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PU	Public	
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RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	X

Approvals

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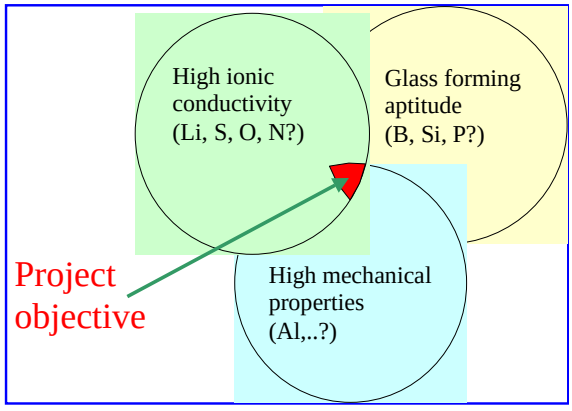
Project execution

Project objectives

Hi-Condelec project was dedicated to the **development of thin films of a high conductive solid ionic conductor for Lithium.** Promising **applications** areas for thin film manufactured materials are **micro batteries** (electrochemical energy storage), **micro-supercapacitors** (energy impulsion) and **electrochromic devices** (ie. smart windows or displays). The challenge lies in the development of solid electrolytes (glasses and crystallized materials) and thin film technology that would provide new physical properties (very high ionic and electronic conductivity) and increased chemical and mechanical stability. Thin film solid electrolytes require rather specific properties that sometimes are difficult to obtain at the same time, therefore the main S&T objective of the HICONDELEC project was to develop **fundamental knowledge in order to enable an optimum design of the solid lithium conducting glass electrolytes with predefined physical and chemical characteristics.** A multidisciplinary RTD approach combining simulation, theory, experiment, validation and use was chosen, in order to maximise the fundamental understanding of ionic and electronic conductivity phenomena and thermo-electro-mechanical behaviour.



HICONDELEC had developed powerful computational tools for materials modelling related to:

- Materials behaviour: for the investigation of the fundamental mechanisms of ionic and electronic conductivity and their interaction with thin film properties, integrating multi-scale simulations from the atomic scale to the glass structure scale (from 0.1 to 10 nm)
- Materials processing and use: for the investigation of the mechanical behaviour and stability of the thin film electrolyte prepared by sputtering, of the stack integration process and of its use.
- In addition, modelling was based on and supported by properties measurements thanks to appropriate characterisation techniques of electrical, mechanical, thermal, environmental and optical properties of the thin film electrolytes

The starting point of the research work were material systems including nitrided borate and sulphate anions of the $(1-y)[0.5B_2O_3\ 0.5Li_2O]\ yLi_2SO_4$ family.

Contractors involved

The HICONDELEC consortium included first Chalmers, TU Ilmenau, NHRF, WWU, UNIMAR, HUT, IST and ENSCPB **high level research centres** with complementary expertise in the fields of modelling and experimental characterisation of ionic and electronic conductivity and thermo-electro-mechanical behaviour of glass like materials (bulk or thin film).

And second, in order to validate the generated knowledge for certain applications, **industrial technology providers** have been added for scaling up and property validation purposes: CTI (PVD target manufacturer), HEF (microbattery), CEA (micro super-capacities), SGR (electrochromic systems).

A consulting company, Alma participated also to the project regarding project management activities.

Full names of **partners** are given below:

HEF R&D (France)

Chalmers University of Technology (Sweden)

Technische **Universität Ilmenau** (Germany)

National **Hellenic Research Foundation** (Greece)

University of **Muenster** (Germany)

Helsinki University of Technology (Finland)

Instituto Superior **Técnico** (Portugal)

Ecole Nationale Supérieure de **Chimie et Physique** de **Bordeaux** (France

Céramiques et Techniques Industrielles (France)

Commissariat à l'énergie atomique (France)

Saint Gobain Recherche (France)

Alma Consulting Group (France)

Phillips-**Universität Marburg** (Germany)

Scientific approach

To achieve its ambitious objectives, apart the management tasks, the HI-CONDELEC work programme has been split down into 5 work packages:

- 1 work package (WP0) dedicated to the **R&D approach strategy and management of knowledge**, including review of the requirements for characterisations and modelling, integration of the results by all partners to give further orientations on electrolyte to consider and knowledge management (intellectual property right, transfer of skills and expertise within the consortium, and exploitation plan)
- 2 work packages dedicated to the set up and running of simulations (**ionic and mechanical)** that will be performed in parallel all along the project to **model the solid state thin film electrolyte** (WP1 and WP2)
- 1 work package (WP3) that will deal with **materials engineering of thin film**, i.e. including the preparation of thin films to be characterised and modelled, the development of appropriate targets for chosen electrolytes and preliminary industrial tests for a first assess of the integration of the new electrolyte into industrial environment by test on large targets
- 1 work package (WP4) dedicated to the **integration** of the selected electrolytes into complete systems: micro-batteries, microsupercapacitors and electrochromic cells for further evaluation

The objectives of main technical WPs are given below:

WP0 - R&D approach and knowledge management

- define requirements for characterisation samples
- ensure integration of the results from the modelling teams (WP1 and WP2) and materials engineering teams (WP3) and update the HI-CONDELEC R&D orientations
- prepare the industrial exploitation of the HI-CONDELEC results
- communicate the results of the projects outside the consortium to ensure their dissemination within the scientific community

WP1 - Ionic and electronic modelling

- suggest favourable anions for glassy electrolytes from ab-initio calculations
- model the fundamental physics of ionic conductivity
- relate the glass structure to transport properties

- conclude on rate limiting factors for high ionic conductivity of thin film solid electrolyte and understand how to obtain high ionic conductivities

WP2 - Mechanical modelling

- develop a complete modelling approach for thin film assemblies under combined thermal, mechanical and electrical evaluation
- carry out optimisation of the thin-film assemblies for the project applications
- validate the model by experimental feedback and recommend the best design of the component
- identify the critical factor(s) controlling fracture point and durability of the system

WP3 - Materials engineering on solid-state thin film electrolyte

- Experimental studies on electrolyte elaboration: determination of the sputtering parameters for the preparation of electrolyte thin films
- Experimental research on materials (gradients of composition): preparation of series of materials in order to investigate the ionic conduction mechanisms
- Preparation of the integration of the thin films into application systems by preliminary studies on large scale targets and deposition parameters

WP4 - Integration into application devices

- integrate the developed electrolyte into the final object. WP1 to WP3 will define optimised composition and structure of electrolyte.
- the electrolyte will be integrated into the stack representative of its application (Microbattery, Microsupercapacity, Electrochrome).
- for each of its application it will be necessary to adjust the optimisation according to its specific stack.

Work performed

WP0 - R&D approach and knowledge management

This work package allowed the consortium to have a common meeting place for managing scientific, technological, communication and exploitation issues. Through this WP samples were defined (nature, shape, number), results from modelling and experiment were synthesised and provided material guideline for their selection along the project, dissemination issues were discussed, and exploitation results were identified and selected.
An exploitation seminar was organised. No specific issue regarding IPR strategy was raised. The very high level of dissemination and related quality is acknowledged thanks to 11 publications done within the project. Some exploitable results have also been identified among which target manufacturing (secret), target bonding (patent) and mechanical design software for thin film stacking (copyright).

WP1 - Ionic and electronic modelling

We have used several different tools in order to model the structure and properties of the thin-film glass electrolytes. The methods range from ab-initio calculations, modelling structure and interactions on a local scale (up to 100 atoms), through molecular dynamics (MD) simulations (up to 1000 atoms) to reverse Monte Carlo/bond valence sum calculations and Monte Carlo simulations over large configurations (up to 10000 particles). The combination of these methods provides a multi-scale approach to the project. The ab-initio calculations provided information on most probable local structures in the glasses and on Li-ion sites. MD-simulations and RMC/BVS methods provided information also on the conduction pathways and their connectivity in the structure and thus connecting to the long-range ionic transport in the material. The Monte Carlo simulations, were together with analytical theoretical calculations, used to investigate confinement effects and non-linear conductivity effects in disordered structures such as glassy electrolytes. An integration of the modelling tools was in particular made by using ab-initio methods for the development of new potentials for MD-simulations of borate glasses as well as the evaluation of Li-ion sites and conduction pathways by combining MD and BVS results.

As input for, and validation of, the simulation methods we have performed extensive characterization of the thin-film electrolytes prepared in WP3. We have used vibrational spectroscopy (micro-Raman and infra-red) and x-ray diffraction to investigate the structure and dielectric spectroscopy to characterize the conducting properties of the thin film electrolytes. In almost all cases the application of these methods to thin-film samples was by no means standard at the start of the project. Thus a considerable effort was devoted to develop methodologies to suite thin-film applications. A prime example is here the development of a theory to model the infra-red (IR) spectra of thin-film materials based on optical constants of bulk materials. Another key development was the implementation of the dot-shaped electrode geometry to measure the conductivity of the thin-film electrolytes.

In addition to determining basic materials properties, the characterization also provided valuable information from a technological point of view. For instance, the homogeneity, with respect to both composition and conductivity, of the thin-films was investigated as well as annealing effects, of importance for the long term practical use of the thin-film electrolyte.

Combining the modelling and characterization results we have been able to guide the direction of the development of new electrolyte compositions in the project. An example is the Midterm review where we suggested two new glass compositions: $0.7Li_2SO_4$-$0.1LiPO_3$-$0.2LiBO_2$ and $0.2Li_2SO_4$-$0.8LiBO_2$. After synthesis and characterization it was clear that these two materials show promising conductivity ($5\cdot10^{-6}$-$1.5\cdot10^{-5}$ Scm^{-1}) even though there are indications that the sulphate rich glass has stability problems. In detail the highlights of the combined effort of the work package include:

- Showing that the actual composition of the glass electrolytes differs from the nominal target compositions. Specifically there was a loss of Li-ions in the sputtering process and thus we are moving in the phase diagram during the preparation procedure compared to the target composition. This effect, found to be more pronounced for materials sputtered in Argon compared to Nitrogen, is important to take into account when deciding on the target composition in an R&D project on thin-film electrolytes.
- Revealing the role of nitrogen in thin-film glass structures. It has been a well know, but poorly understood, fact that the incorporation of nitrogen in the sputtering plasma increases the stability of the material. By combining ab-initio calculations and vibrational spectroscopy we showed that in the most probable structure in a salt glass the nitrogen atoms are located in close proximity, almost forming a nitrogen-nitrogen bond. This provides a steric constraint on the structure and thus increases the stability towards crystallization.
- Showing that the nitrogen flow rate is a key parameter for determining the properties of thin–film electrolytes. From modelling of IR-spectra it was found that the structure of Li-borate glasses is progressively changed as the flow rate is increased and new structural species could be identified.
- Showing that the dot shaped electrode geometry results in more reliable values of the conductivity. This is an important result as it was found that the bar-shaped geometry, which is the standard method both in academic and industrial research, overestimates the conductivity by a factor of 3. The origin of this effect is most likely linked to a coupling between the electrodes in the bar geometry through surface conductivity
- Establishing a new scheme to develop inter-atomic potentials for MD-simulations, based on ab-initio methods. In this new scheme a start configuration, based on an educated guess or a known structural unit, was geometry optimised and the potential energy landscape scanned. The potential is then determined in a parameter fitting routine that includes the comparison of calculated vibraitonal modes to experimental results. This approach allows the development of MD-potentials for a wide range of glass materials without extensive a priori knowledge of the glass structure.
- Developing a theory for the interpretation of non-linear conductivity experiments. This is of importance for investigations of thin film electrolytes where the electric field can be very high even for moderate applied voltages due to the small thickness of the film. The theory was developed by combined analytical calculations and Monte-Carlo simulations.

- Determining the connection between the intermediate range order in the glass structure and the conductivity from RMC/BVS calculations. It was shown the a large intermediate range order is not always beneficial for the conductivity

With these results we have increased the knowledge of the ion conducting process in glasses in general and those in thin-film glasses in particular. We have also added valuable information on technical and process related issues of importance for industrial R&D. The work has resulted in a number of presentations at international conferences and in a number of scientific articles published in international journals of high repute, see further in section 2 below.

WP2 - Mechanical modelling

The mechanical characterization of thin films deposited from different Li-contained targets under N_2 and Ar atmosphere was performed and elastic and deformation properties have been identified. Bend tests were performed using nanoindenter to assess Young modulus, yield strength, rupture and fracture deflections. Young modulus and yield strength were also assessed with ultramicrohardness testing and they are in a good agreement with the data reported in the literature. Density was estimated by Rutherford Backscattering Spectroscopy.

Using these data, a complete thermo-mechanical modelling approach was developed and analyzed for thin film assemblies (2-D linear plate theory) which simulate the whole process of coating of different layers with variable thicknesses and processing parameters as well as 3-D modelling has been done.

Algorithm for analytical calculation of stresses and strains of thin film assemblies (TFA) under elastic regime (including assembly processing and thermal cycling) was developed. The linear plate theory application for a TFA microbattery was applied to get thermal stresses originating due to processing because layers made on the substrate are being made in rather different conditions. TFA curvature, stress and strain distributions were calculated versus processing history. The data indicate substrate temperature and the consequence of processing cycles may give an additional degree of freedom to manipulate stress state in the TFA. Additional heating or cooling of the substrate at some stage might change thermal strain and its distribution to produce lower stresses.

TFA have been simulated from the point of view of thermal and mechanical evaluation. As the result of such simulations the optimisation of these assemblies has been done. The processing history was for the first time accounted and incorporated into calculation of residual stresses and strains by iterative procedure. These different factors were used with micromechanical modelling and linear plate theory and the whole procedure was implemented into a “Working Model” (WM) Excel file, which presents an important tool for quick assessment of the TFA manufacturing process. Special software to (a) count anisotropy of elastic properties and (b) to implement a working model for flat TFA stress, strain and curvature analysis has been developed. The software was proven to be useful for estimation of the planar TFA instead of FEM before moving into a realistic 3-D design.

Numerical FEM analysis was implemented in both 2-D and 3-D cases to see effect of anisotropy and to discover whether LPT model would provide an adequate estimation of stresses. Tests were made with silicon and TGO layer. CTE values for silicon single crystal in the range of 20…850°C have been experimentally determined using dilatometry and the anisotropy was explicitly introduced into calculations. Experimental independent data ensure an excellent agreement with calculated data in both LPT and FEM approximations. The realistic 3-D model of the microbattery was created and has been analysed in respect to stresses and strains.

WP3 - Materials engineering on solid-state thin film electrolyte

The best thin film electrolytes up to now are made from oxide materials deposited using reactive radiofrequency sputtering under a pure nitrogen atmosphere. The resulting amorphous oxynitride thin films exhibit an improved ionic conductivity and a better chemical stability. The nitridation mechanisms are still much debated, and the role of the various sputtering parameters (pressure, power, target-substrate distance, etc) is not well understood. However, it is a crucial point to incorporate as much nitrogen in the thin film as possible. In this project, a new key parameter for the incorporation of nitrogen has been evidenced. It has been shown that the role of the nitrogen flow, at a given pressure, is decisive. A flow variation at a constant pressure in the chamber is obtained by varying also the pumping flow thanks to a throttle valve. The amount of incorporated nitrogen in the thin film, measured using electronic microprobe and nuclear reaction analysis, increases with increasing nitrogen flow rates. It can be modified from a value close to 0 to one third of the initial oxygen content. This phenomenon has been explained by taking into account the outgasing of the chamber. The materials studied in this project were mainly borate glasses, which have been shown to be nitrided such as phosphate glasses.

Various thin film compositions were prepared and sent to the characterisation teams. They are based on lithium borate glasses, but the effect of the addition of a doping salt has been studied, as well as the mixed former effect. Thin films were deposited on various substrates depending on the characterisation method to be performed: amorphous carbon for Rutherford backscattering spectroscopy and nuclear reaction analysis, silicon for infrared spectroscopy, nitrided silicon for ionic conductivity measurements, with stacked blocking electrodes (platinum or stainless steel) and lithium cobalt oxide non-blocking electrodes. The thickness of the thin film electrolyte was between 200 nm and 4 µm. For the best material that has been prepared, the ionic conductivity is 10^{-5} S/cm. A slightly different material has a lower ionic conductivity but with a very good chemical stability. These materials are among the best thin film electrolytes.

Large size sputtering targets have been fabricated during this project. For laboratory sputtering machines, the target is usually a 5 cm diameter disk, with a thickness of few millimetres. Industrial or semi-industrial sputtering machines are equipped with far larger targets, in order to increase the deposition speed. They can be typically rectangular targets, with sides of few tens centimetres. The preparation of such targets by pressing commercially available powder chemicals is a challenge, and at the beginning of the project, no company in Europe was able to produce such targets. One of the partners of the project has developed a

preparation procedure that enables to fabricate dense and solid targets. It involves special additives and a particular thermal treatment. It is important to note that the knowledge gained in the field of the fabrication of targets for electrolyte thin film can be extended towards many other thin film materials such as zirconium oxides for fuel cells, or conducting transparent oxides for solar cells, or perovskite oxides for thin film capacitors etc.

These large targets have been tested in semi-industrial facilities by some of the partners of the project. It has been shown that they behaved satisfactorily under the application of high power plasmas. In particular, they do not delaminate nor brake and the plasma is stable. A special care has been taken to bond the ceramic target to its copper baking plate. One of the partners has developed an original and simple bonding procedure. This procedure was satisfactorily tested by several partners to deposit electrolyte thin films and finally to prepare microbatteries and electrochromic devices.

WP4 - Integration into application devices.

Three types of applications were targeted: thin solid film microbatteries; microsupercapacitors and electrochromic windows. Solid state electrolytes developed within the project and selected in WP0 were integrated into the devices. The most promising materials ranged in the $10^{-5}Scm^{-1}$ ionic conductivity at room temperature so that it was not interesting to integer it into microsupercapacitors that require $10^{-4}Scm^{-1}$. Thus, it was decided to try two types of electrolyte for microbatteries, one material at HEF premises with sulphur from a Li3PO4-LiBO2-Li2SO4 target and another material at CEA premises without sulphur from a Li3PO4-Li2SiO3 target. All the target ceramic tiles were assembled to their backing plate thanks to an original and patented process developed by HEF during the project. The best laboratory result with a 50mm diameter target sputtered under nitrogen and with the sulphured electrolyte ranged in the $10^{-5}Scm^{-1}$ ionic conductivity at room temperature, but when applied in a bigger reactor with 440x140mm squared sputtering targets, the conductivities obtained only ranged in the $10^{-7}Scm^{-1}$. This was explained by the particular sputtering situation (small target, large chamber and high nitrogen flow on one side and big target -30 times bigger- and lower nitrogen flow; this is more detailed in WP3). In addition, it was found that the statistic of shorted batteries was too high with this electrolyte.

A second material based on a Li3PO4-Li2SiO3 target sputtered under nitrogen was integrated into microbatteries stacking, provided very promising results with conductivity in the $10^{-6}Scm^{-1}$, a bit higher than LiPON. It exhibited a perfect mechanical resistance to thermal cycling like Solder reflow one that is necessary for integrating the batteries into Microsystems. All the characteristics of this LiSiPON type electrolyte are valid for the building of microbatteries.

Electrochromic windows sandwich incorporated a sulphur free electrolyte. A LiSiPON type electrolyte were also selected and deposited at SGR by sputtering under nitrogen from a Li3PO4-Li2SiO3-Li2O target. In this case, the distance from target to substrate is small (few cm) and the electrolyte thickness is also smaller than in batteries (1µm range for the batteries that must withstand large Li transfer to optimise capacity; 0.2µm range for smart windows that must optimise commutation time with the lower Li amount). Electrochromic windows require large area ($1m^2$ range while microbatteries are in the cm^2 range). While the theoretical ionic conductivities obtained with this LiSiPON are largely sufficient, sputtered electrolyte

films exhibited a two large number of pinholes (short circuits) to match the electrochromic windows requirements. It was successfully attempted to build-up a composite electrolyte made of three layers with the same total standard 0.2µm thickness, the sputtered LiSiPON between two standard SGR electrolyte films. The commutation time became 5 times the standard one, probably because of additional interface resistance thus created. Thus, it was demonstrated that the LiSiPON electrolyte properties could match the electrochromic windows requirements but that a particular attention should be paid to film defects.

In conclusion, good laboratories results can hardly be transferred to integration into devices on industrial or semi-industrial plant. Some scale effects are to be understood and taken into account. Special attention should be paid to vacuum quality, nitrogen feeding and nitrogen flow. For large surfaces and small thickness like the one used in smart windows, a specific development should be done regarding pinholes managing. This imply composition adjustment and also reactor geometry, deposition mode (is sputtering adapted to this application?). Nevertheless, one LiSiPON composition provided very encouraging results for microbatteries, slightly better than the LiPON reference, as well from ionic conductivity than on thermomechanical behaviour.

Achievements versus objectives and state-of-the-art

WP réf	State-of-the art at project start	Project objective	Project achievement	Additional comment
WP1	Relation between the structure and conductivity of thin-film electrolytes not well developed.	Determine factors related to increased conductivity to guide synthesis of new materials	Key factors of thin-film electrolytes established, such as the role of nitrogen, and new directions for the synthesis of thin-film electrolytes in the project proposed.	-
	Structure and properties of thin-film electrolytes not well characterized and no standard methods available	Characterize thin-film electrolytes to determine properties and provide input for simulations.	Developed several new methodologies to investigate thin-film electrolytes enabling characterization of materials in a standardized way.	Several of the methodologies will become standard in both academic and industrial projects on thin-film materials
	Non-linear effects of ionic transport not understood	Study non-linear conductivity effects by analytical calculaitons and modelling	New theory for non-linear conductivity in disordered structures developed	-
WP2	Stresses evolution during TFA manufacturing and use were not exactly known	Predict maximum stress and strain distributions that can be generated in the electrolyte and in the stack during its preparation, assembly and use	Materials behaviour in TFA was simulated vs. processing parameters, geometry and state of charge (SOC)	Algorithm for calculation of stresses and strains of TFA under elastic regime (including TFA processing and thermal cycling) was established
	Factors affecting stability of TFA from thermal-mechanical point of view were not exactly known	Determine critical factors of TFA structure vs. mechanical stability	Several critical factors have been identified for microbattery, micro-ultracapacitor and electro-chromic glass	New data on properties of deposited electrolyte glasses (modulus, Poisson's ratio, thermal conductivity, thermal behaviour, yield, density, deflection, etc.) were experimentally measured

WP réf	State-of-the art at project start	Project objective	Project achievement	Additional comment
WP3	Nitrided lithium phosphate based thin films were the only competitors	Design thin film materials with high ionic conductivity, good mechanical and chemical properties and glass forming ability	Lithium borate based thin films can be nitrided and exhibit performances at least similar to the existing materials	A decisive break-through in terms of performances probably requests a new design concept
	Sputtering parameters effect on nitrogen incorporation were not clearly understood	Determine the role of the sputtering parameters	A new key parameter for nitrogen incorporation evidenced: the nitrogen flow rate	This result can be used to design chambers for reactive sputtering more efficiently
	No European company able to fabricate large size oxide sputtering targets	Prepare large size targets for thin film electrolyte deposition	Development of a fabrication process for large size targets	This knowledge can be applied to other fields than electrolyte deposition
	Target to baking plate bonding methods expensive and inefficient	Test large targets in semi-industrial equipments	New target bonding procedure	This method can be used for any sputtering target
WP4	For microbatteries: LiPON or LiPON(B) type electrolyte.	10 times better conductivity with good thermomechanical stability and good chemical stability.	One LiSiPON with slightly better conductivity, excellent chemical stablility and better thermomechanical stability.	Unexpected scaling effects detected and partly understood, providing new reactor design input.
	For microsupercapacities: no reference available.	10 times better conductivity with good thermomechanical stability and good chemical stability. But exact specifications not well known.	No electrolyte with a sufficient conductivity achieved. 100 times better than LiPON is required	
	For smart windows: proprietary electrolyte	10 times better conductivity with good thermomechanical stability and good chemical stability.	No satisfactory result because of film defects.	Is sputtering adapted to large area and thin electrolyte?

Impact of the project on its industry or research sector

WP ref.	Expected impact at project start	Actual estimated impact of the project	Further activities to carry on to bring results to the market
WP1	Developing an understanding of factors influencing the conductivity thin-film electrolytes to be able to guide synthesis	Several factors determined concerning both basic structural property relationships as well as relations to process parameters and conditions. New optimum compositions suggested based on the acquired knowledge.	Both the new scientific results and new methodologies developed in the project are expected to be used in future R&D projects in both academia and industry. All results are published and thus available to the scientific community.
WP2	Improvement of mechanical stability of Li-ion TFA	Algorithm of the mechanical optimisation of mechanical parameters (stresses and strains) was developed, critical factors have been identified and the procedure established.	A new knowledge for thermal-mechanical behaviour of TFA was obtained (influence of processing and geometry on stresses and strains) – not previously considered in industry. To exploit it, a software tool was developed and delivered for partners for further testing.
WP3	New thin film electrolyte materials	New families of materials have been developed.	More industrial development is required
	Creation of industrial know-how to fabricate oxide sputtering target	A target fabrication procedure and a target bonding procedure have been developed	A market study is required
WP4	New exploitable electrolyte for microbatteries, microsupercapacitors and smart windows.	One exploitable electrolyte for microbatteries, but none for microsupercapacitors and maybe one for smart windows but after huge development at reducing film defects (pinholes).	Integer the microbattery containing the new electrolyte into devices. Microbattery is not as usual batteries, to provide its all potential it should directly be integrated into Microsystems.

Dissemination and use

Exploitable results:

Result (description)	**Sector**(s) of application	**Timetable** for commercial use	Patents or other IPR **protection**	**Owner** & Other Partner(s) involved	**Contact details** (name, phone, e-mail)
Target bonding procedure	Target sputtering manufacturing. Flat plate assembling.	Can be used now.	French Patent pending Mars 2007	HEF	Michel Martin mmartin@hef.fr +33 438 78 31 47
Algorithm of stress state calculation of TFA	Mechanical modelling of thin film stacking.	Integrated in the modelling software	None sought	HUT	Michael Gasik mgasik@cc.hut.fi +358-94512769
Thin film stack mechanical modelling	Mechanical design software tool for thin film stacking.	To be evaluated, first release at M36, updated release Summer 2008.	Copyright is applied	HUT	Michael Gasik mgasik@cc.hut.fi +358-94512769

List of publications:

- Comparative Study of Ion Conducting Pathways in Borate Glasses A. Hall, S. Adams, J.Swenson Physical Review B 74, 174205 (2006)
- Modelling multilayer systems with time dependant heaviside and new transition functions by Y. Bilotsky et al Proceeding of the Nordic COMSOL Conference 2006 Copenhagen, p.11-14
- Comparison of ionic sites and diffusion paths obtained by molecular dynamics simulations and bond valence analysis, C. Müller, E. Zienicke,S. Adams, J. Habasaki, P. Maass Physical Review B 75, 014203 (2007)
- Structure of glass thin films by infrared techniques, E.I. Kamitsos, M. Dussauze and C.P.E. Varsamis, Review article accepted for publication in Phys. Chem. Glasses: Eur. J. Glass Sci. Technol. B. (2007)
- IR spectroscopy of Li-diborate glassy thin films" E.I. Kamitsos et al. J. Non-Crystalline Solids 353,1818 (2007).
- Thin film glassy electrolytes: structure and composition by experimental and simulated infrared spectra", E.I. Kamitsos, M. Dussauze, C.P.E. Varsamis P. Vinatier and Y. Hamon, J. Phys. Chem. C 111, 8111 (2007)
- Structure of glassy lithium sulfate films sputtered in nitrogen (LISON):Insight from Raman spectroscopy and ab initio calculations, C. Muller, M. Karlsson, P. Johansson, A. Matic, and P. Maass, Physical Review B 77, 094116 (2008)
- Thermal expansion of silicon at temperatures up to 1100°C, A. V. Mazur, M. M. Gasik, J. Mater. Proc. Technol., 2008, in press (available on-line). doi; 10.1016/j.matprotec.2008.02.041
- Nitrogen flow rate as a new key parameter for the nitridation of electrolyte thin films, Y. Hamon, P. Vinatier, E.I. Kamitsos, M. Dussauze, C.P.E. Varsamis, D. Zielnok, C. Roesser, B. Roling , Solid State Ionics , accepted for publication
- Conductivity study of thin film ion-conducting LiSON, LiBSO and LiBSON amorphous electrolytes, D. Zielniok, C. Rösser, B. Roling, Y. Hamon, P. Vinatier, submitted to Solid State Ionics
- Jeppe C. Dyre, Philipp Maass, Bernhard Roling, and David Sidebottom - Some fundamental questions relating to ion conduction in disordered solids, arXiv:0803.2107, submitted to Phys.Rev.B

Presentations:

- Abstract from FEMLAB-2005 conference (Stockholm, 2-5.10.05) on simulation basics principles (abstract about Thermo-Mechanical behaviour of multilayers).
- Poster : day of Physical Chemistry, Marburg (Germany): presentation of a poster about the project
- "On the nitridation process of electrolyte thin films" presented at IMLB by Y Hamon
- IR spectroscopy of Li-diborate glassy thin films" by E.I. Kamitsos et al. at 10th Int'l Conference on the Structure of Non-Crystalline Materials - NCM10 ((Prague, Czech Republic, Sept. 18-22, 2006)
- Modelling multilayer systems with time dependant heaviside and new transition functions" by Y. Bilotsky et al given. at COMSOL 2006
- P. Maass: Invited talk at the Workshop ``Ion Dynamics and Relaxation in Ion Conducting Disordered Solids, Le Mans, France: Hopping Models for Ion Dynamics in Glasses: Effects of Disorder and Coulomb Interactions
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