S et al., Electrochimica Acta, 10.1016/j.electacta.2020.136944

77. **Prelithiation of silicon/graphite composite anodes: Benefits and mechanisms for long-lasting Li-Ion batteries**
Berhaut, CL et al., Energy Storage Materials, 10.1016/j.ensm.2020.04.008

78. **Post-Mortem Analysis of Lithium-Ion Capacitors after Accelerated Aging Tests**
El Ghossein, N et al., Journal of Energy Storage, 10.1016/j.est.2020.102039

79. **Simplified anode architecture for PEMFC systems based on alternative fuel feeding: Experimental characterization and optimization for automotive applications**
Rodosik, S et al., International Journal of Hydrogen Energy, 10.1016/j.ijhydene.2020.05.014

80. **Practical implementation of Li doped SiO in high energy density 21700 cell**
Reynier, Y et al., Journal Of Power Sources, 10.1016/j.jpowsour.2020.227699

81. **Operando investigation of the lithium/sulfur battery system by coupled X-ray absorption tomography and X-ray diffraction computed tomography**
Tonin ,G et al., Journal of Power Sources, 10.1016/j.jpowsour.2020.228287

82. **Lithium-ion batteries - Current state of the art and anticipated developments**
Armand, M et al., Journal Of Power Sources, 10.1016/j.jpowsour.2020.228708

83. **Influence of electrolyte composition on high energy lithium metal cells**
Mercier-Guyon, B et al., Solid State Ionics, 10.1016/j.ssi.2020.115321

84. **Evaluation of chemical stability of conducting ceramics to protect metallic lithium in Li/S batteries**
Castro, L et al., Solid State Ionics, 10.1016/j.ssi.2020.115402

85. **Influence of Electrolyte Additives on the Degradation of Li2VO2F Li-Rich Cathodes**
Kallquist, I et al., Journal Of Physical Chemistry C, 10.1021/acs.jpcc.0c02840

86. **Fingerprinting Mean Composition of Lithium Polysulfide Standard Solutions by Applying High-Energy Resolution Fluorescence Detected X-ray Absorption Spectroscopy**
Robba, A et al., Journal Of Physical Chemistry Letters, 10.1021/acs.jpclett.0c01120

87. **Stabilization of Li-Rich Disordered Rocksalt Oxyfluoride Cathodes by Particle Surface Modification**
Naylor, AJ et al., ACS Applied Energy Materials, 10.1021/acsaem.0c00839

88. **In Situ Measurement of Ionomer Water Content and Liquid Water Saturation in Fuel Cell Catalyst Layers by High-Resolution Small-Angle Neutron Scattering**
Lee, J et al., ACS Applied Energy Materials, 10.1021/acsaem.0c00853

89. **Impact of Silicon/Graphite Composite Electrode Porosity on the Cycle Life of 18650 Lithium-Ion Cell**
Profatilova, I et al., ACS Applied Energy Materials, 10.1021/acsaem.0c01999

90. **Degradation Mechanisms of Supported Pt Nanocatalysts in Proton Exchange Membrane Fuel Cells: An Operando Study through Liquid Cell Transmission Electron Microscopy**
Impagnatiello, A et al., ACS Applied Energy Materials, 10.1021/acsaem.9b02000

91. **A Scalable Silicon Nanowires-Grown-On-Graphite Composite for High-Energy Lithium Batteries**
Karuppiah, S et al., ACS Nano, 10.1021/acsnano.0c05198

92. **Closing the loop: life cycle assessment and optimization of a PEMFC platinum-based catalyst recycling process**
Duclos, L et al., Green Chemistry, 10.1039/c9gc03630j

93. **On The Impact of the Locality on Short-Circuit Characteristics: Experimental Analysis and Multiphysics Simulation of External and Local Short-Circuits Applied to Lithium-Ion Batteries**
Sturm, J et al., Journal Of The Electrochemical Society, 10.1149/1945-7111/ab8873

94. **Impact of Lithium-Ion Cell Condition on Its Second Life Viability**
Coron, E et al., Journal Of The Electrochemical Society, 10.1149/1945-7111/aba703

95. **Probing Silicon Lithiation in Silicon-Carbon Blended Anodes with a Multi-Scale Porous Electrode Model**
Lory, PF et al., Journal Of The Electrochemical Society, 10.1149/1945-7111/abaa69

96. **Review of optimization methods for the design of power electronics systems**
Delhommais M. et al., 2020 22nd European Conference on Power Electronics and Applications, 10.23919/EPE20ECCEEurope43536.2020.9215683

97. **Smart fuel cell module (6.5 kW) for a range extender application**
Bazin, P et al., 2020 22nd European Conference on Power Electronics and Applications, 10.23919/EPE20ECCEEurope43536.2020.9215856

98. **Modelling Carbon Corrosion during a PEMFC Startup: Simulation of Mitigation Strategies**
Randrianarizafy, B et al., Energies, 10.3390/en13092338

99. **Unraveling the properties of biomass-derived hard carbons upon thermal treatment for a practical application in Na-ion batteries**
Saavedra Rios, CDM et al., Energies, 10.3390/en13143513

100. **Looking Inside Polymer Electrolyte Membrane Fuel Cell Stack Using Tailored Electrochemical Methods**
Piela, Piotr et al., Journal of Electrochemical Energy Conversion and Storage, doi.org/10.1115/1.4046106

101. **Nano-Architectured Composite Anode Enabling Long-Term Cycling Stability for High-Capacity Lithium-Ion Batteries**
Kumar, P et al., Small, 10.1002/smll.201906812

102. **Study of (La,Sr)(Ti,Ni)O$_{(3\text{-delta})}$ materials for symmetrical Solid Oxide Cell electrode - Part B: Conditions of Ni exsolution**
Arrive, C et al., Ceramics International, 10.1016/j.ceramint.2019.11.034

103. **Study of (La,Sr)(Ti,Ni)O_3-delta materials for symmetrical Solid Oxide Cell electrode - Part C: Electrical and electrochemical behavior**
Arrive, C et al., Ceramics International, 10.1016/j.ceramint.2020.06.114

104. **Lithium-rich layered titanium sulfides: Cobalt- and Nickel-free high capacity cathode materials for lithium-ion batteries**
Flamary-Mespoulie, F et al., Energy Storage Materials, 10.1016/j.ensm.2019.12.033

105. **Integration of life cycle assessment with energy simulation software for polymer exchange membrane (PEM) electrolysis**
Sharma, H et al., Procedia CIRP, 10.1016/j.procir.2020.02.139

106. **New Interpretation of X-ray Photoelectron Spectroscopy of Imidazolium Ionic Liquid Electrolytes Based on Ionic Transport Analyses**
Morales-Ugarte, JE et al., Journal Of Physical Chemistry B, 10.1021/acs.jpcb.0c04090

CIRCULAR ECONOMY & MATERIALS

107. Experimental and CFD investigation of inert bed materials effects in a high-temperature conical cavity-type reactor for continuous solar-driven steam gasification of biomass
Boujjat, H et al., Chemical Engineering Science, 10.1016/j.ces.2020.115970

108. Power-to-Liquid catalytic CO_2 valorization into fuels and chemicals: Focus on the Fischer-Tropsch route
Panzone, C et al., Journal of CO2 Utilization, 10.1016/j.jcou.2020.02.009

109. Solar chemical looping reforming of methane combined with isothermal H2O/CO2 splitting using ceria oxygen carrier for syngas production
Chuayboon, S et al., Journal Of Energy Chemistry, 10.1016/j.jechem.2019.05.004

110. Modelling the sintering of nickel particles supported on γ-alumina under hydrothermal conditions
Champon, I et al., Catalysts, 10.3390/catal10121477

111. Fluidised Bed Gasification of Diverse Biomass Feedstocks and Blends-An Overall Performance Study
Valin, S et al., Energies, 10.3390/en13143706

112. Solar-hybrid Thermochemical Gasification of Wood Particles and Solid Recovered Fuel in a Continuously-Fed Prototype Reactor
Boujjat, H et al., Energies, 10.3390/en13195217

113. Biomass steam gasification kinetics: relative impact of char physical properties vs. inorganic composition
Dahou, T et al., Biomass Conversion and Biorefinery, 10.1007/s13399-020-00894-9

114. Towards understanding the role of K during biomass steam gasification
Dahou, T et al., Fuel, 10.1016/j.fuel.2020.118806

115. Test blanket modules (ITER) and breeding blanket (DEMO): History of major fabrication technologies development of HCLL and HCPB and status
Forest, L et al., Fusion Engineering And Design, 10.1016/j.fusengdes.2020.111493

116. Performance assessment of thick W/Cu graded interlayer for DEMO divertor target
Richou, M et al., Fusion Engineering And Design, 10.1016/j.fusengdes.2020.111610

117. Dynamic simulation and control of solar biomass gasification for hydrogen-rich syngas production during allothermal and hybrid solar/autothermal operation
Boujjat, H et al., International Journal Of Hydrogen Energy, 10.1016/j.ijhydene.2020.01.072

118. Waste wood characterization and combustion behaviour in pilot lab scale
Gehrmann, HJ et al., Journal Of The Energy Institute, 10.1016/j.joei.2020.02.001

119. Study of the elaboration of high entropy material from powder by laser additive manufacturing
Huser, G et al., Procedia CIRP, 10.1016/j.procir.2020.09.051

120. On the path toward day and night continuous solar high temperature thermochemical processes: A review
Rodat, S et al., Renewable & Sustainable Energy Reviews, 10.1016/j.rser.2020.110061

121. Combustion-assisted solar gasification of biomass particles in a high temperature conical jet spouted bed reactor
Boujjat, H et al., AIP Conference Proceedings, 10.1063/5.0028585

122. Effect of hydrogen content in natural gas blend on the mechanical properties of a L485-MB low-alloyed steel
Ez-Zaki, H et al., American Society of Mechanical Engineers, Pressure Vessels and Piping Division, 10.1115/PVP2020-21746

123. Solar Biomass Gasification Combined With Iron Oxide Reduction for Syngas Production and Green Iron Metallurgy
Bellouard, Q et al., Frontiers In Energy Research, 10.3389/fenrg.2020.00066

124. Joining of Oxide Dispersion-Strengthened Steel Using Spark Plasma Sintering
Naimi, F et al., Metals, 10.3390/met10081040

125. Transparent Heaters: A Review
Papanastasiou, DT et al., Advanced Functional Materials, 10.1002/adfm.201910225

126. Impact of Morphology on Charge Carrier Transport and Thermoelectric Properties of N-Type FBDOPV-Based Polymers
Bardagot, O et al., Advanced Functional Materials, 10.1002/adfm.202000449

127. Moving Ions Vary Electronic Conductivity in Lead Bromide Perovskite Single Crystals through Dynamic Doping
Garcia-Batlle, M et al., Advanced Electronic Materials, 10.1002/aelm.202000485

128. Flexible large-area multi-fingerprint sensors based on thermal mass detection
Roose, FD et al., Digest of Technical Papers - SID International Symposium, 10.1002/sdtp.13831

129. Selective Laser Melting of $Al_{0.3}CoCrFeNi$ High Entropy Alloy: Printability, Microstructure, and Mechanical Properties
Peyrouzet, F et al., JOM, 10.1007/s11837-020-04149-w

130. A unified electrical model based on experimental data to describe electrical transport in carbon nanotube-based materials
Dini, Y et al., Nano Research, 10.1007/s12274-020-2803-z

131. A solution to the hot cracking problem for aluminium alloys manufactured by laser beam melting
Opprecht, M et al., Acta Materialia, 10.1016/j.actamat.2020.07.015

132. Large improvement of CNT yarn electrical conductivity by varying chemical doping and annealing treatment
Dini, Y et al., Carbon, 10.1016/j.carbon.2019.09.022

133. Growth, charge and thermal transport of flowered graphene
Cresti, A et al., Carbon, 10.1016/j.carbon.2020.01.040

134. Y-TZP, Ce-TZP and as-synthesized Ce-TZP/Al_2O_3 materials in the development of high loading rate digital light processing formulations
Cailliet, S et al., Ceramics International, 10.1016/j.ceramint.2020.09.251

135. Deterioration mechanism of insulated circuit substrates in thermoelectric modules operating at medium–high temperatures in air atmosphere
Arai, K et al., Engineering Failure Analysis, 10.1016/j.engfailanal.2020.105088

136. Use of composite voxels in FFT based elastic simulations of hollow glass microspheres/polypropylene composites
Chariere, R et al., International Journal Of Solids And Structures, 10.1016/j.ijsolstr.2019.08.002

137. Experimental measurements of the residual solidification duration of a supercooled sodium acetate trihydrate
Beaupere, N et al., International Journal of Thermal Sciences, 10.1016/j.ijthermalsci.2020.106544

138. The necessity of investigating a freshwater-marine continuum using a mesocosm approach in nanosafety: The case study of TiO_2 MNM-based photocatalytic cement
Chatel, A et al., Nanoimpact, 10.1016/j.impact.2020.100254

139. Stability and thermoelectric performance of doped higher manganese silicide materials solidi fied by RGS (ribbon growth on substrate) synthesis
Pichon, PY et al., Journal Of Alloys And Compounds, 10.1016/j.jallcom.2020.154602

140. Thermal stability of $Mg_2Si_{0.55}Sn_{0.45}$ for thermoelectric applications
Mejri, M et al., Journal Of Alloys And Compounds, 10.1016/j.jallcom.2020.156413

141. Effect of contact alignment on shrinkage anisotropy during sintering: Stereological model, discrete element model and experiments on NdFeB compacts
Hugonnet, B et al., Materials & Design, 10.1016/j.matdes.2020.108575

142. High performance metallic joints from screen-printed Cu@Ag nanopastes
Michaud, T et al., Materialia, 10.1016/j.mtla.2020.100871

143. Photocurrent deviation from linearity in an organic photodetector due to limited hole transport layer conductivity
Euvrard, J et al., Organic Electronics, 10.1016/j.orgel.2019.105450

144. Progress in understanding structure and transport properties of PEDOT-based materials: A critical review
Gueye, MN et al., Progress In Materials Science, 10.1016/j.pmatsci.2019.100616

145. Lifecycle modeling for the eco design of the Internet of Things
Quisbert-Trujillo, E et al., Procedia CIRP, 10.1016/j.procir.2020.02.120

146. Unraveling the mechanism behind air instability in thin semiconducting polymer layers p-doped with molybdenum dithiolene complexes
Nunes Domschke, T et al., Synthetic Metals, 10.1016/j.synthmet.2019.116251

147. Optimization of the Growth Conditions for High Quality $CH_3NH_3PbBr_3$ Hybrid Perovskite Single Crystals
Amari, S et al., Crystal Growth & Design, 10.1021/acs.cgd.9b01429

148. Probing the Electronic Structure of Hybrid Perovskites in the Orientationally Disordered Cubic Phase
Nandi, P et al., Journal Of Physical Chemistry Letters, 10.1021/acs.jpclett.0c01386

149. Safer-by-design biocides made of tri-thiol bridged silver nanoparticle assemblies
Marchioni, M et al., Nanoscale Horizons, 10.1039/c9nh00286c

150. Combined treatment of phonon scattering by electrons and point defects explains the thermal conductivity reduction in highly-doped Si
Dongre, B et al., Journal of Materials Chemistry A, 10.1039/c9ta11424f

151. Spray-coated PEDOT:OTf films: thermoelectric properties and integration into a printed thermoelectric generator
Yvenou, E et al., Materials Chemistry Frontiers, 10.1039/d0qm00265h

152. Twofold advantage of gas bubbling for the advanced solvothermal preparation of efficient YAG:Ce nanophosphors
Cantarano, A et al., Journal Of Materials Chemistry C, 10.1039/d0tc02347g

153. Modeling of demagnetization processes in permanent magnets measured in closed-circuit geometry
Fliegans, J et al., Applied Physics Letters, 10.1063/1.5134561

154. Effect of thermal annealing on the morphology of sol-gel processed barium strontium titanate thin films: Consequences on electrical properties
Mansour, C et al., AIP Advances, 10.1063/5.0007242

155. An insight into the charge carriers transport properties and electric field distribution of CH3NH3PbBr3 thick single crystals
Baussens, O et al., Applied Physics Letters, 10.1063/5.0011713

156. **Integrated thermoelectric sensors based on quantum dot superlattice for thermal management applications**
Savelli, G et al., Journal of Physics D: Applied Physics, 10.1088/1361-6463/aba310

157. **Fabrication and characterization of sensitive vertical P-i-N germanium photodiodes as infrared detectors**
Aliane, A et al., Semiconductor Science and Technology, 10.1088/1361-6641/ab6bf7

158. **Anisotropy and temperature dependence of the spin-wave stiffness in Nd_2Fe_{14} B: An inelastic neutron scattering investigation**
Naser, H et al., Physical Review B, 10.1103/PhysRevB.102.014443

159. **Long- To short-junction crossover and field-reentrant critical current in Al/Ag-nanowires/Al Josephson junctions**
Murani, A et al., Physical Review B, 10.1103/PhysRevB.102.214506

160. **Relativistic stable processes in quasiballistic heat conduction in semiconductors**
Chakraborty, P et al., Physical Review E, 10.1103/PhysRevE.101.042110

161. **High-throughput study of the static dielectric constant at high temperatures in oxide and fluoride cubic perovskites**
Van Roekeghem, A et al., Physical Review Materials, 10.1103/PhysRevMaterials.4.113804

162. **A Fully-Printed Organic Smart Temperature Sensor for Cold Chain Monitoring Applications**
Fattori, M et al., Proceedings of the Custom Integrated Circuits Conference, 10.1109/CICC48029.2020.9075908

163. **Parameter Extraction and Compact Modeling of OTFTs From 150 K to 350 K**
Cortes-Ordonez, H et al., IEEE Transactions On Electron Devices, 10.1109/TED.2020.3032082

164. **Soft Ferrite Material by Powder Injection Molding Process for Power Electronics**
Soupremanien, U et al., IEEE Transactions On Magnetics, 10.1109/TMAG.2020.3027248

165. **Compensation of disorder for extraordinary optical transmission effect in nanopore arrays fabricated by nanosphere photolithography**
Ushkov, A et al., Optics Express, 10.1364/OE.408772

166. **Powder Injection Molding in the Fabrication of Soft Ferrite material for Power Electronics**
Ngoua-Teu, JS et al., 2020 22nd European Conference on Power Electronics and Applications, 10.23919/EPE20ECCEEurope43536.2020.9215957

167. **Dispersion and Stabilization of Exfoliated Graphene in Ionic Liquids**
Bordes, E et al., Frontiers In Chemistry, 10.3389/fchem.2020.00556

168. **Corrigendum: Assessing Sunscreen Lifecycle to Minimize Environmental Risk Posed by Nanoparticulate UV-Filters – A Review for Safer-by-Design Products**
Labille, J et al., Frontiers in Environmental Science, 10.3389/fenvs.2020.597861

169. **Experimental Devices to Investigate the Long-Term Stability of Phase Change Materials under Application Conditions**
Rathgeber, C et al., Applied Sciences-Basel, 10.3390/app10227968

170. **Influences of nanoparticles characteristics on the cellular responses: The example of iron oxide and macrophages**
Dalzon, B et al., Nanomaterials, 10.3390/nano10020266

171. **Key role of the dispersion of carbon nanotubes (Cnts) within epoxy networks on their ability to release**
Pras, M et al., Polymers, 10.3390/polym12112530

172. **Water content control during solution-based polymerization: a key to reach extremely high conductivity in PEDOT thin films**
Schultheiss, A et al., Journal Of Materials Chemistry C, 10.1039/d0tc04899b

173. **An electrochemical method to rapidly assess the environmental risk of silver release from nanowire transparent conductive films**
Omaña-Sanz, B et al., Nanoimpact, 10.1016/j.impact.2020.100217

174. **Insight into the Degradation Mechanisms of Highly Conductive Poly(3,4-ethylenedioxythiophene) Thin Films**
Schultheiss, A et al., ACS Applied Polymer Materials, 10.1021/acsapm.0c00301

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