

SCIENTIFIC REPORT 2019



Director's foreword

The year 2019 was marked by some major energy transition milestones. The European Green Deal was set up, effectively transforming the EU's ambition of sustainable growth and a more equitable economy into policy – one that includes an unprecedented bid to transform Europe into the world's first carbon-neutral bloc by 2050. Guided by an integrated and carbon-free vision of tomorrow's energy systems, CEA-Liten's research, development, and innovation programs are closely aligned with the carbon-neutral movement.

In 2019 our scientists studied renewable energy production and storage, drove advances in the integration of renewable energy into interconnected and interoperable grids, and investigated new and highly energy efficient use cases. Our R&D approach – from proof-of-concept to pre-production prototype – incorporates circular economy principles to ensure that our technologies are environmentally relevant.

Our capacity to take technologies through to the demonstrator stage won us several awards in 2019. Our Li-ion battery recycling process earned a *Trophées d'Innovation Recyclage* grand prize. CEA-Liten startup Power Up won the Cleantech Open France competition for its connected mobile battery life extender built on a charge-optimizing algorithm.

CEA-Liten also continued to cultivate a culture of excellence in science and technology, nurturing 145 PhD students who defended 33 dissertations in 2019, publishing nearly 200 articles in peer-reviewed journals, and filing 210 patents throughout the year. And, with an additional three CEA-Liten scientists earning the accreditation to supervise research, a total of 38 of our staff now hold this habilitation.

Our partnerships with academic institutions in France, Europe, and around the world grew stronger in 2019. We set up two new joint research units: one with G2Elab (UMR CNRS 5269) on smartgrids, and another with LEPMI (UMR CNRS 5279) on PEMFCs. We extended our partnership with ITRI in Taiwan and started a new one on materials for energy with AIST in Japan.

Together, these initiatives and results – within our broader mission of scientific excellence and economic value creation – helped CEA-Liten getting appreciable positive and constructive feedback from HCERES, French High Council for Higher Education and Research Evaluation.

This year's Scientific Report showcases our R&D over the past year – work that allowed us to make some very real scientific advances that will undoubtedly shape tomorrow's energy landscape.



Florence Lambert,
CEA-Liten CEO



Florence Lefebvre-Joud,
Deputy Director for Science



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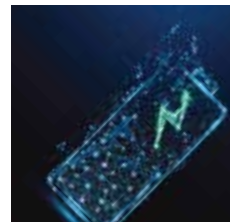
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SCIENTIFIC OUTPUTS



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

We work on projects at different stages in the lifecycle of a given technology with partners from 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 laboratory prototype to functional demonstrator at a scale representative of the target application.

At Liten, 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. This year's Scientific Report is organized around three R&D pillars. For each pillar, you will find an in-depth article on the evolution of our research on a flagship topic that generated major results in 2019, followed by three significant results selected to give you deeper understanding of the kinds of scientific and technological advances happening at CEA-Liten.

- The first pillar, solar photovoltaic energy, stood out in 2019 namely due to our research on perovskite-on-silicon tandem cells at an industrial scale. We made progress on the mechanical resistance of silicon wafers regardless of thickness, validated tests suitable for PV components for space applications, and more effectively controlled the trapping of impurities within silicon cells using passivated contacts.
- Energy grids is our second pillar, with two focuses: energy grid management and energy storage. The first in-depth article is on the interoperability of

grids and cities, and describes our cyberphysical-systems approach to this challenge. We also present the results of our investigations into the impact of electricity storage on variable supply-side and demand-side management for isolated maritime regions and the impact of energy storage on multi-energy grids. The second in-depth article explores our research on Li-ion batteries and our advances toward 100% solid-state batteries. We also achieved significant results in the field of hydrogen, another one of our flagship topics, developing new composite electrode materials for solid-oxide electrolysis cells, 3D modelling of heterogeneous water distribution in fuel cells, and *operando* characterization of fuel cells on large scientific instruments.

- Energy efficiency, our third pillar, was marked by research to reduce the critical elements used in magnetic materials for energy applications. Our other results included using modelling to optimize fluidized-bed thermal storage systems, developing models of low-tech, low-cost closed-loop turbocompressor electricity production systems to respond to spikes in demand for residential applications.

This year's Scientific Report offers up an in-depth look at the three pillars outlined above and a complete panorama of all of our publications in 2019, our PhD candidates' dissertations, and awards that will raise CEA-Liten's profile in our flagship research areas.

CEA-Liten was evaluated by HCERES, French High Council for Higher Education and Research Evaluation, in 2019. The audit provided us with an opportunity to perform a quantitative and qualitative assessment of our research, development, and innovation activities over a five-year period (2014 to 2018) and present our strategy for the next five years (2019 to 2023).

The evaluation committee was selected to ensure a clear understanding of our science and technology strategies. The majority of the evaluators appointed by HCERES were academic researchers; several represented international organizations and industrial companies. After reviewing our self-evaluation documents and spending three days on site in early December, the committee released its report*.

This exhaustive review by an external informed panel provided us with several key insights into our scientific strategy. Several areas for progress were pointed out – ones that will generate internal projects to help us help our scientists get published, raise our profile internationally, improve our educational programs, and build more partnerships with academic research labs.

We received positive feedback for the clarity and relevance of our research positioning, and congratulations for our *“unique place in the French research landscape, downstream from the universities and CNRS (France’s national center for scientific research), similar to CEA-Liten’s European peers like Fraunhofer in Germany and international research organizations like NREL (the National Renewable Energy Laboratory) in the United States.”*** CEA-Liten’s *“outstanding ability to respond to industrial R&D demand with a brisk contract R&D business”* was also commended. Finally, the evaluators deemed our strategy for the next five years *“excellent”*, stating that our *“priorities are clearly articulated and are relevant to the context of climate change.”*

*<https://www.hceres.fr/fr/rechercher-une-publication/liten-laboratoire-dinnovation-pour-les-technologies-des-energies-o>

** Direct translation of the HCERES report.



RENEWABLE ENERGY PRODUCTION

LITEN'S R&D CAPABILITIES COVER THE ENTIRE PHOTOVOLTAIC COMPONENT VALUE CHAIN. THE INSTITUTE LEVERAGES INDUSTRIAL-GRADE EQUIPMENT TO OBTAIN YIELDS OF 25% ON SILICON AND – ULTIMATELY – YIELDS OF 30% WITH TANDEM TECHNOLOGIES. LITEN IS DRIVING ADVANCES IN MORE THAN JUST COMPONENTS. THE INSTITUTE ALSO DEVELOPS INNOVATIVE SYSTEM ARCHITECTURES DESIGNED TO BRING CONVENTIONAL “ON-THE-GROUND” SOLAR POWER PLANTS TO GREATER LEVELS OF PRODUCTIVITY AND TO SUPPORT THE EXPANSION OF PV INTO BUILDINGS, INDUSTRIAL PARKS, VEHICLES, AND ALONG ROADS AND RAILWAYS.

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FROM PEROVSKITE MATERIAL TOWARDS TANDEM PV CELLS ON SILICON

The global Photovoltaic (PV) Market has witnessed an annual growth rate of 24% between 2010 and 2017¹. To fulfill the strategic climate goals the PV-markets in both Europe and the rest of the world will continue to grow between 10% and 30% up to 2030². In order to enable the realization of this gigantic PV deployment, improved, new and widely accepted PV technologies will be required, besides the current existing PV technologies. The LCoE (Levelized Cost of Electricity) of PV is already competitive and in some cases even the lowest as compared to other existing energy harvesting sources.

There is a large room for improvement for which new generation PV technologies are needed to further reduce costs as well as to overcome the current theoretical efficiency limits. Hybrid perovskites are a class of low cost semiconducting materials, which has been the subject of very active scientific investigations in the last decade. The potentials of lower cost, high conversion efficiency, easy integration, low carbon emissions lifetime as well as higher recyclability are the merits that perovskite (PK) based PV have and is ideally positioned to deliver and therefore constitute the best candidate to become the next generation PV technology. The worldwide experiences gathered in thin film PV technologies last decades as well as the unique chemical properties of perovskite material allowed its efficiencies to increase from 3.8% at its discovery in 2009 to an astonishing 25.2%³ in 2019 in a single-junction architecture turning it into the fastest-advancing solar technology to date. Beside these developments, Perovskite materials can also be combined to silicon solar cells leading to highly efficient tandem architecture with target of 30% PV efficiencies. At CEA-Liten, we chose the combination of perovskite technology with the silicon heterojunction one to develop the next premium generation of silicon solar cells. We expose below our recent achievements. The first part describes the control of the crystallization of the perovskite material leading to high efficiency single junction devices and the second part, the tandem integration into the silicon cell.

CONTROL OF THE CRYSTALLIZATION OF THE PEROVSKITE LAYER

While impressive record efficiencies, up to 25%, are now achieved in single cells, a number of challenges are still to be met to ensure a bright industrial future for perovskite solar cells (PSCs). Device area increase, process upscaling and long-term stability are arguably among the most important ones as of today.

For instance, while few groups have been able to demonstrate large scale PSCs, most of the worldwide current research is indeed focusing on small area lab-scale devices ($\ll 1 \text{ cm}^2$). Significantly improving device area without sacrificing efficiency first relies on the crystallization control of the perovskite too (e.g. absorption, crystallinity, grain size). From the practical

point of view, this was achieved for a multi-cation multi-halide perovskite $\text{FA}_x\text{Cs}_{(1-x)}\text{Pb}(\text{I}_y\text{Br}_{(1-y)})_3$ via joint optimization of SnO_2 layer [1] on which perovskite is formed, and of perovskite deposition process. Thanks to structural and chemical characterizations [T1], we have evidenced the influence of the chemical composition of the transport layer surface on the perovskite microstructure, as well as the complexity of the formation mechanisms of the perovskite [2,3]. These studies also strongly benefited to the degradation understanding and hence, stability improvement. As of today, good thermal and photochemical behavior with limited degradation *i.e.* 20% loss at 1000h (mostly initial burn-in then a plateau) and less than 10% losses at 1200h, respectively are achieved.

When going from cells to modules (Figure 1), we also tackled a variety of challenges to realize efficient devices. Building upon some previous knowledge from OPV (organic photovoltaics), a laser scribing protocol was developed ensuring high selectivity and registration accuracy. The serial association of the multiple cells was optimized through contact resistivity measurements and geometrical design was tuned through resistive power losses calculations. All this work culminated in the realization of about 10 cm^2 module yielding efficiency in excess to 20% with high active area ratio ($> 93\%$). To our knowledge, this represents the current state-of-the-art. Perovskite material developments (e.g. 2D perovskite passivation, chlorine incorporation, ionic liquids) will be envisaged to try and further improve efficiency and stability.

1 / <https://www.ise.fraunhofer.de/content/dam/ise/de/documents/publications/studies/Photovoltaics-Report.pdf>
 2 / <http://itrpvdma.org/documents/27094228/29066965/ITRPVo2019.pdf/78cb7c8c-e91d-6f41-f228-635c3a8abf71>
 3 / <https://www.nrel.gov/pv/cell-efficiency.html>

Regarding the process upscaling, a gas-knife assisted slot-die coating process enabling fast and parsimonious formation of high quality perovskite films is developed to replace spin coating in the framework of a joint PhD scholarship with Nanyang Technological University at Singapore [T2]. In such an approach, the interplay between ink formulation and quenching conditions is of paramount importance. We built an in-house quenching system and tuned ink composition - more specifically increasing the Caesium content - to reach pinhole-free perovskite films showing high absorbance and appropriate crystallinity and grain morphology. This resulted in the realization of proof-of-concepts small-scale devices with efficiency higher than 16 % [4]. Further work is needed to improve large-scale homogeneity to pave the way to realization of large area devices.

DEVELOPMENT OF TANDEM INTEGRATION ON SILICON SOLAR CELLS

Similarly impressive were the improvements of silicon/perovskite tandem devices culminating today at 29.1% with a certified record efficiency from HZB⁴. However, there is a lag between the improvements in single junction and those in tandem devices. This may stem from additional challenges posed by the two-terminal tandem architecture integration:

First, in the two-terminal architecture, where the sub-cells are serially connected, current density of both sub-cells must be balanced and maximized. This implies a rigorous management of optical processes occurring within the whole stack. The challenge is to maximize photon absorption in both sub-cells by playing on absorbers' band-gap, thickness, and optical indices of each layer, in order to minimize parasitic absorption and reflection.

Secondly, from the processing point of view, the perovskite top cell has to be fabricated directly on the silicon bottom cell. One of the major challenge of the tandem integration is to find a perovskite deposition process that is compatible with the textured silicon surface or to adapt the silicon surface morphology. Also, in most devices, the sub-cells are connected via a so called tunnel/recombination junction (TRJ) [T3], [5] that may have different surface properties from the classical electrode used in single junction (SJ) PK devices (nature, surface, roughness, wettability). This may necessitate important process modifications for adapting the perovskite cell in a tandem structure.

Third, scaling up perovskite solar cells is challenging as evidenced by the difference in record efficiency between 1 cm² cells and 0.1 cm² cells, 21.6 vs 25.2%⁵. This relates to the difficulty of depositing very thin contact layers void of any defects that would cause local shunts. Tandem devices are usually larger than 1 cm² because smaller devices would suffer from extra recombination in the non-illuminated area because of the conductivity of silicon.

Fourth, record SJ PK devices feature full rear metallic electrode to reflect light and enhance absorption and to minimize resistive losses. Tandem devices require semi-transparent top cells. This implies a contact of one of the charge-extracting layer to a TCO (transparent conductive oxide) which might require some optimization.

We tackle the upscaling challenge from the early development stages. We work to improve the homogeneity of the deposition process on relatively large area

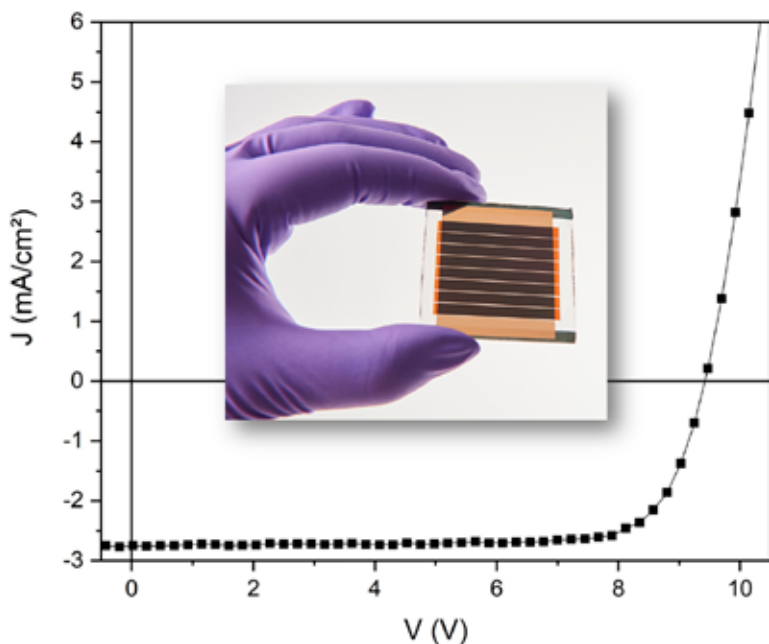


Figure 1: IV curve of a perovskite-based module with an area higher than 10 cm² showing an efficiency higher than 20 %

4 / https://www.helmholtz-berlin.de/pubbin/news_seite?nid=21020;sprache=en;seitenid=1

5 / Green, M. A., Dunlop, E. D., Hohl-Ebinger, J., Yoshita, M., Kopidakis, N., & Ho-Baillie, A. W. Y. (2020). Solar cell efficiency tables (Version 55). Progress in Photovoltaics: Research and Applications, 28(1), 3–15. <https://doi.org/10.1002/pip.3228>

devices (9 cm²) and improve the electrical performances of the complete devices. The tandem integration of perovskite device with high performances in single junction proves to be challenging. We developed characterization techniques to pinpoint the limiting loss mechanisms in our tandem devices which architecture is shown on Figure 2. Performances as high as 23.7% on active area were achieved (Figure 3).

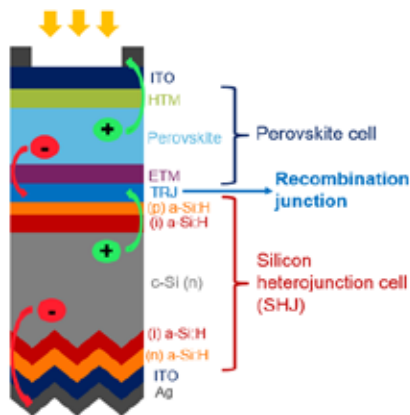


Figure 2: Tandem device architecture.

Optical simulations and characterizations that provide clues regarding optical losses and give guidelines for further device optimizations, targeting efficiencies as high as 30%, support all these developments. Figure 4 shows the simulated external quantum efficiency (EQE) of such an optimized architecture.

We focus our next efforts on the fabrication of tandem devices on full wafers (M2 sized). This implies the development of slot die coating for the perovskite layer to replace the spin coating technique used in earlier works and that is not compatible with industrial processes. We also plan to upscale the processes for the interfacial layers and consider physical vapor deposition (PVD) or atomic layer deposition (ALD) [T4] techniques as well as the solvent approach by slot die.

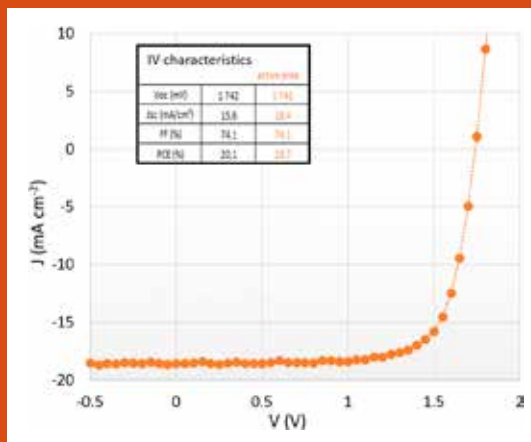
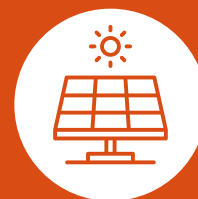


Figure 3: IV curve and characteristics of the tandem device measured in reverse scan.



YIELD OF

23.7 %

ON A SURFACE OF 9 CM²
(ACTIVE AREA,
WITHOUT SHADING)

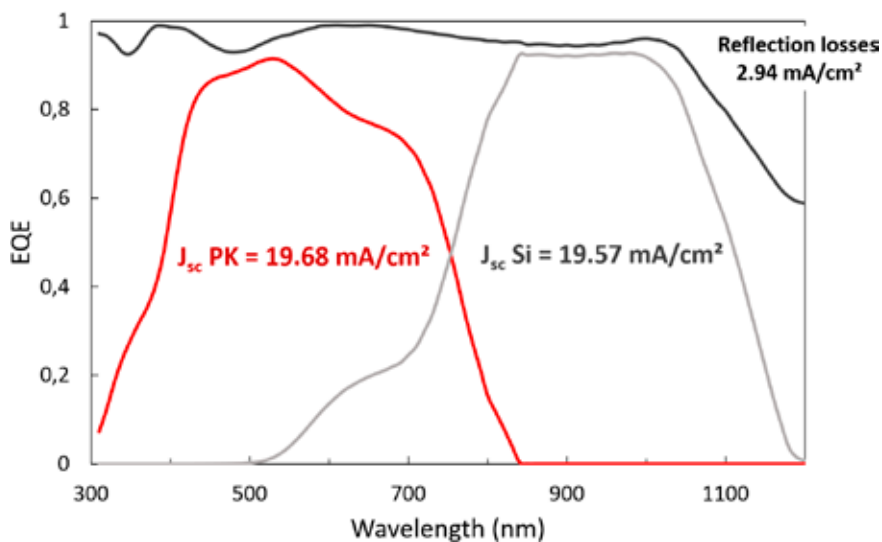
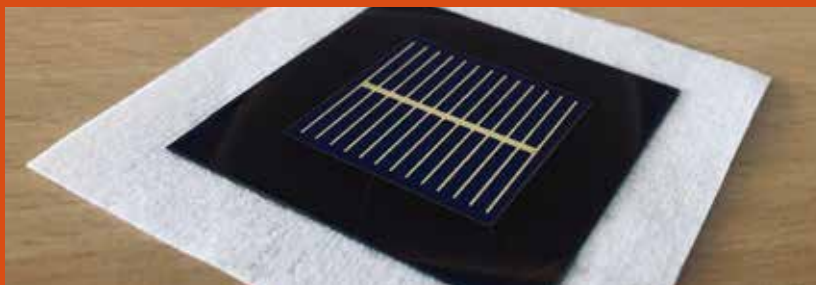


Figure 4: Simulated External Quantum Efficiency (EQE) of an optimized tandem architecture producing current density above 19.5 mA.cm⁻²: EQE of top (red) and bottom cells (grey). The black curve represents 1 - total reflectance of the whole stack, from which reflection losses are calculated taking into account AM1.5 spectrum.

GENERAL PERSPECTIVES

The control of the crystallization of the perovskite layer was achieved on 11 cm² active area devices leading to 20 % PV efficiency in the single junction devices and 22 % in the tandem architecture. These developments are now transferred at the industrial scale to increase the surface area of the final device by using printing processes, fast ALD or PVD steps. Moreover, CEA-Liten teams are making improvements for the tuning of the bandgap of the perovskite material and for the optical management in the interfacial layers and top electrode to reach 30 % efficiencies.

In parallel, the stability assessment should be continued at the cell and module scale to pass soon the IEC requirements and to evaluate the technology in real outdoor conditions.

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Thesis defended

- [T1] P. Dally, “Perovskite based solar cells: From material characterizations to improvement of device performances and stability”, PhD thesis, Grenoble, 2019.
- [T2] M. Fievez, “Slot die coating of double cation perovskite: From ink tuning to high efficiency devices”, PhD thesis, Grenoble & NTU Singapore, ongoing.
- [T3] A. Puaud, “Understanding and optimization of transport mechanisms in silicon heterojunction / perovskite tandem solar cells”, PhD thesis, Grenoble, ongoing.
- [T4] F. Gayot, “ALD deposition technique for interfacial layer deposition in silicon /perovskite tandem architecture”, PhD thesis, Grenoble, ongoing.

Projects

- [P1] Si-Premium project, Carnot Énergies du Futur internal project.
- [P2] Print-Rose project, CEA internal project.
- [P3] HETNA4 project, bilateral partnership CEA-Enel Green Power.

MECHANICAL STRENGTH OF DIAMOND-SAWN SILICON WAFERS: EFFECT OF THICKNESS AND CRYSTALLINE NATURE

Reducing the thickness of silicon wafers cut using diamond wire technology is one of the key issues to lower manufacturing costs in the photovoltaic (PV) industry. To avoid higher breakage rates, it is crucial to understand how the sawing process affects the mechanical resistance of wafers. It is shown that for a given silicon quality, bending fracture stress of a wafer is independent of its thickness. Nevertheless, mono-like and multi-crystalline wafers are less resistant than monocrystalline ones.

APPROACH

Currently, the typical thickness of as-cut wafers (the time when they are most likely to break) is around 180 to 160 μm and there is almost no work focusing on the mechanical properties of thinner ones. Therefore, it is essential to understand if the sawing induced damage for thinner wafers could become critical and lead to greater breakage rates during the following handling steps. In our study, we therefore proposed a rigorous analysis to evaluate the mechanical strength of diamond-sawn wafers of different thicknesses and silicon qualities. Bricks from each ingot

quality (Mono, Mono-like & Multi) were cut in a diamond wire saw using a special wire guiding system with a variable pitch, which enables the slicing of wafers of three different thicknesses (180, 160 and 140 μm) in the same brick. As-cut 156 x 156 mm^2 wafers were then tested through 4-line bending until breakage, the effective stress being calculated by finite elements analysis, because of the wafers large deflections.

RESULTS AND PERSPECTIVES

The experiments confirm the well-known dependency of the mechanical strength on the orientation of the saw

marks for diamond-sawn wafers (two to three times stronger when rollers are parallel to striations = “cut direction”, see Figure 1). The main result is that the characteristic fragile (calculated by Weibull’s analysis) is the same for thicknesses 180, 160 and 140 μm in the cut direction, no matter the crystalline structure. In wire direction, breaking stresses for a given crystallinity are also comparable for all tested thicknesses but they are lower with mono-like and multi than for monocrystalline silicon. It is suggested that the difference in mechanical strength is not explained by differences in surface defects, since the three types of silicon have similar morphologies, but rather by a more pronounced subsurface damage of mono-like and multicrystalline wafers due to interactions of diamond grains with the dislocations or grain boundaries present in these materials. /

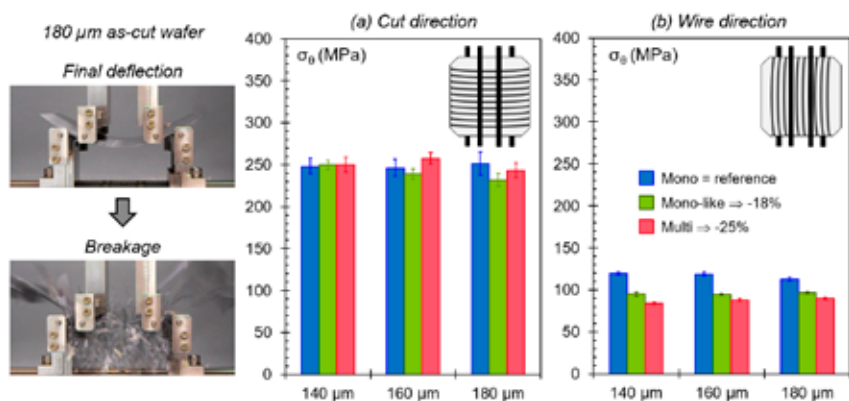


Figure 1: Characteristic fracture strength of mono-Si, mono-like and mc-Si wafers of different thicknesses tested in 4-line bending in (a) cut and (b) wire direction.

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IMPURITY GETTERING BY POLYSILICON PASSIVATED CONTACTS FOR ADVANCED CAST SILICON



APPROACH

Polysilicon on oxide passivated contacts spark interests for reducing carrier recombination at the metal-substrate interface of solar cells. In parallel cast silicon is an interesting challenger to mono-crystalline (Czochralski) silicon, particularly due to its lower carbon footprint. Nowadays, small grain multi-crystalline silicon ingots feature low amounts of dislocation clusters by using seed-assisted directional solidifications. We recently brought new insights into the mechanisms by which, the nature of the seeds and the melting parameters influence the crystallographic properties [1]. Beyond dislocations, cast silicon usually contains more metal impurities than Czochralski silicon. Therefore, to be compatible with this material, the elaboration pro-

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Polysilicon on oxide passivated contacts spark interests for reducing carrier recombination below the electrodes of silicon solar cells. We formed these structures on dislocation-poor multi-crystalline wafers obtained by seed-assisted directional solidification. Interestingly their elaboration processes provide external gettering effects (metals extraction). This opens the path for low carbon-footprint premium photovoltaic devices.

cesses of polysilicon passivated contacts have to provide external gettering effects (bulk extraction of metals), in the manner of phosphorus thermal diffusion doping. To assess this possibility, we formed both p- and n-type passivated contacts, and conducted thermal diffusions, on dislocation-poor multi-crystalline wafers obtained by seed-assisted directional solidification. The carrier lifetime of the processed wafers as well as the remaining dissolved iron concentration were monitored.

RESULTS AND PERSPECTIVES

Interestingly, the elaboration processes of both p- and n-type polysilicon passivated contacts provide strong external gettering effects: important increases of the carrier lifetime and reductions of the dissolved iron concentration [2]. For instance, the n-type passivated contacts formation process extracted more than 99 % of the ini-

tially dissolved iron atoms (Figure 1). These improvements are close to those provided by the phosphorus diffusion, known for its excellent gettering efficiency. Notice that the boron diffusion (particularly used for the fabrication of bifacial devices) degrades the material quality (dissolution of metal precipitates). Therefore replacing a boron-diffused layer by a p-type passivated contact could improve both the efficiency potential of the cell and its material tolerance. We investigated the mechanism behind the p-type passivated contact gettering. We showed, by combining secondary ion mass spectrometry with electro-chemical analyses, that the p-type polysilicon film would contain boron-silicide precipitates, known in the literature as segregation sites for metals. These results open the path towards high efficiency passivated contacts solar cells prepared from low-carbon footprint cast materials. /

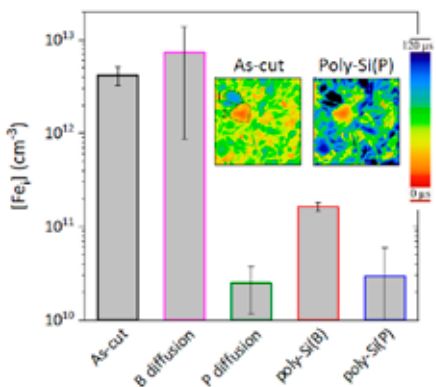


Figure 1: Dissolved iron concentrations ([Fe]) determined on p-type multi-crystalline “sister” wafers (bottom part of the ingot) that experienced various processes (thermal diffusions and polysilicon passivated contacts formation steps). Maps (3x3 cm²) of the carrier lifetime for a non-treated (as-cut) sample and a sample that experienced the n-type polysilicon passivated contacts formation, highlighting two different natures of grains (labelled 1 and 2 in the As-cut).

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ACURATE MULTI-JUNCTIONS SOLAR CELLS CHARACTERIZATION APPLIED ON SPACE MICRO-CONCENTRATORS

High efficiency III-V multi-junction solar cells (MJSCs) make it possible to envisage photovoltaic modules for application fields that involve high energy densities such as space missions and Internet of Things (IoT). To support these developments, we designed an improved testing process for the MJSCs electrical characterization that take into account their particular structure with only two terminals and the inappropriate spectrum of the existing solar simulators.

APPROACH

In order to make this measurement reliable, it is therefore essential to control appropriate calibration methods and testing means at one's disposal and not to be dependent of the reference solar cells (isotypes) which are very hard to provide. The proposed method [1], based on pseudo-isotypes made with silicon and germanium photodiodes filtered reproduces the cut-on and the cut-off of each MJSC sub-cell, as shown for the middle sub-cell (Figure 1). The use of pseudo-isotypes requires the development of a simple and accurate calibration method in order to obtain the constants associated with these references without sending it to a certified laboratory. Therefore, reference solar cells (isotypes) and pseudo-isotypes are lighted by solar simulators but also by calibrated lamps from NIST. Currents are compared in order to choose the good constants with a discrepancy under 5%. Moreover, in order to consolidate this method, spectro-radiometers are espe-

cially assembled to carry out solar simulator spectra from 300 to 1700 nm with a very short time of 100 μ s.



RESULTS AND PERSPECTIVES

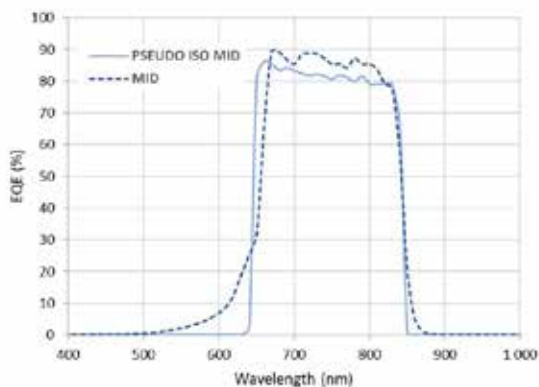
We applied this new method to the characterization of concentrator photovoltaics technology that can be a cost-effective solution for powering specific spatial missions. Compared to classical

concentrators, micro-optical systems reduces the weight, the need in materials and the cost of solar arrays while increasing the efficiency. This work led to a new concept especially dedicated to space application: a linear Total Internal Reflection (TIR) module, operating at a low concentration (7.6X), and called SLIT (Space Linear TIR) module (see picture). Requiring no deployment system for optics, extremely angular independent, the efficiency of the first prototype is around 18 % for a spectrum AMO. Preliminary thermal tests also enhance a stable behavior for optics [2]. Now our work aims at increasing the theoretical CPC (Compound Parabolic Concentrator) efficiency. A 94 % efficient parabolic shape is under study, providing a gain of about 19 % respect to the present model. /

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Figure 1: External Quantum Efficiency (EQE) of an isotype made with AlGaAs (MID) and a pseudo-isotype made with silicon and appropriate interferential filters (PSEUDO ISOMID).



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ENERGY GRID MANAGEMENT

LITEN IS DESIGNING NEW HARDWARE AND SOFTWARE TO DELIVER REAL-TIME, MULTI-SCALE GRID MANAGEMENT CAPABILITIES AND INTEGRATE INTERMITTENT RENEWABLE ENERGY. AS INTERMITTENT RENEWABLE ENERGY INTEGRATION RATES INCREASE, GRIDS WILL NEED TO BECOME MORE FLEXIBLE. LITEN IS ALSO DEVELOPING HYDROGEN AND BATTERY-BASED ENERGY STORAGE SOLUTIONS THAT CAN PROVIDE THIS FLEXIBILITY. THESE TECHNOLOGIES ARE A NECESSARY STEP TOWARD THE CONVERGENCE OF ENERGY VECTORS AND APPLICATIONS IN AREAS LIKE CLEAN MOBILITY.

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INTEROPERABILITY IN THE DEVELOPMENT OF SMART GRID AND SMART CITIES

The sharp increase in the rate of integration of distributed and renewable energy sources (DRES) into electricity networks, accompanied by a rapid digitalization via growing penetration of advanced information and communication technologies (ICT) introduces a significant impact to the architecture of the system (i.e. communicative and bidirectional). It also transforms the conventional power system into a cyber-physical energy system (CPES) (i.e. the “smart grid”) consisting of a juxtaposition with several layers of technologies of different natures and of different abstraction levels. The diversification of energy supply leads to new challenges in the operation of the power system, in terms of maintaining energy quality (i.e. voltage, frequency, harmonics, etc.) and improving reliability against the intermittency of the renewable resources. On the other hand, the digitalization in power system paves the way to enable new applications; both at operator level (e.g. coordinated voltage and frequency control, optimized energy management system, etc.) and at end-user level (e.g. auto-consumption, peer-to-peer energy transaction, load planning, shifting and shedding, etc.). In this context of technological development, the power system is required to become communicative and interactive, capable of exchanging data and taking into account the actions of all actors of the power system in a holistic manner and in real time. This will enable a wide range of new smart applications as well as to fulfill the complete operational data requirement of the network. Interoperability, defined as the ability of two or more networks, systems or applications to exchange and use this information in an efficient and secure manner, is the enabler and the core requirement to complete the integration and proper functioning of the smart grid. Achieving this interoperability is however challenging due to the vast scale of the multi-domain smart grid and of the multitude of equipment, communication protocols and policies. The research requires also advanced and holistic assessment at system level with adequately sophisticated validation platform, which exceeds the capability of traditional methods that mainly work at component level. At CEA Liten, our research team focus on the development of interoperability architecture in smart grid and the technical implementation of interoperability for novel applications such as distributed control of microgrid, energy internet or cyber-security. The team works also on the validation aspect where we integrate advanced simulation and experimental techniques to create a combined physico-virtual environment for the assessment of such a complex and large-scale system. In this article, we summarize firstly our work on the development of interoperability in smart grid, from conceptual architecture to technical implementation using the concept of hybrid cloud SCADA¹ and PaaS/SaaS² deliverance model, harmonizing CIM³ (IEC 61970/61968) and OPC UA⁴. We then cover the deployment of interoperability as enabler of several novel smart grid applications in the framework of our research. Finally, we present our combined physico-virtual validation environment where we can electrically plug physical devices to a digital twin of the interested CPES, for a realistic and holistic assessment both at local and global level.

ENABLING INTEROPERABILITY: ARCHITECTURE AND IMPLEMENTATION

Advanced and coordinated applications require information in real-time from multiple entities in the power system that communicate in a wide range of protocols, sometimes over different or overlapping abstraction layers. While the concept of interoperability involves all the abstraction layers, from physical devices

to high level policy making, we focus only on the technological aspect in the framework of our research [P1, P2]. We develop interoperability architecture for CPES based on hybrid cloud SCADA concept and propose the deliverance of SCADA service via PaaS model, or SCADA-as-a-Service approach [1] (Figure 1). The proposed architecture [2] provides an infrastructure for interoperability among multiple platforms, while maintaining

security and reliability of the system operation. We employ in the architecture the usage of CIM semantic over OPC UA protocol [3], two important standards in the development of smart grid, thank to our developed automatic implementation procedure [4]. A wide range of SCADA services can be deployed using this hybrid cloud based architecture (e.g. remote coordinated control, congestion management, etc.) [P3].

1/ Supervision, Control and Data Acquisition

2/ Platform-as-a-Service/Software-as-a-Service

3/ Common Information Model

4/ Open Platform Communication Unified Architecture

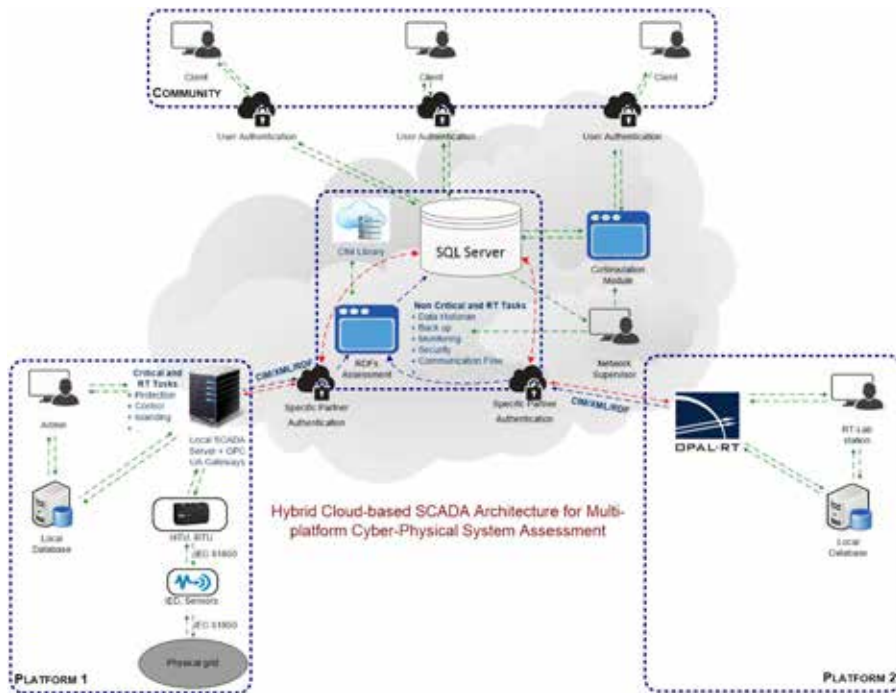


Figure 1: Interoperability with SCADA-as-a-Service Approach [7]

INTEROPERABILITY AS THE ENABLER OF THE NOVEL APPLICATIONS

Going beyond the development of technical solutions for interoperability, we seek also to implement it as the enabler of the novel architecture and applications smart grid. Notably, our deployment of interoperability in power system targets two types of application: i) stability of a micro-network with distributed control of DRES and flexibility that must provide system services in the objective of dynamic optimization; ii) aggregate management of a pool of DRES, in the perspective of electricity market integration. In the first applications, we developed a distributed voltage and frequency control using multi-agent approach [T1]. Contrary to the traditional centralized approach, the agent only requires local information of its neighborhood to actualize the algorithm; the global optimization is then

achieved via a consensus among the agents. In the vision of interoperability, the agents are configured in a plug-and-play manner (i.e. the network detect and self-reconfigure automatically when a device connect or shut down

from the grid) [5, 6]. This approach enables the interoperability and the seamless integration of DRES in a micro-grid (which may come from multiple vendors) and ensures that the technical exigencies in terms of power quality are satisfied. Integrated to the electricity market layer, we deploy the control system to contribute to establishment of an Energy Internet concept, in collaboration with the universities of Strathclyde and Nanyang. A cross-continental demonstration was carried out over the three platforms located in France, Scotland and Singapore [7] (Figure 2). We investigated also the potential application of distributed ledger technologies (e.g. block chain, block lattice or the Tangle) as the register of such peer-to-peer energy transaction framework [8]. These results open interesting perspectives for our researches in terms of developing technical framework for energy transaction eventually at micro-grid to macro-grid scale [P4].

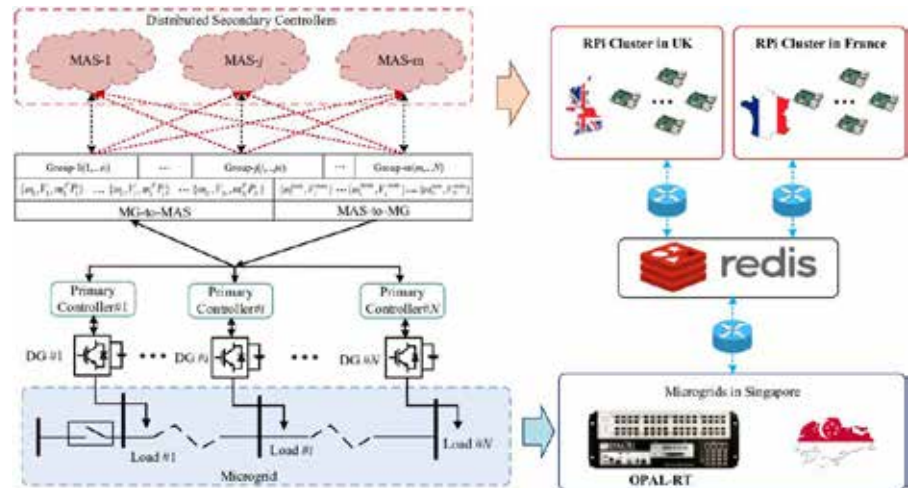


Figure 2: Interoperability of three platforms in CEA (France), UST (Scotland) and NTU (Singapore) for a cross-continental implementation of Distributed Control in Energy Internet Paradigm [7].

COMBINED PHYSICO-VIRTUAL PLATFORM FOR CPES ASSESSMENT: DIGITAL TWIN AND POWER-HARDWARE-IN-THE-LOOP

In the case with CPES, as a juxtaposition of multiple domains, a single domain approach by simulation or hardware testing does not suffice. A holistic consideration at system level is necessary due to several reasons: i) the integrity and the interdependency of the subsystems in different domains need to be well reflected in the validation framework; ii) a local solution obtained by a single domain test may not be (or compatible with) the global solution [9]. In order to put in place and to demonstrate our CPES solutions [P5], we explored advanced validation methods for interoperability of co-simulation with different domains (electrical, informatics), time scales (μ s to days), simulation mode (dynamic, steady state, phasor, temporal or frequency) and solvers (continuous, discrete event) [P6, 10]

with eventually integration of physical devices (i.e. hardware-in-the-loop) [11] (Figure 3).

Eventually, using these results, we are capable of constructing a combined physic-virtual platform for CPES holistic assessment at system level. We developed a linkage with the OPC UA SCADA system in Python with which the grid data and services are synchronized to create a digital twin of the real grid in real-time simulation [12]. This digital twin continuously updates itself to represent the current state of the real-world counterpart. We can gain an in-depth insight of the CPES to improve, optimize the performance or to study extreme or rare scenario of this system. We can also connect a physical electrical device to any coupling point of this digital twin via a power interface (i.e. power-hardware-in-the-loop) to study its impact to the CPES, locally or globally [13], in a most realistic and holistic manner.



*vRES = variable renewable energy sources

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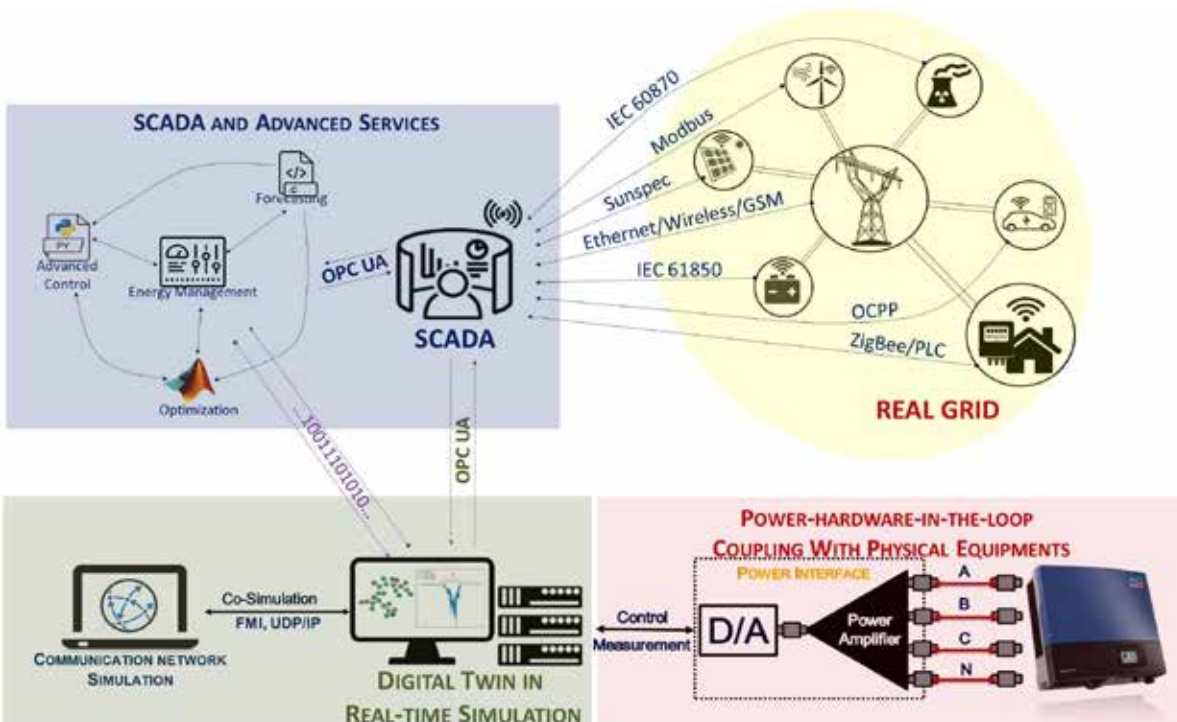


Figure 3: Combined physico-virtual environment for a holistic validation of CPES.

GENERAL PERSPECTIVES

We presented here a brief summary of our works on the development of interoperability in smart grid, from conceptual architecture to technical deployment for several novel smart grid applications. We developed also a combined physico-virtual validation environment for a realistic and holistic assessment of CPES.

The proposed interoperability architecture is going to be used as the base for development of more innovative smart grid applications, as well as in our upcoming projects [P7, P8]. /

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- [P2] PPInterop 2, CARNOT “Énergie du futur” project, 2017-2018
- [P3] United Grid, European H2020 project, <https://united-grid.eu/>, 2017-2021
- [P4] m2M, European H2020 project, <https://m2m-grid.eu/>, 2017-2021
- [P5] ERIGrid, European H2020 project, <https://erigrd.eu/>, 2015-2020
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ELECTRICITY STORAGE TO MANAGE VARIABLE SUPPLY AND DEMAND AT VARIOUS TIME SCALES

The rising share of Variable Renewable Electricity Sources, and the shrinking share of distributable production (in France: nuclear) lead to new challenges in balancing production and consumption at all times. The present work provides new insights on how electricity storage could handle this variability, focusing on the different time scales involved, due to human rhythms, meteorological and climatic cycles.

APPROACH

We decompose the French production and consumption patterns using a wavelet transform, over time scales ranging from one hour to one year. For each time scale, we can calculate the necessary size of storage from the previous decomposition. As storage efficiency is less than 100 %, some energy is lost in the process and it is necessary to oversize the production. We define the “flexibility service” as the amount of electricity needed to fill the gap when production is not sufficient to meet consumption. Several indicators are used to quantify the cost (including both storage and oversizing) for providing the service: either economical cost, CO₂ emissions, or embodied energy of the devices. This last indicator, divided by the service, has the interesting property of being dimensionless. Through both several extreme cases and practical cases, we studied the competition

and collaboration between storage technologies, and with the production oversizing.

RESULTS AND PERSPECTIVES

Unsurprisingly, PV features high variability at the daily and seasonal scales (out of phase of consumption). Wind power rather shows high variability around the week scale. As the figure below shows, the necessary storage size grows heavily with the time scale. Consequently, storing excess electricity in summer to use it in winter when demand is high is very expensive, whatever the technology considered. We observed a tradeoff between storage cost and efficiency, the most efficient technologies being suited to short time scales, and the cheaper ones to long time scales. Batteries appear well suited up to daily storage, which encourages the development of Vehicle-to-Grid. Pumped Hydro is very good up to weekly

storage, but severely constrained by available potential. Hydrogen is relevant up to one or two months, above which the cost of the bottles dominates. This pushes towards studying geological storage of hydrogen. Compressed Air Energy Storage was not found to be particularly relevant. The low efficiency of the hydrogen route implies that the oversizing of the production system is a dominant cost. It is therefore less suited to high variability or high costs of electricity, which imply higher and more costly oversizing. An optimization using realistic production and consumption patterns shows a dominant usage of Li-ion up to one day, and of hydrogen and oversizing for longer time scales. The perspectives include the conversion of electricity into heat that is easier to store for later use in winter. That way, the flexibility is obtained by changing the consumption pattern rather than the production pattern. /

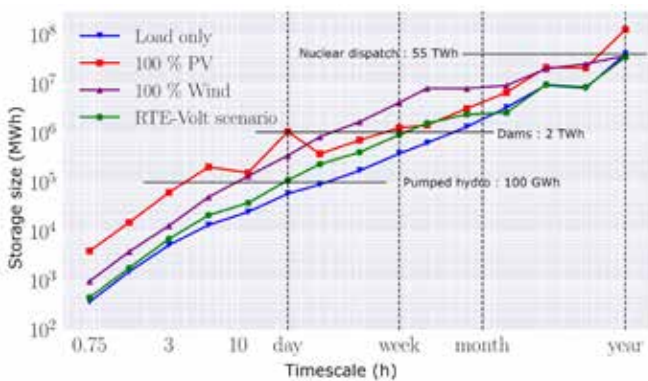


Figure 1: Size of the storage necessary to provide flexibility, depending on the time scale considered. The size increases rapidly with time scale up to 40 TWh for seasonal storage. 4 scenarios are considered: Load only (production is not variable), 100% PV, 100% wind power, or RTE-Volt scenario (10% PV, 26% wind). Three existing flexibility levers are shown for comparison: pumped hydro storage, hydraulic dams, and nuclear dispatch (mainly choosing the dates of nuclear maintenance).

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OPTIMAL ENERGY MANAGEMENT FOR A REMOTE MARITIME AREA

The deployment of renewable energy resources for electricity supply of islands is challenging due to multiple technical and economic constraints. To provide more degrees of freedom for these off grid networks, a multi-level algorithm based on several Demand Side Management (DSM) strategies is proposed in this work with an application for an island supplied by a multi-source system including solar, wind, tidal, wave energies and a battery energy storage solution.

APPROACH

To limit the inconvenience for users, we studied a hierarchical application of the proposed strategies, according to day-ahead forecast. The excess of generated power is prioritized for electric room heaters and water heaters, using anticipation strategy. Load shifting and load shedding are used for the most critical situations. Optimization is done with genetic algorithm.

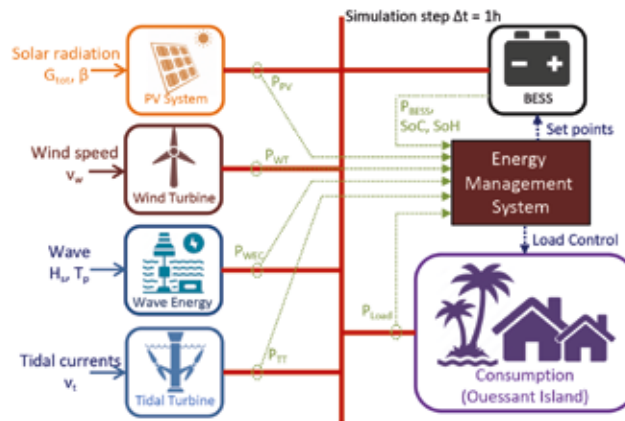


Figure 1: Studied multi-source system for a remote maritime area

RESULTS AND PERSPECTIVES

The proposed DSM algorithm was found to help reduce the unmet load demand rate and to adapt load demand according to the power generated (see

table). The main results obtained from this study show the benefits to anticipate shiftable loads when enough energy is generated by the sources, according to the reduction of the unmet load rate.

Our next target is to study the impact of a forecast error concerning resource and consumption data and the aging of sources. /

DSM mode n° (priority order)	DSM strategy	Main goal	Method/ Tool	Load and DSM strategy considered
1	Without DSM	Evaluate the expected state of charge evolution over the scheduling period	Rule-based	None
2	Water heaters anticipation	Use the excess of generated power when it occurs whatever the power balance in the future	Rule-based	Water heaters load shifting by anticipation
3	Electric room heaters anticipation	Use the excess of generated power when it occurs if a lack of power is expected in the future	Rule-based	Electric room heaters load shifting by anticipation
4	Scheduling for critical situations	Schedule the three load profiles while limiting the modification of initial demand	Genetic algorithm	Water heaters and electric room heaters loads: load shifting and load shedding. Other loads: load shedding

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FLEXIBLE CONSUMPTION AND PRODUCTION FOR THERMAL GRIDS

District heating systems should continue to grow rapidly in France in the next years. In this context, the smart coupling between the electricity and thermal sectors is of crucial importance. However, the design and operation of flexible thermal grids is still a challenge. This paper highlights our latest research achievements on this topic.

APPROACH

Transporting electricity is efficient, storing it is expensive; comparatively, transporting heat is more complex yet storing it is cheaper. We therefore focus our research efforts on the design and operation of flexible district heating systems. By “flexible system”, we mean a system that can satisfy consumers’ demand relying on a variety of production plans. At the consumer’s level, we worked on the development of control strategies exploiting thermal mass in the building and space-heating systems. The challenge here is to identifying relevant thermal inertia with a minimal and non-intrusive set of sensors. We carried this work using simulation means complemented with a real-world demonstration. At the production level, we focus on systems combining power-to-heat components and heat storage capacities. These systems are potentially interesting in a low carbon content electricity mix context such as the one existing in France. However, evaluating and sizing such systems remains a delicate task. We propose a solution based on optimization and simulation to tackle this challenge.

RESULTS AND PERSPECTIVES

At the consumer’s level, we developed a methodology for modeling and identifying a building model only with data available at the substation level [1-2]. In particular, no measurement inside buildings is required. We believe this can significantly improve the replicability and dissemination potential of the solution. We also showed that such an identified building model is accurate enough to design an efficient controller able to minimize energy costs while guaranteeing thermal comfort inside the building. We have implemented such a controller and we are testing it in a demonstrator building located in the city of Grenoble. At the production level, we studied a production plant composed of a

biomass generator, a heat pump and a heat storage in the French, German and Danish energetic contexts [3]. We assessed the techno-economic performances of this system using Mixed Integer Linear Programming. We applied a multi-objective parametric optimization method to size the system using the available quantity of biomass, the maximum CO₂ content and a minimum renewable energy ratio (REnR) of the heat production as ϵ -constraints (see figure below). Our analysis shows that without strong constraints, heat pump and daily storage are used. However, when the amount of biomass becomes a limiting factor, we show that investing in an inter-seasonal storage is necessary to reach high renewable energy ratio. /

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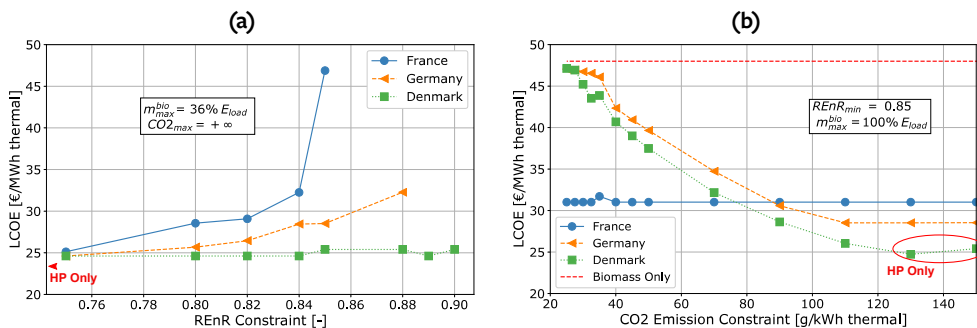


Figure 1: Pareto fronts – (a) LCOE/REnR and (b) LCOE/CO₂ emission – for France, Denmark and Germany. Biomass-only and HP-only scenario are highlighted.

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THE COMPLEMENTARITY OF SKILLS WITHIN THE PARTNERSHIP OF INSTITUTE CARNOT ÉNERGIES DU FUTUR

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Yvon Besanger

Professor, Grenoble Institute of Technology,
and Co-Head of the SYREL (electrical systems and grids)
research group at G2Elab (a multi-partner electrical
engineering lab in Grenoble)



“A uniquely well-rounded partnership”

“ Our team at LEPMI has been working with Liten for years. However, the relationship grew much stronger a year and a half ago, when we started collaborating on a co-supervised a PhD research project to limit the use of platinum in the active layers of PEMFCs (proton exchange membrane fuel cells) without adversely affecting performance or lifespan. One of the reasons we would now like to set up a joint lab or research group is because our skillsets round each other out so nicely. Together, LEPMI and Liten cover the entire PEMFC value chain from materials through to testing stacks and systems. LEPMI’s research is on the basic science. In addition to innovative materials (catalysts and membranes) and conventional electrochemical characterization methods used to analyze what happens to electrodes during fuel cell operation, we can also contribute more advanced spectroscopy methods like DEMS and ICPMS to analyze the durability of materials. Liten’s work addresses more mature technologies and, specifically, scaling up the technologies developed in the lab so that they can be transferred to industrial companies. This comprehensive range of know-how covers all stages in PEMFC development, an advantage that is absolutely crucial to winning EU research grants. So, working together with Liten was only natural.”

“Sharing resources makes us all more efficient”

“ Our team is investigating system-level approaches to research on smartgrids in the broad sense of the term, from network components like electric vehicles to transmission and distribution networks.” We have been working with Liten regularly since one of our PhDs doing his dissertation here was hired at INES around ten years ago. In 2017 we made it official when we set up a joint research team of around twelve people. Today, the team is working mainly on smart grids. We have several large projects going on right now with interoperability aspects that are keeping us pretty busy. The PRISME testing lab at INES is home to solar panels, 1:1 scale test homes, electric vehicle charging terminals, energy storage solutions, real-time simulation software, and smart-grid equipment. Back at G2Elab, we have several technology platforms located at the Grenoble Institute of Technology PREDIS test facility. These include two micro-grids with reduced-scale equipment, a hybrid real-time simulator, and a grid supervision system. Because our facilities are interoperable, we can do things like share our resources by getting them to work together at the same time remotely. The partnership is win-win. We have the critical mass we need to move things forward, and it has raised all of our profiles, positioning us to work on more projects and secure more grants. We are collaborating with organizations such as the Carnot “Energies du Futur” institute, the Auvergne-Rhone-Alpes regional government, and the French national research agency (ANR) on interoperability projects at the regional and national levels. We also recently completed the EU ERIGRID project.”



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BATTERIES FOR THE FUTURE

The development of intermittent renewable energies requires sustainable energy storage for the adjustment of production to consumption without resorting to high carbon impact means of production (oil, gas, coal). One of the relevant way of storing excess energy is the use of high-efficiency electrochemical energy storage systems, such as batteries. However, the batteries must have a favourable energy return on investment (EROI) and provide the required service at an acceptable cost [1]. Batteries are evolving as demand rises owing to electric vehicles. Several industrials have already staked out positions on this market, including the leaders who are mainly in Asia. Europe, which has lagged in the production of batteries, is starting to set up ambitious programs for competing with the Asian monopolies. Nonetheless, several technological and economic issues must be addressed to create a durable battery industry for electric vehicles [2]. One solution to amortize the costs of batteries in electrified vehicles is also to use them to store energy from the grid and supply energy to it. A target of \$120 / kWh at system level seems to be achievable in 2025 for battery electric vehicles. It should be noted, however, that this cost, together with volume effects, will become increasingly dependent on the price of raw materials and thus on their fluctuations as it is already the case for the most critical material, cobalt.

In this context, CEA-Liten is following a scientific research strategy that take into account the industrial demand in this field that is (i) increase of energy density at the cell and pack level, (ii) ever-faster recharging which requires increasing power density, and (iii) ever-increasing lifetime of the systems. These increasing are conditional (i) by the need to demonstrate identical or even improved safety than previous solutions despite performance improvements, (ii) by a strong cost pressure (at all levels: materials, cell, and system), and (iii) by a need to guarantee the durability of the solution by using fewer and fewer strategic or critical materials. For Li-ion batteries, the increase in the maximum energy density at the cell level requires a technological breakthrough on the materials to exceed 300 Wh.kg⁻¹ and 800 Wh.L⁻¹ through new generations of batteries (e.g. all-solid battery, sodium-ion...) and using less costly production processes (e.g. solvent-free), without degrading the service life and environmental impact. We show the strong involvement of CEA-Liten in these improvements through the results of the work performed on three types of materials: Na-ion technology, Si for Li-ion technology and post-Li-ion “all-solid” electrolytes.

NA-ION TECHNOLOGY

The question of replacing Li-ion technology with a technology that consumes less critical materials seems to be relevant. Na-ion technology could answer this question, under certain conditions [3]. The main weakness of this technology lies in its lower energy density. Indeed, the redox potential of the Na⁺/Na couple above that of the Li⁺/Li couple limits the voltage at the battery terminals, and therefore the energy density. The supply of negative and positive electrode materials appears limited for the moment. The search for competitive materials in terms of energy density therefore remains one of the major challenges of this technology.

Liten’s work on this technology addresses all the active materials [4-6]

and the full cell [7, T1]. The use of a disordered carbonaceous material, such as hard carbons should overcome the limited intercalation of graphite by sodium for the anode side. V. Simone’s thesis work has made it possible to correlate the physico-chemical properties of this material with electrochemical performance [T1]. On the cathode side, since lamellar materials have poor performance and generally contain critical materials, Liten focuses on other promising compounds [P1]. They include Na₃V₂(PO₄)₂F₃ (NVPF), studied for the first time by Barker’s team. This polyanionic compound has a high operating voltage for a specific capacity of 120 mAh.g⁻¹, leading to a high specific energy that makes it the reference material as an alternative to lamellar oxides. It is

worth noticing that vanadium might pose abundance and toxicity limitations for the deployment of this electrode material on a large scale. Following these successful results at laboratory scale, Liten has carried out an up-scale synthesis to assemble several cylindrical 18650 Na-ion cells (Figure 1) based on hard carbon anode and NVPF based cathode [8]. The performance tests demonstrated the potential interest of the technology [9]. We integrated (Figure 1) storage modules based on this technology in a stationary application [P2] and in a robot [P3]. The commercial deployment of such mature technology seems to depend on the future evolution of the markets for lithium and transition metal resources.



Figure 1: First Na-ion accumulator in cylindrical 18650 format (left) [P1]. Sodium robot (middle) [P2]. Na-ion module (right) for stationary application [P3].

SILICON FOR LI-ION TECHNOLOGY

The second class of material aim directly at outperforming conventional lithium-ion. The development of very high-capacity cathodes such as Ni-rich or Li-rich (or even Rock-salt) requires an increase in the capacity of the anode, traditionally composed of carbon whose capacity is limited to 372 mAh.g^{-1} . To meet this requirement, the industry has been trying for several years to integrate silicon-based compounds into carbon. However, the progress is limited due to the high volume expansion of the structure during the formation of the Li_ySi_x alloy [10]. In order to understand better the limits of this promising technology, we studied the ageing mechanisms of silicon-based anodes [11] in the frame of several partnerships with academia. This work allowed to understanding the impact of silicon particles on the mechanical stresses induced and to introducing new core-shell particle morphologies [12,13]. The composite materials that contain silicon reduce the interface with the electrolyte and limit the impact of volume changes. Various research avenues have been considered: SiO_x [14,15], silicon-carbon and alloy composites. We integrated the original materials in electrodes for accumulators [P5] that shown very high specific capacities (Figure 2) [16] with acceptable lifetimes [17,18].

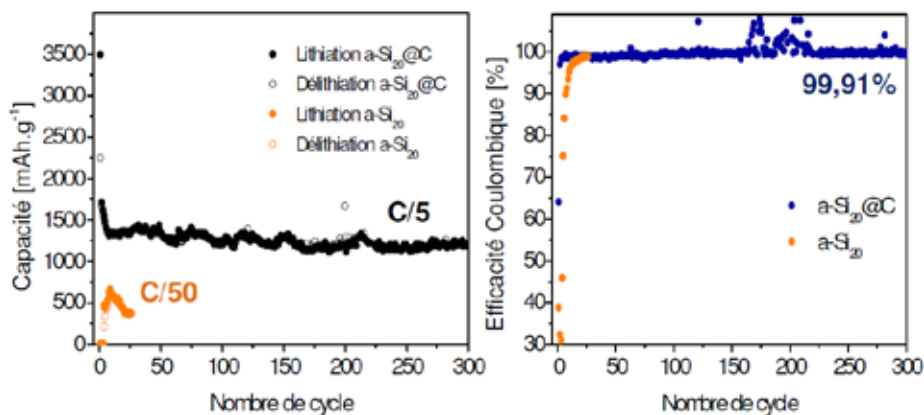


Figure 2: Evolution of the capacity of silicon particles covered with carbon ($a\text{-Si}_{20}\text{@C}$) compared to the amorphous silicon material ($a\text{-Si}_{20}$) and coulombic efficiency of these two materials in cycling (cycling between 5 mV and 1 V vs Li metal, at C/5 rate).

POST-LI-ION “ALL-SOLID” ELECTROLYTES

The “all-solid” systems aim to replace the graphite electrode by metallic lithium and are a real technological breakthrough compared to conventional Li-ion batteries. Although the interest in terms of energy density is easily demonstrated, it involves the use of solid electrolytes present both between the two electrodes and in the cathode. This solid electrolyte must be conductive at room temperature, have very good electrochemical stability with respect to lithium and cathode materials, generate a very good interface with all the components for which it must transport the ions (electrolyte/

cathode material, electrolyte/anode interfaces) and above all not be toxic or contain critical materials while being easy to use (process aspect).

The work carried out at Liten focus both on the material aspects of inorganic electrolytes and on polymer electrolytes with the advantage of being much easier to process. We consider the use of polymer electrolytes instead of liquid organic systems to be relevant for improving the safety of lithium batteries. In addition, it may allow the transition to high-energy lithium metal anodes. However, an intrinsic limitation is their ionic conductivity - rather low at room temperature. Nevertheless, we suggested overco-

ming this limitation by decoupling the transport of ions and the loosening of polymer chains [21]. In fact, although the understanding of the underlying transport mechanisms has improved considerably in the recent years, it is still quite difficult to outperform poly(ethylene oxide) (PEO) electrolyte systems. Then we directed our studies [P4] towards original materials, ionic liquid crystals, to understand the mode of transport in these

new electrolytes [T2,22,23], breaking with the traditional conductive polymer materials based on PEO [24]. One of the first approaches is to identify the relationship between polymer characteristic distances, viscosity and conductivity using different polymers chain lengths (Figure 3). These materials show promising performance and we continue the work to improve their properties [T3].

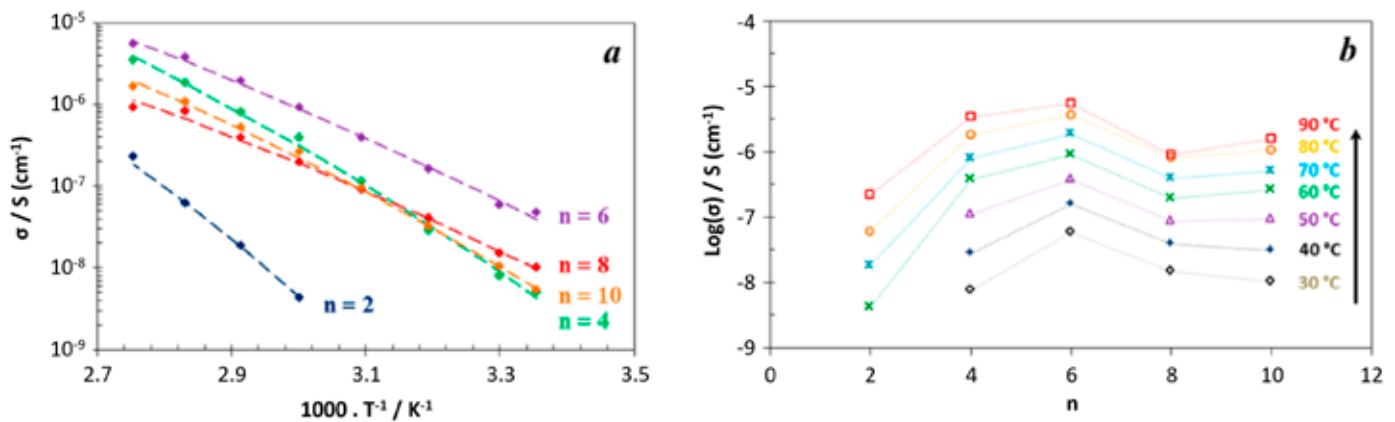
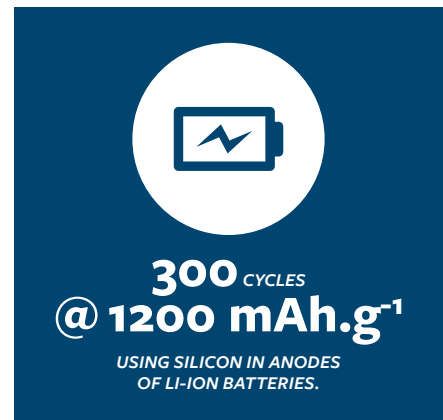


Figure 2: Ionic conductivity of $p(\text{C}_n\text{VIm-TFSI})$ poly(ILs) as function of (a) temperature and (b) chain length n for temperatures between 30°C and 90°C. The role of interdigitating here is preponderant over performance.

GENERAL PERSPECTIVES

Silicon anode based systems are the legitimate evolutionary path for Li-ion batteries, if they demonstrate increased lifetime and safety. The current efforts will most certainly be the intermediate path with higher energy density between conventional Li-ion and the emerging “all-solid” Li-metal. In the race for energy density improvement, the lithium metal anode breakthrough is the most eagerly awaited. However, power density targets, particularly for rapid vehicle charging, and the demonstration of acceptable lifetime at standard operating temperatures require significant improvements in the performance of the electrolytes and the interfaces between the various cell components. Only a coupling between modelling and simulation at different scales and understanding of the different transport mechanisms will reveal the relevant systems.

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- [P5] SPICY project, H2020, 2015-2018.

MICROSTRUCTURAL AND ELECTROCHEMICAL MODELING FOR SOLID-OXIDE-CELL ELECTRODES OPTIMIZATION

CEA-Liten has developed original models to generate synthetic electrode microstructures of Solid Oxide Cells (SOCs). We have used them to validate microstructural correlations related to the key properties controlling the electrode performances. We implemented these correlations in an electrochemical model to propose a numerical optimization of the air electrode microstructure.

APPROACH

The performances and the durability of SOC's still need to be improved to envisage the industrial deployment of this technology. In this objective, the electrodes microstructure can be optimized as it plays a key role on the SOC's efficiency and lifetime. A first strategy consists in manufacturing and testing a large number of electrode microstructures by changing the composition, the porosity and the distribution of the powders used for the preparation. However, this experimental approach is time consuming and does not allow the deep understanding of the complex relations between the microstructural properties and the electrode response. To overcome this issue, we adopted an alternative solution by the development of an integrated multiscale modeling approach. We applied this methodology to optimize the air electrode microstructure of a composite material made of lanthanum-strontium-cobalt ferrites (LSCF) and ceria doped gadolinium oxides (CGO).

RESULTS AND PERSPECTIVES

A pure mathematical model based on geo-statistical simulations and an original sphere-packing algorithm have been developed to produce digital twins of the electrode microstructures [1] (see a in the figure below). The representativeness of the synthetic volumes has been validated on electrode reconstructions obtained by X-ray holo-tomography. Afterwards, semi-analytical microstructural correlations have been proposed and validated on a large dataset of representative synthetic microstructures [2]. These equations allow establishing the links between

the microstructural properties controlling the electrode performances to their geometric attributes (composition, porosity and particle size distribution (see b in the figure below)). The correlations have been implemented in an electrochemical model specifically developed for the LSCF-CGO composite electrode [3] (see c in the figure below). The optimized numerical microstructures have been used as a manufacturing guide and a gain in performances has been obtained for the cells prepared at CEA. The methodology will be adapted to the hydrogen electrode to define mitigating solutions to limit the degradation. /

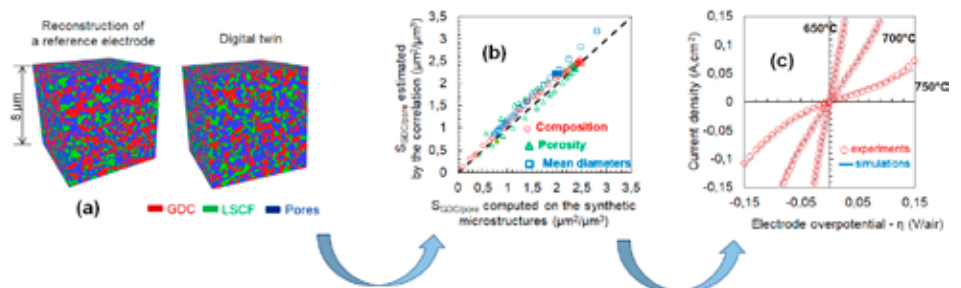


Figure 1: Integrated modelling tool with (a) synthetic microstructure for a LSCF-CGO electrode, (b) the development of microstructural correlations validated on the 3D numerical volumes and (c) the electrochemical modelling illustrated with the plot of the electrode polarisation curves under air at 650 °C-750 °C.

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INFLUENCE OF OPERATING CONDITIONS ON LIQUID WATER DISTRIBUTION IN PEMFCs

Liquid water distribution is a key parameter for the optimization of Proton Exchange Membrane Fuel Cell (PEMFC) performance and durability in various operating conditions. A deeper analysis of experimental and simulation results both at large and small scale contribute to the improvement of the tools dedicated to this optimum research.

APPROACH

Proton Exchange Membrane Fuel Cells (PEMFCs), as many other fuel cells, reject only water when they deliver electrical power from hydrogen. Their interest is continuously growing for many applications, either stationary or mobile. However, cost and durability remain some key issues for a large commercialization of this technology. Water has a key function in PEMFC operation, and impacts performance and lifetime. As a byproduct of the reaction, its evacuation from the electrochemical cells is mandatory. Liquid and vapor forms usually coexist inside the cells, and liquid accumulation can obstruct the reactant supply. However, a lack of water decreases the conductivity of the membrane. Identifying the optimal water quantity inside the cell is thus a promising path for PEMFC enhancement. At CEA, we combine liquid water visualization by neutron radiography, mappings of current density and temperature at cell

level, and finite element simulation to constitute a unique comprehension tool for the optimization of PEMFC operation.

RESULTS AND PERSPECTIVES

Several PEMFC stacks equipped with the same cell technology were necessary to combine the different experimental techniques, due to their particular requirements (for example, neutron radiography requires the development of dedicated terminal plates; current density mapping requires the integration of a current scan device in the stack). In parallel, we have pursued the development of our pseudo-3D model of

PEMFC stacks. Our previous work have shown that a simplified approach for the description of two-phase flows could deliver some simulation results in good agreement with experiments [1]. As the justifications of this agreement required some complementary investigations, our recent studies aim at a more detailed analysis of the water localization and flux from the cathode to the anode at channel-rib scale (see figure below), and on the comparison of several formulations for two-phase flow models [2]. Therefore, we expect a significant improvement of the reliability of our next generation of models. /

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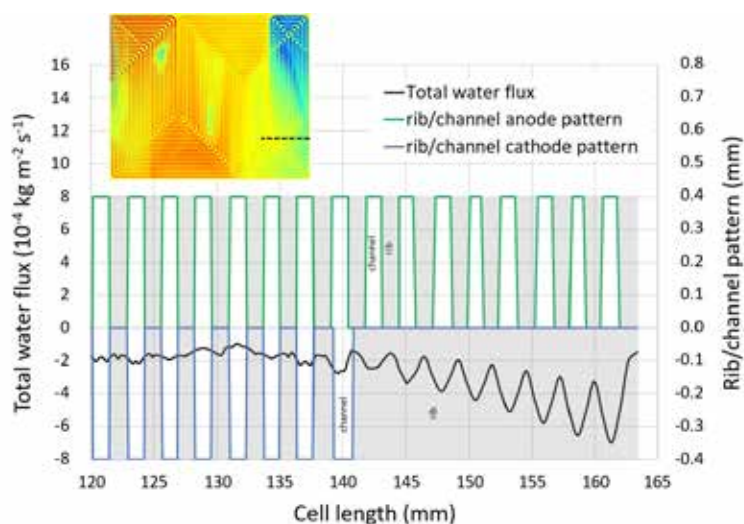


Figure 1: Water flux from the anode to the cathode at rib/channel scale, along a cut line of the cell total water flux mapping [2]

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WATER DISTRIBUTION AND MEMBRANE DEGRADATION IN PROTON EXCHANGE MEMBRANE FUEL CELL

By coupling original techniques based on neutron and X-Ray we are providing unique and invaluable information for understanding and improvement of Proton Exchange Membrane Fuel cells (PEMFCs). This is essential for the large-scale commercialization of this clean and efficient power source for vehicles, portable devices and stationary applications.

APPROACH

Proton Exchange Membrane Fuel cells (PEMFCs) are considered as one of the most promising carbon-free alternative energy conversion system for transportation and stationary applications. They produce electricity and heat from hydrogen with high yield, water being the single byproduct. Their efficiency and durability have been considerably improved since their early development. However, in view of extending their use to a broad range of customers, progress has still to be done in terms of cost, performance and lifespan. In the

PEMFC, all the physical and chemical mechanisms are highly dependent on water. Thus the water distribution, and consequently operation and degradation, are intrinsically heterogeneous along the cell. At CEA, we have been developing original and unique tools based on Neutron and X-Ray probes available at large scale research facilities in order to characterize operando the water distribution and the nanostructure of the polymer electrolyte membrane. This is a prerequisite towards understanding and improving PEMFC components.

RESULTS AND PERSPECTIVES

We identified the relevant scale for probing the physical degradation of the polymer electrolyte membrane and we evidenced the evolution of its nanostructure in dependence of the local hydration [1]. In parallel, by comparing neutron imaging and small angle scattering, we quantified the in-plane and through-plane liquid water distribution but also gradients in relative humidity at the cell level, and also at the mm and sub-mm scales. The results evidence the large heterogeneities of operation, and how two-phase flow with evaporation/condensation plays a crucial role in the water distribution in an operating PEMFC (see figure below) [2]. We are currently developing new methods to increase time and spatial resolutions and to obtain 3D information. We are now focusing our efforts on the most limiting component, the electrodes, by applying our expertise at smaller scale to study the relationships between the water content, the micro/nanostructure of the catalyst layers, and their evolution upon aging. /

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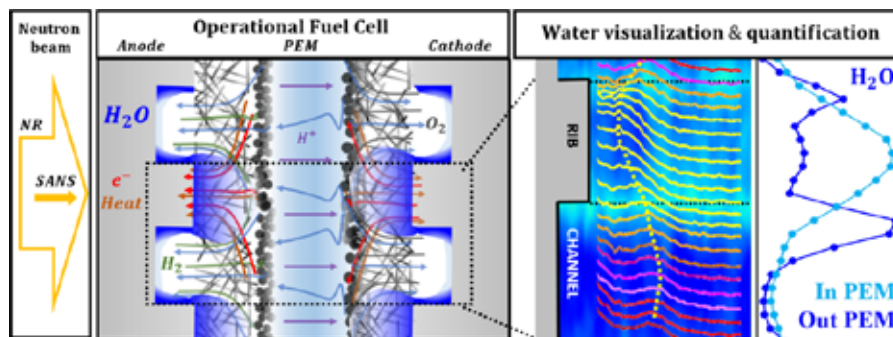


Figure 1: Scheme (left) of the cross-section of the fuel cell with water distribution in the components and (right) of the water quantification inside the membrane and in the cell at the rib/channel scale [2]

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REDUCING THE OVERALL ENERGY FOOTPRINT

IF THE ENERGY TRANSITION IS TO SUCCEED, THE ENERGY FOOTPRINT LEFT BY PRODUCTS AND PROCESSES OF ALL KINDS WILL HAVE TO BE REDUCED. AND THIS MEANS FACTORING IN A NEW SET OF IMPERATIVES. MATERIALS IS ONE OF THESE IMPERATIVES. LITEN IS DEVELOPING NEW TECHNOLOGIES LIKE ADDITIVE MANUFACTURING AND STRUCTURAL ELECTRONICS THAT MAKE MORE ECONOMICAL USE OF MATERIALS. LITEN IS ALSO INVESTIGATING SUBSTITUTES FOR CRITICAL MATERIALS AND APPROACHES TO RECYCLING AND ECO-INNOVATION RELEVANT TO THE INSTITUTE'S FLAGSHIP INDUSTRIES. FINALLY, LITEN IS LEADING THE WAY IN THE THERMOCHEMICAL CONVERSION OF CARBON-CONTAINING BIORESOURCES.

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REDUCTION OF CRITICAL MATERIALS IN PERMANENT MAGNETS: A STRATEGIC CHALLENGE

High-performance permanent magnets are made of metallic alloys that combine chemical elements from the rare earths (RE) series with transition metals. The first element brings the resistance to demagnetization, or coercivity, while the second determines the magnetic strength. Nd-Fe-B compounds are the most powerful magnets produced by industry and enable considerable improvement of the compactness, yield and reliability of electrical machines. The demand for such magnets is rapidly growing (15-20% per year) for the deployment of electrical vehicles (EV) (1 kg of magnets per EV), wind turbines (up to 600 kg per MW) and other industrial equipment. RE used in magnets are mainly light rare earth elements (LREE) such as neodymium but also heavy ones (HREE) such as dysprosium. The European Union points out potential supply risks for RE elements and in particular HREEs, and therefore recommends reducing the dependence on these critical materials. CEA-Liten hosts a semi-industrial pilot line and a powder metallurgy platform (POUDR'INNOV) for investigating the manufacturing of magnets. Besides, advanced characterization tools, numerical simulation as well as life cycle analysis methodologies jointly address the technological and scientific challenges. Reducing the RE content involves three main approaches: (i) rational use of raw critical elements in the material composition, (ii) material saving by net shape process to avoid scraps and machining loss and (iii) recycling end-of-life products through “magnet to magnet” short routes. The objective is to maintain the strength and demagnetization resistance of magnets to comply with motor requirements.

RATIONAL USE OF RAW CRITICAL ELEMENTS

Following a general rule in the science of materials, the performance of magnets depends not only on the basic properties of elements but also on mesoscale features influenced by the material process. Historically the first lever, i.e. an increase in HREE content, allowed complying with the stability requirements for motor operation (150 °C). The rare earth crisis in 2010 triggered unpredictable price fluctuations and revealed that this approach was no more sustainable. For this reason, the second lever, i.e. a better control of the process, is preferable but implies a quantitative understanding of the extrinsic properties. The standard powder metallurgy process involves the crushing of precursor alloys into fine particles followed by the compaction and sintering of the powder. In the last stage, the particles packing evolves toward a continuous network of faceted grains separated by very thin intergranular phases. In this dense product, due to inherent defects, the vicinity of grain boundaries (GB) are the weakest points where demagnetization nucleates. Thus, homogeneous phase distribution along

GBs and grain downsizing tend to favor the magnets' coercivity.

The thesis of B. Hugonnet [T1] investigated the role of the intergranular liquid phase formed during the sintering stage in standard magnets [1]. The work determined the optimal combination of alloying elements and annealing conditions liable to cure such defects [T1]. Localization of HREEs at the periphery of grains also improves the coercivity and mobilizes a small amount of critical materials. Diffusion treatment of some HREE compounds coated on the magnet surface produces such resistant core-shell structures. In the process, the intergranular liquid phase favors the diffusion of HREE at low temperatures along GBs, while the consump-

tion by grains is limited and forms thin enriched shells. This approach is only applicable for thin parts due to the HREE depletion in the core of magnets. Diffusion mechanism of HREE into the grains upon localization is actually not well established. The synthesis of large Nd₂Fe₁₄B monocrystals in collaboration with CEA-INAC [P1] supplied a grain model from which the dependence of diffusion profiles on crystallographic directions was finely resolved (Figure 1). The thesis of J. Fliegans [T2] focused on the diffusion gradients encountered in sintered magnets treated with DyCo alloys. Simulation with a polycrystalline 3D model [2-4] accounted for the HREE depletion effects when the thickness of magnets exceeds a few mm.

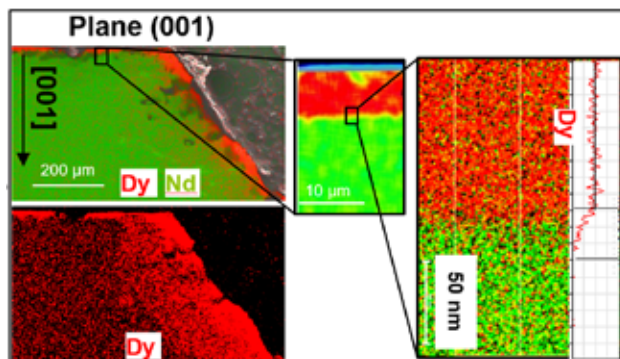


Figure 1: EDX Dy mapping on NdFeB monocrystal after diffusion from sample surface exhibiting lower penetration along the [001] direction and an abrupt diffusion front [P1]

CEA-Liten also developed an alternative process liable to overcome this dimensional limitation. Blending the HREE and magnetic powders before sintering tends to reduce the diffusion length and favors HREE homogeneity [5]. The challenge consisted in performing the powder densification and HREE diffusion at the same temperature, keeping in mind that sintering requires temperatures higher than 1000 °C while GB diffusion is optimal around 900 °C. A larger amount of liquid phase at GB contributed to reduce the sintering temperature, paving the way for HREE localization in thick magnets. Further work will focus on the achievement of full densification and the optimization of thermal annealing.

Besides GB engineering, grain downsizing from 5 to 3 μm proved to enhance the coercivity by 40 % without adding HREE. However, tailoring homogeneous microstructure in the final products with an effective decoupling of the magnetic small grains becomes a significant challenge and has not been deployed at

the industrial scale yet. One limitation comes from the early stage of magnet manufacturing, i.e. the synthesis of precursor alloys whom microstructure itself requires refinement and homogenization. The rapid solidification technique also named *strip-casting* (SC) (Figure 2) yields the starting alloys under the form of ribbons: raw materials are melted in an inductive furnace, the molten alloy is cast on a water-cooled rotating wheel and undergoes fast cooling (10^4 K/s) and solidification. Thanks to the range of solidification rate, SC advantageously produces well-defined crystalline and dendritic microstructures without undesirable alpha-iron phase.

In the frame of the UPGRADE project [P2], CEA-Liten implements its platform to optimize the SC process and to demonstrate the achievement of finer microstructure on large batches (up to 50 kg) of ribbons. The project implies European industrial partners playing a key role in the magnet value chain.

MATERIAL SAVINGS BY ADVANCED SHAPING PROCESS

The standard manufacturing route massively yields simple geometrical parts. Yet, the brittleness of sintered magnets upon machining leads to costly operations with high material loss (>30 %). Research on advanced shaping process of new magnets paves the way for a virtuous combination of innovation in machine design and raw material saving.

In this context, CEA-Liten is exploring Additive Manufacturing (AM) of magnets, notably the Laser Powder Bed Fusion (LPBF) process, and already obtained promising results, i.e. nearly dense 3D-printed parts with excellent magnetic properties (Figure 3). AM magnets performance intricately depends on the process parameters and a trade-off has been found to maintain the coercive microstructure of initial powder after fusion and re-solidification. A non-standard but commercially available gas-atomized coercive powder was used in the feasibility study. The scientific activities turn now to the upscaling of powder production [P3] as well as to a better understanding of the microstructure of NdFeB after LPBF.



Figure 2: Strip casting equipment for synthesising ferromagnetic alloys at CEA-LITEN.

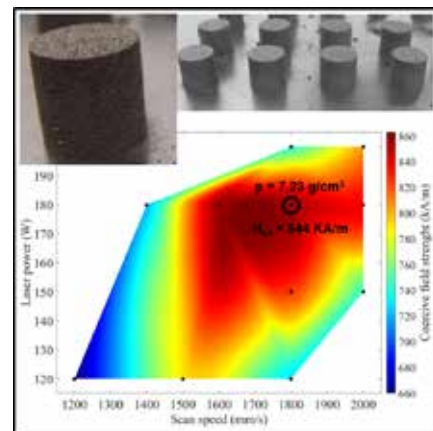


Figure 3: Cylindrical NdFeB magnets built by additive manufacturing with optimisation of process parameters (laser power and scan speed) leading to the best properties (coercivity and density)

Bonded magnets are an interesting alternative to sintered magnets despite their weaker magnetic strength because these composites are made of HREE-free ferromagnetic particles and are well suited for moulding. A specific application of bonded magnets consists in the direct injection of molten composite into rotors of electric machines. In the framework of the MODULED project [P4], an industrial partner developed a high-speed 150 kW electric vehicle motor with two variations of the rotor (with sintered / injected magnets). CEA-Liten was in charge to design a specific injection equipment for the rotor “overmoulding” operation; it includes a multipole coil-based magnetization system with advanced magnetic flux management, proper mechanical clamping, monitoring of the composite flux and thermal management. The challenge was to achieve high magnetic field (1 T) uniformly distributed in the rotor’s cavities during the injection. Extensive 3D electromagnetic finite-element simulations supported the tool design [6]. CEA-Liten delivered two complete injected and functional sets of rotor stacks. No deformation of the FeSi laminations occurred during injection and magnetic field mapping shows very good consistency with calculations.

RECYCLING THROUGH “MAGNET TO MAGNET” SHORT ROUTES.

The rapidly growing part of electrical machines in the energy transition technologies gives an opportunity to promote eco-design and reuse of end-of-life (EoL) products. With a content of about 300 g of rare earth per kg, EoL magnets constitute a valuable source. The flow of EoL permanent magnets will depend on the lifetime of motors and generators (10-15 years) and the collection efficiency but could cover at the end of the decade about 15-20 % of the rare earth demand for new magnets. The goal of the PERMAFROST project [P5] is to evaluate the efficiency of a short loop process to recycle large blocks of permanent magnets from wind turbines. CEA-Liten studied the feasibility of introducing EoL magnets as starting raw materials of the strip casting technique. After melting, re-solidified alloys can enter as standard semi-products (ribbons) in the manufacturing chain, avoiding REE extraction and separation. Thanks to a better understanding of the role of oxides during solidification, CEA-Liten established the concept feasibility on its magnet manufacturing pilot line and implemented the powder metallurgy route to build new sintered magnets. The magnetic performances of the

recycled magnets are comparable to those of the starting material: remanence $B_r = 1.34$ T and coercivity $H_{cJ} = 1178$ kA/m for the starting magnets and $B_r = 1.3$ T and $H_{cJ} = 1170$ kA/m for the recycled magnets.

The RECVAl project [P6] investigated a shorter route based on the direct conversion of used magnets into sinterable powder. The reaction of hydrogen with EoL magnets leads to the formation of Nd hydrides and, by swelling, to the decrepitation into a coarse powder, which is consecutively refined by jet milling under nitrogen. Lab-scale studies showed that this powder could not reach full densification during sintering due to oxygen contamination. However, mixed with fresh powder, recycled powder can be sintered to give magnets with properties very similar to those of the initial magnets ($B_r = 1.3$ T and $H_{cJ} = 950$ kA/m). The proportion of recycled material can reach 30 % with conventional powder and 50 % using a powder enriched with cobalt, less sensible to oxygen contamination. To achieve further progress on this topic, research on magnet recycling is currently being carried out using hydrothermal decrepitation of used magnets [P7].

THE MAGNETIC PERFORMANCES OF THE RECYCLED MAGNETS
ARE COMPARABLE TO THOSE OF THE STARTING MATERIAL: REMANENCE

<p>$B_R = 1.34$ T $H_{cJ} = 1178$ kA/m</p> <p>FOR THE STARTING MAGNETS</p>	<p>$B_R = 1.3$ T $H_{cJ} = 1170$ kA/m</p> <p>FOR THE RECYCLED MAGNETS</p>
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GENERAL PERSPECTIVES

Thanks to the technological platforms and the involvement of a multi-disciplinary scientific team, CEA-Liten obtained promising results towards the mitigation of critical materials in permanent magnets. Progress on the localization of heavy rare earths for thick magnets, on the additive manufacturing and on the valorization of end-of-life products has been accomplished. CEA-Liten involves European industrial leaders on these topics. Meanwhile, scientific challenges for developing RE-lean magnets are addressed. /

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Thesis defended

- [T1] B. Hugonnet, "Sintering and microstructure evolution during thermal processing of NdFeB magnets: effect on the magnetic properties", PhD thesis, Grenoble, 2016.
- [T2] J. Fliegans, "Coercivity of NdFeB-based sintered permanent magnets – Experimental and numerical approaches". PhD thesis, Grenoble, 2019.

Projects

- [P1] MagMono project, PTC CEA internal programme
- [P2] Upgrade project, KIC EIT Raw Materials
- [P3] 3DRemag project, KIC EIT Raw Materials
- [P4] Moduled project, H2020
- [P5] Permafrost project, KIC EIT Climate
- [P6] Recval project, ANR
- [P7] RAP project, ANR

STUDY OF HIGH TEMPERATURE GAS/SOLID PACKED-BED HEAT STORAGE SYSTEMS

Storage of intermittent renewable energy sources is of main interest to limit the use of fossil ones, especially for large electricity amounts. High temperature packed beds is an efficient solution and a validated simulation tools is of major interest for the development of such solutions. The goal of this work is to present such model and validation cases.



APPROACH

A packed-bed heat storage is a volume filled with rocks (granular) or with a structured media (see images). The model is based on a continuous porous media approach solving one mass conservation equation of the fluid and at least two equations of energy conservation. The model assumes one dimension behaviour (height of the packed bed) with thermal and hydraulic homoge-

neities in the cross-section. The model is discretized with the finite volume approach. Two important points in this model are the choice of correlations for heat transfer coefficient between the fluid and the media, and the effective thermal conductivity, which takes into account thermal conductivity, radiation and other phenomena. We studied experimentally such systems, with a dedicated high temperature (880°C) air loop and two different configurations. In one configuration, the system is filled with plates forming channels with obstacles to increase heat transfer efficiency with a total height of 5 m and a cross section of 0.8 m x 0.8 m. In the other configuration, the system is filled with basalt rocks of equivalent diameter 1.7 cm with a total height of 3 m and a cross section of 1.09 m x 1.09 m.

RESULTS AND PERSPECTIVES

Each packed-bed is instrumented with air flow-rate measures and with thermocouples distributed at inlet, outlet and in planes at different levels along height. Experimental procedure consists in the repetition of successive charge periods, with hot air (800°C) entering from the top and discharge periods with cold air (80°C) coming from the bottom. The analysis of inlet/outlet measurements allows calculating the energy which is loaded/unloaded at each period. After stabilisation process, for structured packed bed this value is 726 kWh_{th}, which lead to a volumetric capacity of 227 kWh_{th}/m³, compared with the granular one of 205 kWh_{th}/m³ (730 kWh_{th}). The model predicts very well these global values but also more detailed results like the evolution of temperature gradients along the height of packed-beds. The result presented on the figure below is interesting to show the good concordance between simulation and measurements but also to show that, during a long period, this storage system can deliver heat at a constant temperature during discharge. /

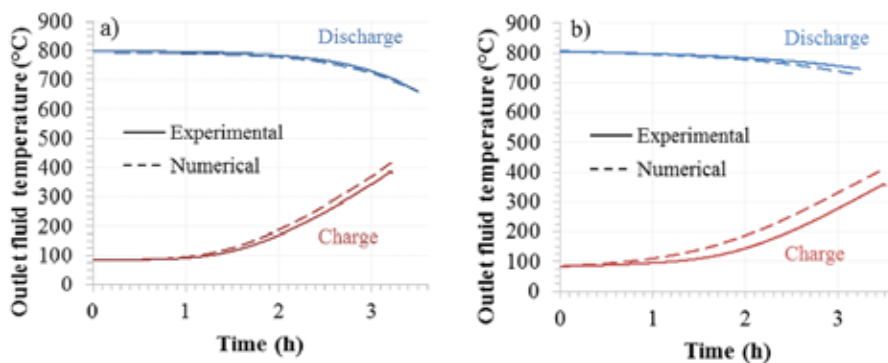


Figure: Evolution of outlet fluid temperature for (a) structured and (b) granular packed-beds.

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THERMALLY DRIVEN CHILLER TO ENHANCE TURBINE PRODUCTION DURING PEAK DEMAND

This numerical study concerns a nitrogen turbo-compressor used to generate electricity from a thermal source. The system is required to have the capacity to keep a reserve of power provided to the grid during peak demand. The additional production comes from an innovative thermodynamic cycle coupled to the main compressor.

APPROACH

An effective mean to efficiently provide a fast power increase during peak demand is to cool nitrogen at compressor inlet at a low level (-15 °C to 10 °C). Our strategy is to use a continuous source of low-grade heat (~100 °C) available at the turbo-compressor pre-cooler and to consider combined power and cooling technology. A first huge effort in this study has concerned the development of a complete dynamic modelling of a closed cycle nitrogen turbo-compressor, including all components (compressors, turbine, pre-cooler, intercooler, recuperation unit, intermediate heat exchangers, valves, tanks). In the frame of an internal collaboration with CEA-ISAS, we used the CATHARE software [1]. In a second step, we propose different architectures for the cold power production and the system optimization. Two technologies of thermodynamic machines using low temperature waste heat have been numerically compared to fulfill variable power and cooling requirements: ammonia-water absorption chiller and a thermally driven heat pump based on two Rankine cycles: Organic Rankine Cycle (ORC) and a vapor compression refrigeration (VCR) system. We have also used thermal energy storage tanks to charge and discharge cold thermal energy produced during low demand.

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RESULTS AND PERSPECTIVES

Three main criteria have been used to compare the different systems and strategies: total size (including machine and storage contributions), net power production and overnight cost (including machine and storage contributions). Size and cost evaluations are estimated through correlative approaches based on various databases. Cross-comparison between the two different combined power and cooling technologies shows the interest of absorption-based system on the three main criteria [2]. A particular configuration including an ammonia expander

to allow a supplementary power production during peak demand appears to be the most attractive (see figure below). Such innovative thermodynamic cycle has not the same technological maturity as other systems and a small prototype design is considered to confirm some numerical hypotheses and to investigate other parameters (complexity, maintenance, etc...). We point out that the ammonia-based solution remains interesting due to its negligible Global Warming Potential. Cross-comparisons with more traditional solutions based on hot temperature storage will complete these evaluations./

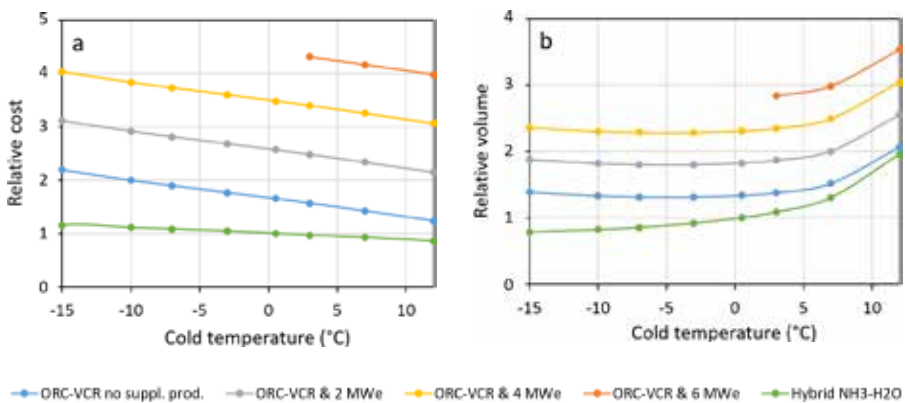


Figure: Comparison of (a) the overnight cost (left) and (b) volume of the different cold and power solutions.

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ECO-EFFICIENT EVAPORATIVE AND GROUND-COUPLED SYSTEM WITH TERRA-COTTA EVAPORATIVE WALLS

An innovative low-energy, low-tech and low-cost cooling system for buildings has been developed. This cooling system simultaneously makes use of three available heat sinks: the ground, evaporation of water and radiation to the sky. A terra-cotta tank is placed along a northern wall of the building to achieve the two last phenomena. This simple, inexpensive and energy-saving system was simulated on a 100 m² house in Bordeaux climatic conditions.

APPROACH

The main components of the system are shown on the figure below. The system follows a daily cycle. During the daytime, when the indoor house temperature exceeds the set comfort temperature, the pump (4) is turned on. The cool water passes from the storage tank (1) to the cooling floor (2), where it removes heat from the building and is then transferred back to the porous tank (3). When this porous evaporator is full, the three-way valve (9) sends water back from the cooling floor directly to the storage tank. During the following night, the water in the evaporator (3) is cooled due to evaporation, radiation and convection at the porous tank surfaces. In the morning, as soon as the temperature of the water

contained in the porous tank (3) increases, the automatic valve (5) opens and cool water flows from the evaporator into the storage tank (1). This closes the cooling cycle. The evaporator (3) is a vertical flat tank. The porous material proposed for this tank is terra cotta because of its very low cost, low embodied energy and it can have adequate properties for the evaporation process [1,2]. The storage tank (1) makes use of ground cooling because it is installed in the basement under the house and is thus in close contact with a large surface of ground. The storage tank can be a plastic flexible container, making its installation in the basement easy and its price low. This component is used both as a storage and as a heat exchanger with the ground.

RESULTS AND PERSPECTIVES

The heat exchanges of the storage tank with the ground in the basement play a very important part in the good functioning of the system and allow the system to adapt to heat waves efficiently. The terra-cotta evaporator, meanwhile, helps to cool down the storage tank and to operate at lower temperature levels, which guarantees high COPs (coefficients of performance) [3]. The complementarity between the different heat sinks allows maintaining good performance throughout the summer. In the Bordeaux climatic conditions, the cooling capacity of the system varies between 4500 and 1000 W depending on the period. The average performance coefficient is 24 in these climatic conditions, which is approximately 5 times greater than a conventional commercial air conditioner.

The system is very cheap and simple, as expected, and could be an efficient alternative to electrical compression chillers technology in terms of performance. Further research remains necessary to analyze long-term behavior and performance of this system. Here the description of the system focuses on a single-family house application. It can also be used, at a larger scale, for a collective building. /

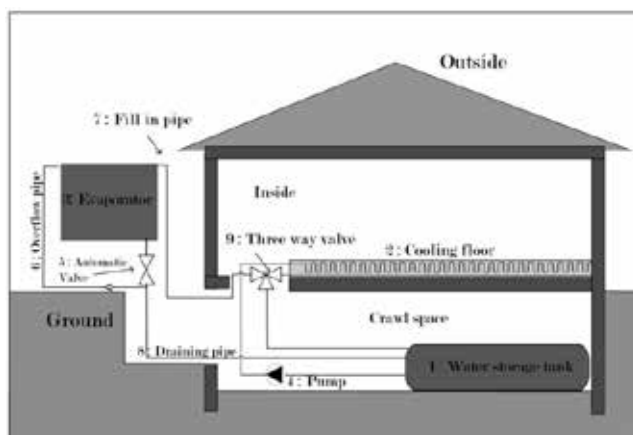


Figure: Cooling system integrated into a dwelling.

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SCIENTIFIC OUTPUTS

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YOUNG RESEARCHERS TESTIMONIALS

Louise Carton

PhD student, Liten

“ I did my graduate degree in engineering at INSA in Lyon. I went on to do my PhD research at Liten on the mechanical properties of the silicon wafers used to make photovoltaic cells with the goal of thinning the wafers to reduce raw materials costs without critically affecting mechanical resistance. I wanted to work in renewable energy, but I also wanted to become an expert in a highly technical field. The INES campus in Chambéry does research across the entire PV value chain and works closely with industrial companies, so it was a perfect fit for me. Winning the Liten PV Dissertation Award in 2019 was a particularly special moment that I will always remember.”

Akash Sonawane

PhD student, Liten

“ I am originally from India. I came to Grenoble to study materials science at an engineering school here. During my student internships, I was able to learn about additive manufacturing and I wanted to go further with it. Liten is a leader in additive manufacturing, so it was the ideal place for me to do my PhD on the 3D printing of aluminum alloy parts using laser beam melting. At Liten, I get an opportunity to interact with people who work in different disciplines and potentially find new applications for my research in other areas. I studied the cracking mechanisms that affect an aluminum alloy used in heat exchangers and came up with a solution to prevent cracking. I won several awards for my research, including Liten's 2019 Best PhD Dissertation award.”

Morgane Briand

PhD student, Liten

“ When I was in engineering school, I did my internship at Liten, where I worked on the technical and economic assessment of a hydrothermal liquefaction process used to produce high lower heating value biofuels from biomass. Liten asked me to stay on as a PhD candidate to pursue the project and support the development of the technology on a larger scale. In three years, we were able to move from batch production to continuous production on a lab-scale pilot line. I was given opportunities to present my research at a conference in Ireland and to a research group made up of biomass stakeholders in France.”

Thibaut Gutel

Habilitation senior scientist, Liten

“ I came to Liten in 2010, working on topics like organic electrode materials for lithium-ion batteries. These materials are derived from biomass or carbon-based chemistry and offer a potentially attractive alternative to critical materials. I had also worked on two EU projects and supervised three PhD dissertations on the topic, which represents around 30% of my research at the CEA. These were all factors that led me to apply for my certification to direct research. I earned the certification in December of 2019. Now that I am certified, I can play a more active decision-making role in the PhD research I supervise, suggest PhD research topics, and be asked to weigh in on PhD research supervised by other scientists. The certification has given me more freedom and broadened my horizons.”



PhD DEFENSE AT LITEN

RENEWABLE ENERGY PRODUCTION

Luis Gabriel ALVES RODRIGUES

Design and characterization of a three-phase current source inverter using 1.7 kV SiC power devices for photovoltaic applications, Univ. Grenoble Alpes (May 28, 2019).

Moussaab BENHAMMANE

Development of a power operational model for concentrated photovoltaic (CPV) systems, Univ. de Corse PASQUALE PAOLI (October 28, 2019).

Vincent BROHA

Thin film encapsulation of organic photovoltaic devices, Univ. Grenoble Alpes (January 31, 2019).

Elise BRUHAT

Development of industrializable homojunction silicon photovoltaic cells with passivated contacts, Univ. de Lyon (December 17, 2019).

Pia DALLY

Characterization of Perovskite systems: Understanding and improving the performance and stability of photovoltaic devices, Univ. Grenoble Alpes (November 29, 2019).

Nouha GAZBOUR

Systemic integration of Eco-design in photovoltaic technologies R&D, Univ. Grenoble Alpes (February 14, 2019).

Marc-Antoine LLOBEL

Development and application of characterization methods applied to stability studies of organic photovoltaic modules manufactured by roll to roll, Univ. Grenoble Alpes (April 2, 2019).

Audrey MORISSET

Integration of poly-Si/SiO_x contacts in silicon solar cells: Optimization and understanding of conduction and passivation properties, Univ. Paris-Saclay (December 11, 2019).

Manon SPALLA

Intrinsic stability of perovskite solar cells: Impact of active layer formulation and charge transport layers, Univ. Grenoble Alpes (October 16, 2019).

ENERGY GRID MANAGEMENT

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Innovative solid electrolytes for Li-ion battery: Multiscale structure and transport properties in ionic liquid crystals, Univ. Grenoble Alpes (January 30, 2019).

Marie BICHON

Evaluation and optimization of the cycle life of water-based electrodes for new generation Li-ion batteries, Univ. De Nantes (November 28, 2019).

Nicolas DUFOUR

Physics-based modeling of graphite electrode inside Lithium-ion battery: Study of heterogeneities and aging mechanisms, Univ. Grenoble Alpes (February 8, 2019).

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Jorge MORALES

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Hamza MOUSSAOUI

Microstructural optimization of Solid Oxide Cells: A coupled stochastic geometrical and electrochemical modeling approach applied to LSCF-CGO electrode, Univ. Grenoble Alpes (April 29, 2019).

Amélia NADAL

Impact of uncertainties on the techno-economic optimization of hybrid energy systems, Univ. Grenoble Alpes (November 22, 2019).

Philip OVERTON

Mono-EndCapped Single-Ion Polymer Electrolytes: Synthesis & Lithium-Ion Transport Properties, Univ. Grenoble Alpes (March 27, 2019).

Sandrine RODOSIK

Study of the Impact of Innovative Fluidic Architectures on the Management, Performance and Sustainability of PEMFC Fuel Cell Systems for Transportation, Univ. Grenoble Alpes (November 8, 2019).

Anthony ROY

Optimal management of a multi-source system for an isolated offshore site, Univ. De Nantes (December 5, 2019).

Guillaume TONIN

Li/S accumulators: Electrochemical mechanism investigation using operando analysis by absorption and X-Ray diffraction tomography, Univ. Grenoble Alpes (June 5, 2019).

REDUCING THE OVERALL ENERGY FOOTPRINT

Materials and processes

Romain CHARIERE

Development of new lightweight polymer composite materials based on modified hollow microspheres, Univ. Paris-Saclay (December 20, 2019).

Mathias COUDRAY

Process for recycling fuel cell membrane electrode assemblies (MEAs) using ionic liquids, Univ. de Lyon (December 9, 2019).

Yoann DINI

Carbon nanotube yarn electrical transport study: From experiments to semi-empirical modeling, Univ. Grenoble Alpes (October 7, 2019).

Jérôme FLIEGANS

Coercivity of NdFeB-based sintered permanent magnets: Experimental and numerical approaches, Univ. Grenoble Alpes (December 16, 2019).

Lucas GIVELET

Detection and characterization of titanium dioxide nanoparticles by AF4-ICP-MS and Sp-ICP-MS, Univ. Grenoble Alpes (June 21, 2019).

Simon PUYDEBOIS

Hydrogen embrittlement on the low cycle fatigue behavior of laser beam melting Inconel 718 (LBM), Univ. Grenoble Alpes (February 13, 2019).

Meryem TAZI

Physico-chemistry of vitreous carbon brazing: Wetting and interfacial reactivity, Univ. Grenoble Alpes (December 6, 2019).

Nicolas TISSOT

Improvement of the LBM process by nanostructuring aluminium powders, Univ. de Lyon (March 29, 2019).

Energy efficiency

Nadine AOUN

Modeling and flexible predictive control of buildings space-heating demand in district heating systems, Univ. Paris-Saclay (December 2, 2019).

Noé BEAUPERE

Controlling the release of heat and studying the ageing of phase change materials, Univ. de Lille (November 7, 2019).

Clément BEUST

Multi-scale modelling of a thermal energy storage system with Phase-Change Material (PCM) for the thermal storage of steam, Univ. de Pau et des Pays de l'Adour (October 24, 2019).

Isabelle CHAMPON

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Tilila DAHOU

Contribution to the understanding of the role of inorganic elements in biomass steam gasification, Univ. Grenoble Alpes (December 13, 2019).

Léa GONDIAN

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Laura GUIMARD

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HDR* DEFENSE AT LITEN

STORAGE FOR ENERGY GRID MANAGEMENT

Thibaut GUTEL

Organic electrode materials, a viable alternative for future batteries? (December 13, 2019)

Loïc SIMONIN

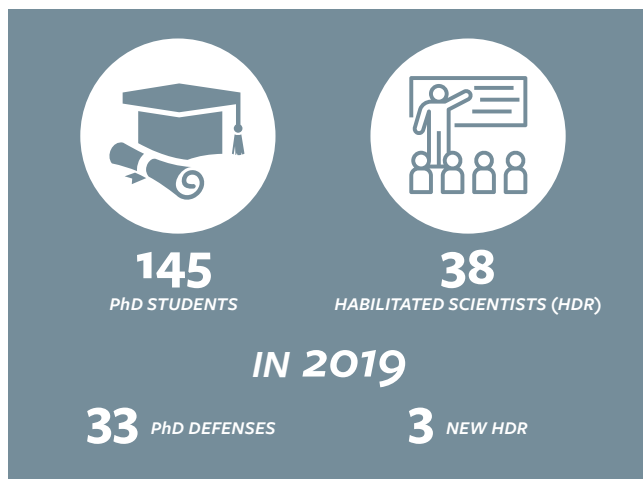
From active battery materials to a complete system (September 26, 2019)

REDUCING THE OVERALL ENERGY FOOTPRINT

Amélie REVAUX

Functional printed materials, from optoelectronics to pyro-electricity (April 30, 2019)

*HDR : accreditation to supervise research



2019 AWARDS



Elise Bruhat
Best student award EU PVSEC 2019



Emmanuel Billy
Improving lithium-ion battery recycling
Recycling Innovation Award in the Innovation in Academic Research category
French Federation of Recycling Companies (FEDEREC)



Maria Gonzalez Martinez
2019 PhD award
Société Française de Génie des Procédés
www.sfgp.asso.fr/2019/10/15/prix-de-these-de-la-sfgp

2019 Innovation award
Académie des Sciences de Toulouse
www.academie-sciences-lettres-toulouse.fr/?p=4634

**Caroline Celle,
Jean-Pierre Simonato,
Djadidi Toybou**

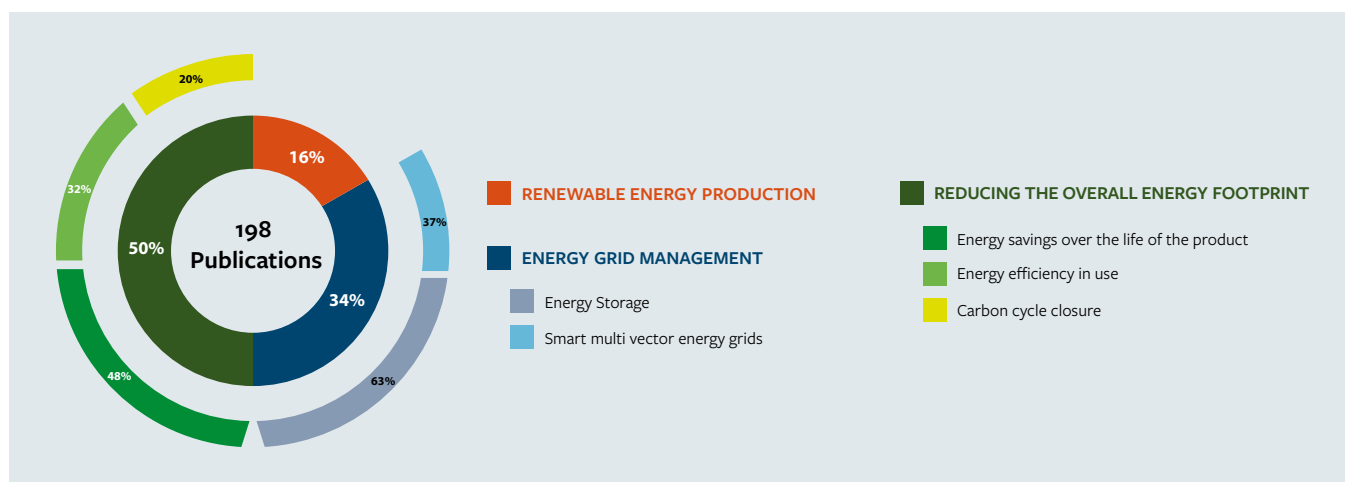
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Didier Bouix
Energy Observer project
Mission Innovation Champions award

Viet Huong Nguyen
2019 PhD thesis award
Division de Chimie du Solide de la Société Chimique de France



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- 3. Round Robin Test for the comparison of spectral emittance measurement apparatuses**
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- 4. Characterization of different Moroccan sands to explain their potential negative impacts on CSP solar mirrors**
A.-C. Pescheux et al., Solar Energy - DOI: 10.1016/j.solener.2019.11.020
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- 6. Modelling of a converging/diverging tube using CATHARE-3 two-phase flow system code for sodium cavitation studies**
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- 9. Characterization of dual-junction III-V on Si tandem solar cells with 23.7% efficiency under low concentration**
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