Scientific Cooperation
between the Institute of Atomic Physics (IFA), Romania
and the Alternative Energies and Atomic Energy Commission (CEA), France

Activity Report on 2010

Bucharest-Magurele, ROMANIA
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Brief overview of IFA & CEA

The Institute of Atomic Physics (IFA) located at Magurele was established in 1956. It spun off from the Institute of Physics of the Romanian Academy founded in 1949 under the leadership of the eminent scientist Horia Hulubei who was also the first director of IFA.

IFA laid the foundations of a Romanian scientific research elite and a renowned scientific research school: IFA is the cradle of the Romanian physics. The development of the Physics Platform located at Magurele reached its peak in the 1970s bringing together a human potential and a research, educational, even a social infrastructure impressive for that time. The science performed at Magurele became widely acknowledged by the international scientific community, setting a high standard for the Romanian scientific research.

In December 2008, IFA was reorganized by government decision with the view to playing a new and enhanced role in the development of the Romanian physics research.

Following its reorganization, IFA's main achievements comprise:

- Research Unit of the Romanian EURATOM-Fusion Association (since 1999)

  Since 1999 when the Contract of Association with EURATOM was signed, the Institute of Atomic Physics has coordinated the participation of Romania in the European integrated scientific research in controlled thermonuclear fusion.

- Cooperation agreement with CEA (since 2009)
- Evaluation and Strategy of the Romanian physics - ESFRO project (2009-2011)
- Executive Agency for the F4E-RO Programme (since 2010)

  The Institute of Atomic Physics was designated by the National Authority for Scientific Research as the executive agency for financing, in the frame of F4E-RO programme, the projects obtained by the Romanian institutions following the calls of European Fusion for Energy Agency.

- Management of the CERN-RO Programme (since 2011)

  The Institute of Atomic Physics was appointed by Government decision, to ensure the management of the participation of Romanian institutions in CERN's programmes and scientific projects.

IFA pursues a pro-active agenda for providing a stimulating scientific policy for the development of the Romanian physics research and to increasing the visibility and impact of physics in our society.

Brief overview of IFA & CEA

The CEA, the French Alternative Energies and Atomic Energy Commission (Commissariat à l'énergie atomique et aux énergies alternatives), is a public body established in October 1945 by General de Gaulle.

The CEA is based in ten research centers in France, each specializing in specific fields. The laboratories are located in the Paris region, the Rhône-Alpes, the Rhône valley, the Provence-Alpes-Côte d'Azur region, Aquitaine, Central France and Burgundy. The CEA benefits from both the strong regional identities of these laboratories and the partnerships forged with other research centers, local authorities and universities.

The CEA leads research, development and innovation in the following fields: low-carbon energies, defense and security, information technologies and health technologies. It conducts also fundamental and applied research into many other areas, including the design of nuclear reactors, the manufacturing of integrated circuits, the use of radionuclides for curing illnesses, seismology and tsunami propagation, the safety of computerized systems, etc. It has one of the top 10 supercomputers in the world, the *Tera-100*.

Regarding the scientific and technical collaboration agreements, CEA negotiates and implements scientific and technical cooperation agreements with foreign organizations from USA, Brazil, Marocco, Tunisia, Russia, India, China, Vietnam, Korea and Japan in both nuclear and non-nuclear fields.

The CEA is a technological research body which has developed extensive expertise in a number of fields – energy, information and health technologies and nanotechnologies, in particular – which are now central to the subjects studied within the European Research Area. The CEA implements an extremely proactive policy regarding the collaboration with its European partners, which is manifested in its highly-committed involvement in a series of research and development framework programmes (FP). In this respect, it is noteworthy to mention that the CEA is currently involved in more than 180 projects.

The CEA plays a significant role in human resources and training throughout Europe, promoting professional development opportunities for researchers and students.

General Agreement for Scientific Cooperation between IFA and CEA

Strengthening the scientific cooperation between France and Romania in the field of physics is an initiative designed to reinforce the importance of scientific dialogue and knowledge transfer as a base for developing a common pool of scientific knowledge and enhancing the competitiveness in this area of research.

The signing of the General Agreement for Scientific Cooperation between CEA and IFA, on December the 2 nd , 2009, was a step envisaged in the Road Map for the Strategic Partnership on science and technology between Romania and France established in 2008.

The two institutions were represented by Florin Dorian Buzatu - IFA Director General and Hervé Bernard - CEA vicepresident The event was also attended by Mr. Gerard Cognet, CEA Director for Eastern Europe and Mr. Marius Enachescu, vice-president of the National Authority for Scientific Research.

The **fields of cooperation** are:

- ***Nuclear Energy***: nuclear safety, development of new generation nuclear power reactors, spent fuel and radioactive waste management, exchange information relating to nuclear energy, education and training;
- ***New Technologies for Energy***: fuel cells, solar cells, energy storage, hydrogen;
- ***Fundamental research on Energy***: nuclear fusion and fission, matter sciences, climate sciences;
- ***Technologies for Information and Health***: micro and nanotechnologies; software technologies, biotechnologies, radiobiology and nuclear toxicology, radioprotection and medical imaging.

Following the first call launched on 3rd May, 2010 for research projects proposed by the Romanian institution together with units of the CEA, the first of its kind in the recently established partnership between IFA and CEA, a total of 9 joint research and development projects are currently funded. The projects will run for three years and will benefit from mixed financing provided equally by the National Authority for Scientific Research and CEA, respectively.

Signing the Cooperation Agreement, December 2nd, 2009

Project C1-01

Photosensitive Azopolymers for Biological Applications

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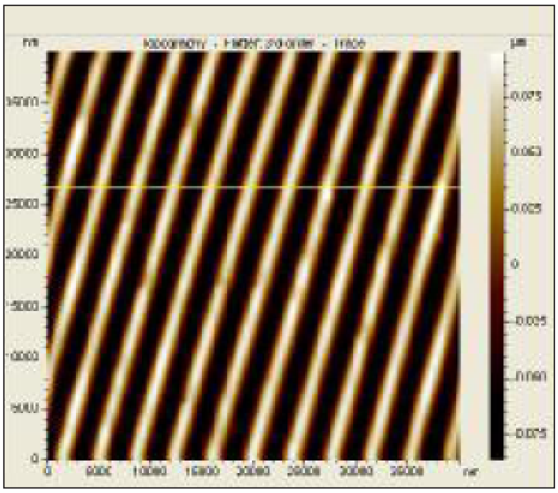
The project has a strong interdisciplinary character, being situated at the interface between chemistry, physics and biology. The project's aim is focused on the synthesis and characterization of «smart polymers» for biological applications, capable to interact with external light stimuli. One of the main objectives is the study of the supramolecular reorganization processes of azo-polymer systems, due to their interactions with UV-Vis laser radiation. Conceptually, the supramolecular reorganizations are related to the *trans-cis* photoisomerization capability of azobenzene groups present in the side chain of a polymer. Amongst the most interesting effects of this *trans-cis* photoisomerization in mass is the possibility of inducing controlled deformation of the surface geometry of a film (deformations that can happen at the micro- or nano-metric level) or directional flowing on the film surface. Moreover, by introducing the hydrophilic groups in the azo-polymeric structure, amphiphilic systems can be obtained. In this case, the photoisomerization process in an aqueous medium may be responsible for aggregation / disaggregation phenomena, which leads to the formation of photosensitive micelles.

There are several possibilities of using the azopolymers in the biological field, and the project will focus on the following: the use of azopolymer nanostructured films as support for directional cell cultures; nano-optical (laser) manipulation of biomolecules immobilized on the surface of azopolymeric films; the study of the photosensitive amphiphilic systems with potential application in the controlled release of drugs.

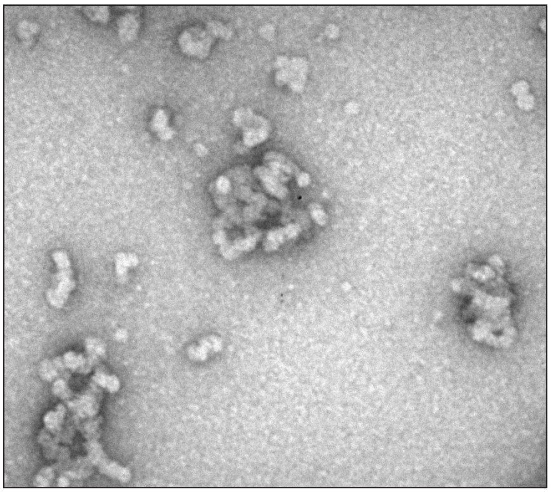
The main stages of the project implementation: **2010** - Azo-polymers synthesis and characterization; **2011** - Surface relief grating formation in different laser irradiation conditions; **2012** - Nano-structuration of the associated azo-polymers and the cytotoxicity preliminary tests of the obtained materials; **2013** - Laser nano-manipulation of the biomolecules on the surface of different azo-polymeric films.

The most important biological application of the new azo-materials obtained during this project is the study of the surface films interactions with the cell membrane. Due to the continuously *trans-cis-trans* isomerization process of the azo-groups resulting even from the interaction with visible light, the film surface is expected to induce very low mechanical stress in the cell membrane, with consequences on the cell division process and cell growth. Moreover, the presence of a certain type relief (at nano- or micro-metric scale) on film surface can induce a strong response in terms of increased cell adhesion, differentiation, proliferation, cytoskeleton development and gene expression. All this aspects are extremely important in understanding the cell's biological activity, or some diseases' mechanism (ex. Alzheimer disease). It must be underlined that only a single type of bloc-copolymer with azobenzenic groups used as support for cell development was reported until now in the literature. Taking into consideration this high interest research opportunity we have carried out the preliminary test of azo-polymers cytotoxicity, the results being extremely favorable.

The first tests to determine the surface nano-structuration capacity, using a continuous laser irradiation were performed and some azo-polysiloxanic structures capable to generate surface patterns with stable geometries were identified [1.]. During the nano-structuration studies some particularities concerning the mass transport mechanism were identified. We suppose a superposition of two different parallel mechanisms that probably will be separated using different azo-polysiloxanic structures. In spite of the fact that the mass transport phenomenon induced by laser irradiation on the films surfaces of the azo-polymeric materials ~~is~~ has been studied from more than 20 years, there are many aspects un-elucidated until now. In parallel with the nano-structuration mechanism using continuous laser irradiation, the Romanian partner from the Technical University of Iasi (National Institute for Laser, Plasma and Radiation Physics, Bucharest - team coordinator Dr. Victor Damian) will investigate the structuration process using a pulse laser technique. These complex studies using pulse or continuous laser irradiation are expected to contribute to the clarification of the mass transport mechanism.



Nanostructured azo-polysiloxane film surface



TEM image of the inter-micellar clusters

As concerns the amphiphilic azo-polymers, their capacity to generate photosensitive micelles which are capable to disaggregate under UV irradiation was demonstrated [2]. As a consequence of the very particular architecture of the azo-polysiloxane (having both hydrophilic and hydrophobic groups connected to the same chain) micelles with amphiphilic surfaces were obtained. Molecular modeling studies confirmed the existence of the amphiphilic surface corresponding to the micellar aggregate [3]. As a function of the polymer chemical structure, photo-sensitive inter-micellar clusters or vesicles can be obtained with potential applications in drug delivery systems.

Taking into consideration all the results obtained until now, the joint research developed by the Romanian and French teams have high chances of being continues and extended. At this moment the research teams prepare the documentation for a FP 7 European project (coordinated by CEA) which supposes the implication of other three research groups from 6 universities from Paris (France), Ecole Polytechnique Fedrale de Lausanne (Suisse) and the Institute of Biochemistry of the Romanian Academy (Romania).

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3. L. Epure, A. Neamtu, N. Hurduc - manuscript in preparation

Project webpage address: http://omicron.ch.tuiasi.ro/~inor/bioazo/en/index.html

Project C1-02

Study of the influence of forced and natural convection on impurity segregation and coating stability in the ingot growth of multicristalline Silicon for photovoltaic applications

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Due to its strategic importance in the development of a new route for feedstock production for photovoltaic applications, the interest for segregation processes in silicon ingot casting has strongly increased. The investigations were mainly done for the case where silicon feedstock was intentionally highly contaminated with C and N by adding defined quantities of carbon and nitrogen to the silicon melt. It is well-known that melt convection plays an important role in the distribution and segregation of impurities. Therefore, one of the project's objective is to study the influence of natural convection on impurity segregation and coating stability in the ingot growth of multicristalline Silicon for photovoltaic applications, in order to ensure a better control of the crystal quality. Due to the electromagnetic skin effect, it is likely that the techniques based on the implementation of magnetic fields that were seen to be quite efficient in Czochralski growth, will not allow and adequate control of heat and species transfer in large crucibles. It is therefore necessary to propose new methods allowing to tailor the convection within the solidifying melt adapted to the crystal growth of large scale silicon ingots. Thus, the objective of the present projects is to focus on these issues by studying stirring devices based on the use of rotating blades. The problem will be addressed using both numerical simulation and experiments.

The specific objectives are:

Objective 1: *Experimental and numerical study of natural convection effect on impurity segregation and coating stability in a Bridgman method for multicristalline Si growth.*

Because of moderate costs (small crucible diameter-max 3cm), the Bridgman equipment from Crystal Growth Laboratory (Fig.1), Faculty of Physics, West University of Timisoara is ideal for a parametrical study. Impurities distribution will be investigated for different growth parameters. Experimental results (temperature and concentrations) will be compared with numerical results in order to validate numerical models. First multicrystalline silicon ingots obtained in Bridgman equipment are presented in Fig.2.

Objective 2: *Modelling of Si crystal growth process in furnaces with stirring devices.*

Numerical simulation will be performed for the experimental configurations of the INES furnaces in order to understand the physical phenomena and to give information for the design of the experimental configuration. Time-dependent computations will be carried out with the software STHAMAS3D, which was developed at the Crystal Growth Laboratory in Erlangen, under the coordination of Prof. Dr. D. Vizman and already validated by experiments for the Czochralski and Bridgman processes. The first results on modelling of dissolution rate were accepted for publication in Int. J. of Heat and Mass Transfer (Numerical study of the melt convection on the crucible dissolution rate in a silicon directional solidification process, A.Popescu, D. Vizman)

Objective 3: *Growth of multicristalline silicon with a stirring device in laboratory and pilot scale furnaces.*

Experimental work will be initiated in a laboratory scale (2 kg ingots) furnace at INES. The laboratory furnace features cylindrical crucibles of appr. 15 cm in diameter. A single rotating blade will be implemented on the crucible axis. The first point to be verified is whether the induced flow damages the Si_3N_4 coating, and whether the results of the release of particles within the melt and/or increased infiltration of liquid Si into the coating are due to a possibly increased de-oxidation rate.

The realization of the current project (by implementation of a stirring device in directional solidification method), will open the door for the improvement of the quality of multicristalline silicon for photovoltaic applications. The technological benefits of understanding the effect of forced and natural convection on the impurity segregation and coating stability will facilitate the further development of directional solidification method for growth of multicristalline Silicon for photovoltaic applications.

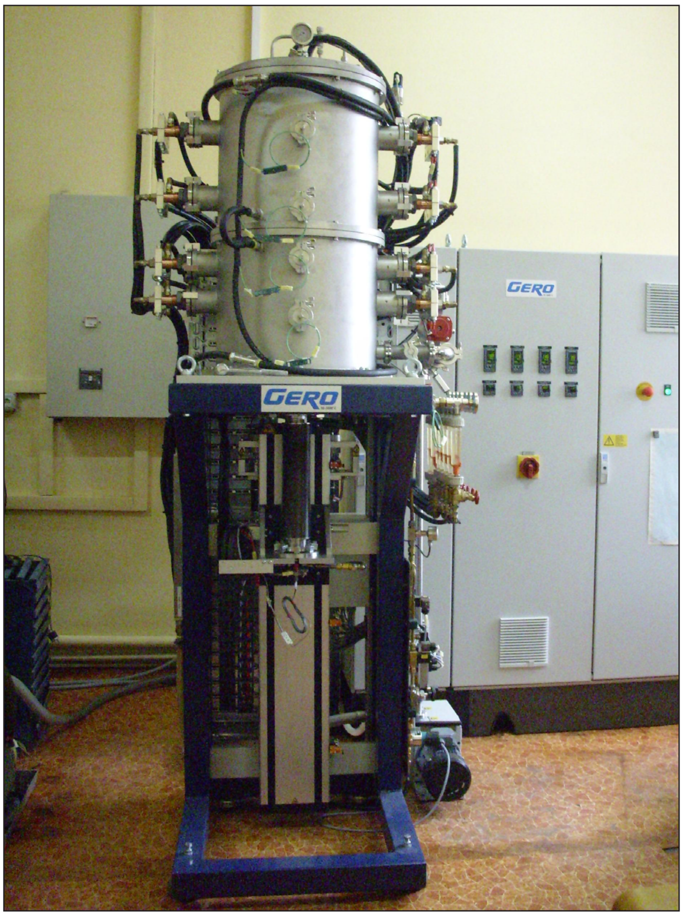

Fig.1. Bridgman equipment

Fig.2. Multicristalline silicon ingots obtained by Bridgman method

Project webpage address: http://www.physics.uvt.ro/~vizman/CONSIL_web_page/

Project C1-03

Numerical Simulations for RAdioactive Waste Disposal – NSRAWD

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NSRAWD aims to establish a collaboration between SCN and CEA in the field of numerical simulation for radioactive waste disposal, combining computational work with experimental activities in order to improve and validate flow and transport numerical models. Numerical models appropriate for each element of the disposal system will be coupled in the Platforme Alliances in order to be applied in performance and safety assessments of the LIL waste repository from Saligny. This project will use CEA's experience in developing numerical models, as well as the experience of SCN team in developing in-field tests and running computer codes.

Objectives

The main objectives of the projects are (1) to improve and validate flow and transport numerical models and codes used in disposal safety assessment through developing new in-field test, collecting experimental data for Alliances codes validations and for better understanding of site characteristics and increasing confidence in the numerical modelling used in radioactive waste disposal and (2) to develop an integrated system for safety assessment of LIL waste disposal applied to Saligny site as an useful tool for further application in the site licence.

Stages of the project

The project is to be implemented between October 2010 and October 2013 (36 months) and is structured in four stages, each containing a series of activities as follows:

(I) Implementing and using the Platform Alliances at SCN. Comparison of different computer codes simulations used by CEA and SCN

- I. 1. Training in the use of Platform Alliances for SCN team;
- I. 2. Benchmark on pumping test simulations using FEHM and Alliancese;
- I. 3. Benchmark on tracer test simulations using FEHM and Alliances.

(II) In situ experimental program for new data acquisition with a special focus on the unsaturated zone

- II. 1. Hydrogeological data collection from the Saligny site for computer codes validation;
- II. 2. Tracer test in the unsaturated zone.

(III) Validation improvement of flow and transport in the unsaturated zone computer codes developed by CEA with 3D data

- III. 1. Computer codes validation for flow;
- III. 2. Computer codes validation for transport.

(IV) Construction of the integrated safety assessment system using Platform Alliances for radioactive waste disposal at Saligny

- IV. 1. Source term modeling;
- IV. 2. Contaminant transport simulation in unsaturated zone;
- IV. 3. Contaminant transport simulation in saturated zone;
- IV. 4. Contaminant transport through the repository cover system;
- IV. 5. Coupling near field and far field models in an integrated performance assessment for LIL waste disposal at Saligny;
- IV. 6. Dose assessment for normal evolution scenario;
- IV. 7. Surface response development using Alliances;
- IV. 8. Benchmark on sensitivity and uncertainty analysis in Alliances and GoldSim.

Expected results, possible applications and impact

From a technical point of view, through the experimental work carried out, the project will contribute to the improvement of Saligny site characterisation, bringing new data and relevant information on the most sensitive parameters of the Saligny site related to the water infiltration and contaminant transport in the vadose zone, as well as concerning water flow and transport parameters in the aquifer. It will be designed to provide also data for the validation of the CEA's codes especially from the point of view of 2D and 3D effects, increasing confidence in their prediction.

The integrated system for safety assessment developed in the project will represent a flexible tool for the safety assessment process and can be used in the Saligny site licensing by AN&DR (Romanian Nuclear Agency and for Radioactive Waste).

But beside the technical impact, the project will contribute to the strengthening of R&D potential of both research centres, generating new experimental and computational achievements. The project will consolidate the existing partnership in numerical simulation for nuclear waste disposal concluded this year between SCN and CEA-DEN, establishing a common working platform and facilitating the communication between the French and Romanian scientists. The joint activities developed under this project will build confidence in the capability and competence of the specialists that will be taken into account in future collaborative research projects.

Perspectives of collaborations

This project opens real perspectives for a further collaboration between SCN and CEA in the field of radioactive waste disposal. For instance, the licensing process of the LIL waste repository at Saligny offers clear opportunities for a future collaboration assisting AN&DR in achieving its objectives.

Implementing of geological disposal is a key issue in the nuclear energy development and still provides ample room for new collaborative research projects in investigating and modelling uncertainty of the long term processes that occur in the complex system of radioactive waste final disposal. The FP7 projects CARBOWASTE and FORGE in which CEA and SCN are partners, represent a promising start point for future participation in the next European collaborative projects.

At international level, there are also other countries concerned by the radioactive waste disposal problem that request assistance for safety assessment. The experience gained through this project can be helpful in potential joint tenders.

Project webpage address: http://www.nuclear.ro/ProiecteInternationale/nsrawd/index.html

Project C1-04

Electrochemical study of iron monosulfide dissolution

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Project motivation

The migration of radionucleides out of deep nuclear repositories in geologic media can be mitigated by interaction with mineral surfaces. Specifically, the minerals which can release redox active species or display surface oxido-reduction properties can significantly alter contamination patterns by redox-sensitive radio-isotopes (see the example of U(VI) reduction to U(IV)). As an example, dissolution of minerals such as iron monosulfides (IMS; pyrrhotite, troilite or mackinawite) releases species of sulfur in intermediate oxidation states, which can diffuse and buffer the redox characteristics of medium [1,2]. The iron monosulfide minerals can be enclosed in geological media or they may be formed by reactions like reduction (in presence of magnetite) of sulfate (S(VI)) to sulfides (S(-II)) with hydrogen released by corrosion of containers with radioactive wastes.

Project objectives and foreseen results

The main goal of this project is to gain insight into the reaction kinetics and mechanisms of sulfur-bearing species released during iron monosulfide dissolution, and into the impact of redox active species transport in media around radionuclide repositories (Figure 1).

In this context, the project will focus on: (1) investigation of IMS dissolution reactions by various electrochemical techniques, (2) characterization of solid reaction products formed on surface of IMS electrodes using FTIR spectroscopy, X-ray diffraction (XRD), Atomic Force Microscopy (AFM), μRaman spectroscopy and Micro-X-ray absorption fine structure (μXAFS) spectroscopy (3) identification of the main factors controlling IMS dissolution, and (4) development of theoretical models to estimate the redox buffer potential of IMS.

Project stages

The main stages of the project are: 1) the chemical and structural characterization of iron monosulfide samples and work electrodes preparation; 2) the investigation of iron monosulfide dissolution in presence of $O_{2(aq)}$; 3) the investigation of iron monosulfide dissolution in presence of $H_2O_{2(aq)}$ and 4) the investigation of iron monosulfide dissolution in presence of $Fe^{3+}_{(aq)}$.

Cooperation perspectives

The project will help to develop new ways of cooperation between the two teams, especially in the strategic interdisciplinary and multidisciplinary domain of Nuclear Energy/Waste Management. Both infrastructure and human resource will be improved. The new acquired skills and knowledge will foster the development of dynamic teams able to approach complex problems of radiocontaminant sequestration and storage.

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[2] P. Chirita, M.L. Schlegel, Oxidation of FeS by $Fe^{3+}_{(aq)}$, Goldschmidt 2011, August 14-19, 2011 Prague, Czech Republic (in preparation).

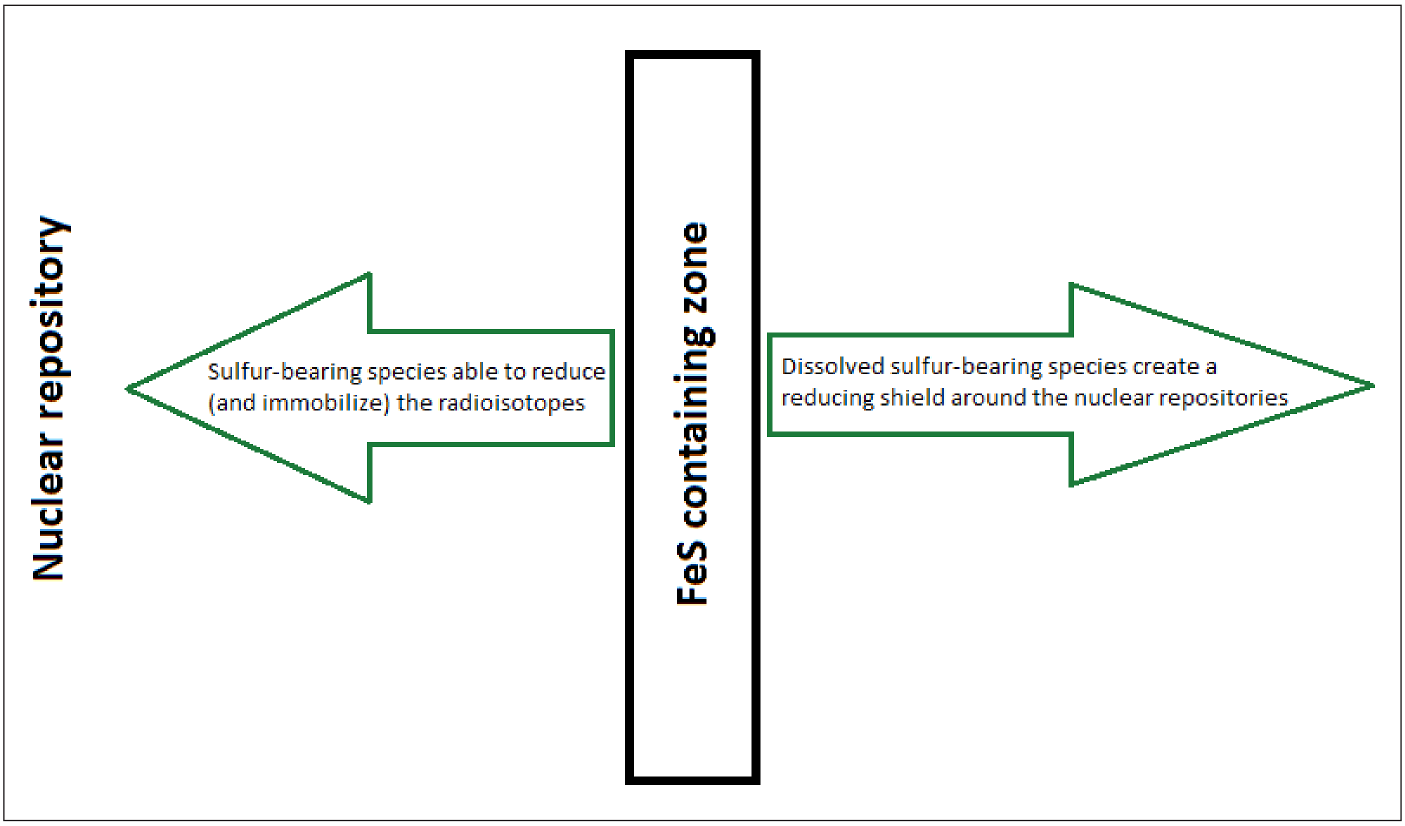

Figure 1. A schematic representation of FeS action on redox characteristics of media around nuclear repositories.

Project webpage address: http://chimie.ucv.ro/facultate/cercetare/proiect_pchirita.pdf

Project C1-05

Plasma and laser processing of powders for nuclear applications

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Powders as materials and powder based technologies are of large interest for engineering and technology. Powder properties depend on material and size. They are obtained from diverse materials (metals, ceramics and polymers), in a wide range of sizes, from nanometric dimensions (clusters) to hundreds of microns. At macroscopic level the powder properties lie between that of a solid and liquid, leading to specific applications: powder metallurgy (by sintering), coating of surfaces by plasma spray for improving surfaces quality, providing them special properties, like chemical inertness, mechanical resistance, or capability to resist to large thermal loads. Recent approaches focus on nanoparticles utilizations in emerging fields from biology and medicine, as markers, drugs carriers, and in the area of energy production and electronics, where the nanoparticles are the basis for ink-jet printable electronics and printable photovoltaics. The research on powders focuses on physical and chemical processes involved in powder production and transformation, characterization and their applications. In the opposite direction, the research focuses often on avoiding the powder formation or presence, in processes and technologies where the powder presence is detrimental (like semiconductor industry, or in thin film deposition by Pulsed Laser Ablation). Also, a very important issue is the dust incidence on operation of fusion machines. In that case, the intense plasma outflow produces, by wall erosion, a large amount of dust containing metal (Be, Al, Mg, Cu, W, etc.) and C particle powders. The created dust is transported in remote areas and in the gaps present in the vessel topology, resulting in deposition of the so called codeposited layers, compromising the long term operation of fusion machines.

With respect to this wide range of research and applications areas, lasers and plasma techniques may address several open issues described above. By this project we aim at fabricating and transforming, by lasers and plasma methods, the particles and powders of materials that have significance for a number of nuclear applications (mainly fusion technology). The materials to be used are C, Be (due to induced cancerous pathologies of Be there will be used Al and Mg as substitute) and W.

The general objective of the project consists in obtaining particulates and powders of the above materials, with fine control of their properties (size, surface chemistry, structure) and their transformation by using plasma and laser methods in order to ensure safer maneuverability with respect to nuclear safety issues.

The novelty of the concepts comes from applying the paradigms established in the field of materials processing by laser and plasma to new environments and situations that favor the interactions with small size objects. According to the work plan for producing metallic powders, two techniques are taken into consideration. The first consists of ablating metals in gases or liquids with various chemistries, where the laser beam will be focused on Al, Mg, or W targets immersed in those media. The second one is a novel concept of plasma deposition method, namely sequential Magnetron Sputtering (MS) / Plasma Enhanced

Chemical Vapour Deposition (PECVD). Particles of C, Al, Mg, W will be incorporated in a carbon matrix by periodical exposure, for defined periods of times, the substrate of the two separated plasma deposition sources, one of them depositing the metal, the other depositing carbon. In a subsequent step the particulates incorporated in the matrix will be revealed by plasma etching of the carbon phase. For plasma treatment of powders and particulates, aiming at their surface modification (nitriding, oxidizing, size reduction), a fluidization method is proposed, in which a plasma jet will be used to spread out and circulate the powder in plasma, ensuring the intimate contact of each particle with plasma species.

The expected results are: i) testing the ability of laser ablation in liquids with respect to producing particulates with controlled morphology and surface chemistry from the mentioned metallic elements; ii) development of a new and reliable plasma based technique (sequential deposition) for producing particulates with controlled size incorporated in a carbon matrix and of revealing the particulates by etching away the carbon matrix; iii) the setting up of a fluidization technique for powder processing, including the enhancement or inhibition of particles oxidation/reducing. In addition, experiments will be performed to assess whether the particle size reduction is possible by plasma and laser processing.

Where applications are concerned, it is of major importance to produce small test particles, similar to the particles observed in current operating tokamaks in order to prepare, in laboratories, the strategy to be used in order to control the in vessel tritium inventory in ITER or in the hot cell present in ITER. Moreover, the handling and safe processing of powders is an issue: due to the large surface area their chemical transformation (as example oxidation) is fast and release energy that can easily lead to explosion. Surface stabilization of powders by plasma treatments is an approach which can prevent or diminish such a danger. Not in the least, the investigation of the effects of small size particles and powders on living organisms, cells and bacteria is a hot research topic. In the last decade the question of the impact that the nanoparticles powders have on health has been at the core of the calls of FP6 and FP7 research programs at European level. As such, dust manipulation, collection and removal is an important issue, being currently in the focus of computational and experimental work of important research groups from different countries.

Project webpage address: http://plasmat.inflpr.ro/tot-projects_international.htm

Project C1-06

Efficient Handling and Processing of PetaByte-Scale Data for the Grid Centers within the FR Cloud (HaPPSDaG)

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The main purpose of the project is to provide the means for improving the handling and processing of large data sets at the Tier2 grid centers which participate in the ATLAS experiment at the LHC computing support. The specific objectives of the project are the following:

- Improving communication and coordination between GRIF and the Romanian associated sites
- Testing and improving the quality of the FR-cloud - RO data link for large dataset transfers
- Implementation of specific measures for increasing the ATLAS job load on sites
- Implementation of specific measures for increasing the storage performance
- Improving the large dataset transfer between RO sites and FR-cloud
- Improving the data analysis in the grid sites which are associated to the FR-cloud.
- Contributing to the grid monitoring and technical support within the FR-cloud
- Providing the necessary training related to the grid monitoring and support
- Dissemination of the results of the project

The work plan of the project comprises three stages: 1) *The analysis of the Tier1-Tier2 communication* (2010), which is mainly dedicated to establishing good communication paths between the partners and to identifying the weak points of the data connection between the grid centres; 2) *Studies and software tools for monitoring and operating the FR Cloud-RO-LCG Grid connection and job loading, as well as testing of data handling and processing within the FR Cloud* (2011) ; 3) *Methods and procedures for improving the performance of the RO sites within the FR Cloud* (2012), which will be dedicated to elaborating and testing of general methods and procedures for achieving a higher efficiency in the handling the peta-byte scale datasets and data analysis in ATLAS clouds, based on the experience gained in the FR-cloud, especially at GRIF and IFIN-HH .

The second stage of the project is focused on implementing the best tools for monitoring data transfer and storage performance of the Grid sites. Through these tools, the reasons for lower performance of the sites were found, which helped to find a means to improve the LAN throughput at IFIN-HH, its connectivity with the FR-cloud, and the job loading of the workernodes. These results are depicted in Fig.1 and Fig.2, respectively.

The improvements of the Grid productivity will be measured through intensive data transfer tests and distributed analysis tests by IFIN-HH and GRIF Grid management teams. HAPPSDAG will present the first complete case study and set of guidelines regarding the improvement in efficiency of grid centers which are associated to an ATLAS cloud. The in-depth investigation of the problem will offer a better understanding on the technical and management factors that significantly contribute to the full coordination of the grid centers.

It is estimated that the project will have a direct result in the improvement of the efficiency of processing and handling of ATLAS data between IFIN-HH and the FR Cloud. Also, the project will offer technical guidance to two smaller Romanian sites which expressed their intention to become FR Cloud associates. The participation of Romanian and French team members in the activities of support and monitoring of the FR-cloud will continue beyond the end of the project.

Besides the immediate beneficial impact on the FR Cloud – RO-LCG common activity, the project will provide strategies for improving grid-computing environment for all the users. Smaller grid sites, especially those in more remote places, and their users will be the primary beneficiaries through the provision of detailed guidelines on how to better operate with huge amounts of grid data in international collaborations. Sharing best practices in system management and site hardware and software configurations will result in an improved quality of service for all clients. The usability of the computing infrastructure will improve, lowering the threshold for the everyday utilisation of the infrastructure by researchers and engineers.

The project will facilitate the sharing of best practice when dealing with data-intensive applications at grid sites and will therefore improve the effectiveness with which researchers can use the available computing resources. This is expected to lead to an increased global efficiency in the usage of existing computing resources by researchers in Europe. Also, on a longer term, it will contribute to the transfer of knowledge on best operational procedures from sites operating larger grid computing centres to medium and small sites.

The project will also contribute to the intensification of the scientific exchanges between the Romanian Grid community and the French Grid professionals. In this respect, the project has the potential for leading to the development of new cooperations to be concretized in projects proposed for funding through regional, European and international programs or initiatives.

Due to the fact that the LHC-based scientific research is scheduled to take place during the next 20 years, it is plausible that CEA/IRFU and IFIN-HH will receive the funds to sustain the cooperation in the future. Both IFIN-HH, which is the largest R&D institute from Romania, and IRFU, have the scientific capacity and the manpower required to successfully continue this cooperation in the years to come after the end of the project.

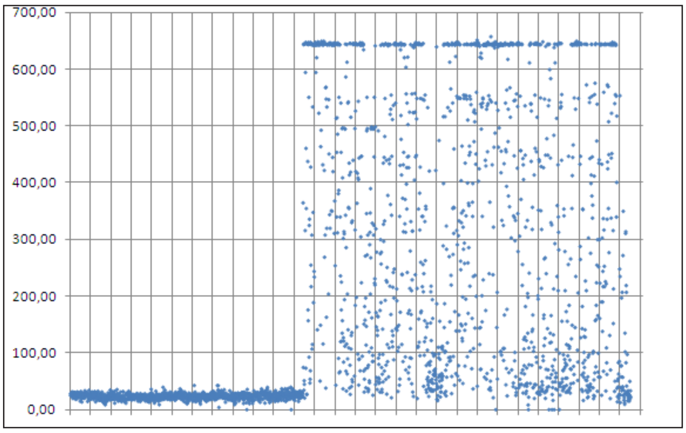

FIG.1: Results of file transfer bandwidth measurements, showing a dramatic improvement since February 2011.

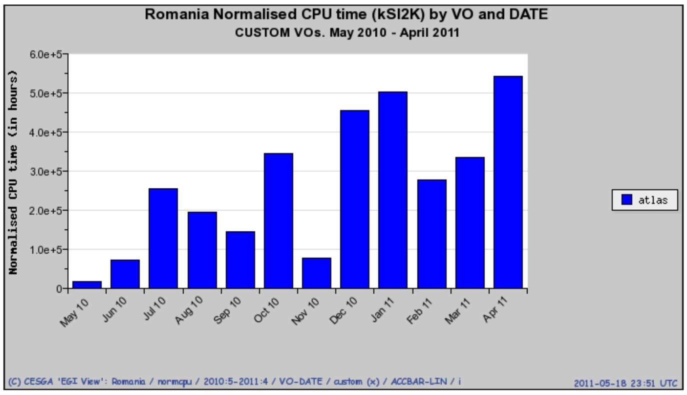

FIG.2: CPU time provided by RO-LCG to the users of the ATLAS VO during the last 12 months (kSI2k units)

Project webpage address: http://happsdag.nipne.ro

Project C1-07

TiO_2-based nanoparticles for applications in photovoltaic cells or bactericide elements

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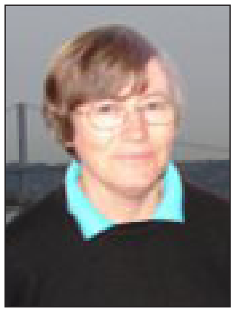


The worldwide interest for TiO_2 is due to its exceptional properties. In the anatase form, TiO_2 is widely used for its photocatalytic properties. Titania appears as an interesting component in new generation photovoltaic cells such as hybrid cells (organic /inorganic). A limitation is provided by its low efficiency for absorption of solar light in the visible range therefore, intensive research are carried out in order to shift the optical gap toward lower energy. The most explored idea is that of incorporating heteroatoms such as N, C, S or F. Numerous methods have been developed for the synthesis of nanoparticles e.g. the liquid phase synthesis methods (co-precipitation, solvo-thermal or hydrothermal methods, electrochemical synthesis, sol gel synthesis) or the high energy ball milling. However, all these methods suffer the same drawback: powders are produced by batches and the methods allowing continuous work are often preferred for industrial developments. The l*aser pyrolysis* has also been used in research laboratories for production of $TiO_{2,}$ mainly from titanium tetraisopropoxide (TTIP) - precursor or $TiCL_4$. Unlike chemical methods where several synthesis steps are required to synthesize doped or composite materials, doped TiO_2 nanoparticles are easily obtained in a one step reaction by this method, just by mixing the precursors containing the dopants with the titanium precursor before the laser irradiation.

Our objective is to prepare TiO_2 nanoparticles doped with various hetero elements (F, V, N, S, C) obtained by laser pyrolysis for the elaboration of solar cells and/or with improved antibacterial properties.

Specific objectives:

i) the synthesis of anion-doped TiO_2 particles (with N, C and S dopant) using the *laser pyrolysis method* and the obtention of particle dimensions about 10-30 nm average diameter, with low diameter dispersion (lower than 30% of the average value); ii) *the use of different gas phase precursors* (titanium tetrachloride, oxidizers, hydrocarbons, nitrous oxide, sulfur hexafluoride, hydrogen sulfur) for the in situ obtention of different kind of synthesized doped TiO_2 nanoparticle systems; iii) *the complex characterization* of nanoparticles for studying their structural, chemical and morphologic properties and *gaining understanding of the photocatalytic behavior of the TiO_2-based pure and modified nanoparticle; iv) the use of laser pyrolysis for simultaneous coverage of the doped nanoparticles with a siloxane polymer* which represents one of the hottest interest worldwide in the study of Titania-based antibacterial nanostructres; v) *structural and morphological analysis through transmission electron microscopy* (TEM, HRTEM, SAED)

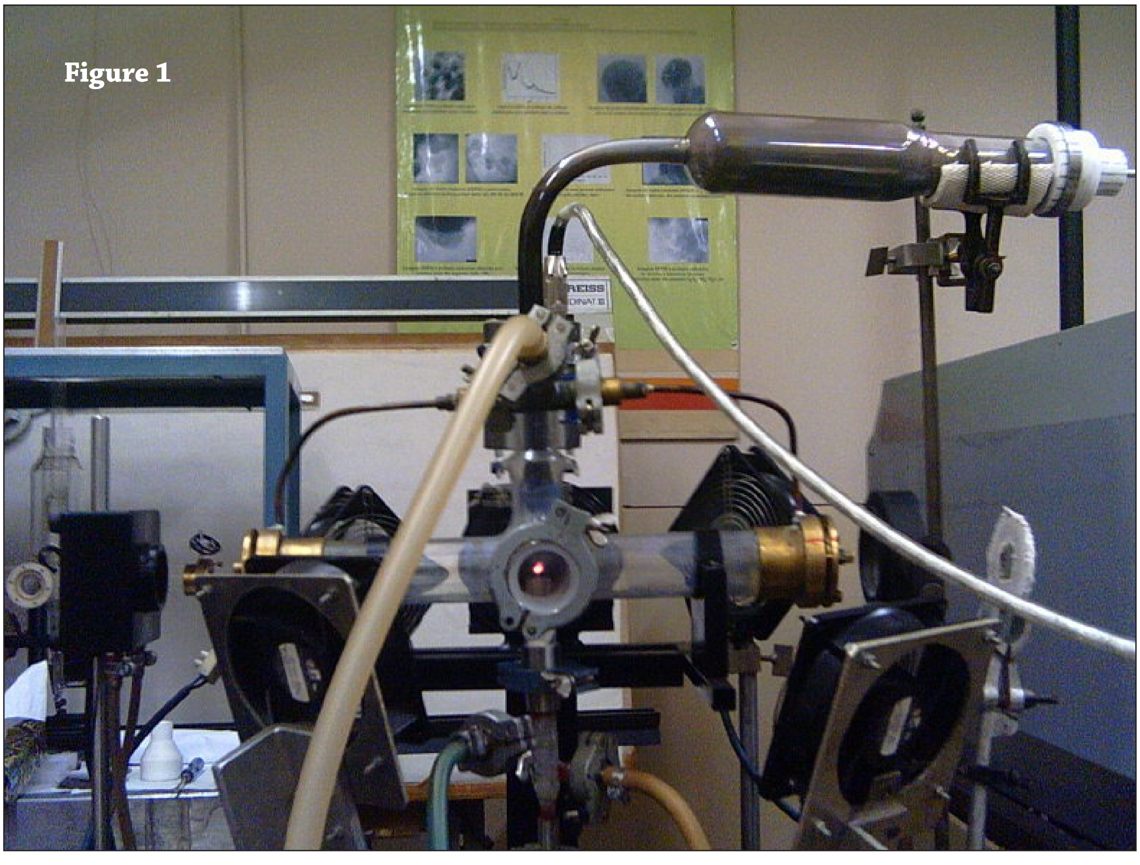
Work plan and foreseen results:

- In the first step of the Project (end of 2010) a report has been issued on the elaboration of conceptual models and theories as concerning the synthesis methods for the nanostructure preparation of TiO_2-doped compounds.

- *The following task of the project (2011) consists in investigating*: TiO_2 nanoparticles doped with various hetero elements (F, V, N, S,...) , synthesized by laser pyrolysis (Fig. 1) by both Romanian and French team, from different combinations of precursors (TTIP as TiO_2 source in France, $TiCl_4$ - as Ti as TiO_2 source in Romania). We will study the structural and optical properties of the different nanoparticles with special attention to the determination of the position of the absorption edge as compared to pure TiO_2 - this last measurement can be done in France. The Romanian team will focus on the experimental model of carbon doped TiO_2 nanoparticles. The French team will investigate the experimental model of nitrogen doped nanoparticles. Samples will be exchanged between the teams for a complex characterization of the obtained nanopowders.

- In the third year of the project, selected batches of powders will be optimized in order to obtain a composite powder, containing TiO_2 cores implanted in a polymer matrix (mainly core-shell structures). Samples of the doped TiO_2 nanoparticles will be characterized in Bucharest and Saclay. The elaboration of a stage report will be performed which will contain details about the obtention of doped TiO_2 based nanopowders and about the description of their spectral, morphologic, crystallographic and other specific properties. The joint publication of scientific results obtained with the French partners is envisaged.

Figure 1



Project webpage address: http://llp.inflpr.ro

Project C1-08

Ferroelectric and diluted magnetic semiconductor based multiferroic heterostructures for energy applications

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Ferroelectrics and multiferroics materials have a potentially great importance for a wide range of applications, due to the presence of the spontaneous polarization, high dielectric constant, non-linear optical properties, piezoelectric and pyroelectric effects, magnetoelectric coupling in multiferroics, etc. Diluted magnetic semiconductors (DMS) where ferromagnetism is established through indirect RKKY interaction, that allows electrical or optical control of the ferromagnetism have also a high technological potential. DMS oxides with room temperature ferrimagnetism are natural candidates to be interfaced with ferroelectrics, as recently demonstrated. MULTIFERRODMS will be the first project to combine both materials by synthesizing multiferroic heterostructures engineered from ferroelectric and DMS layers. The main goal is to provide a route to robust electrical polarization from rather weak magnetic polarization, triggered by light absorption. This way, sufficiently high voltages may be provided by such devices to induce electrolysis in an integrated thin film light absorber - hydrogen generator. In the first stage of this project we will carry out a systematic investigation of a prototype ferroelectric, $PbZr_xTi_{1-x}O_3$ (PZT), epitaxially grown as a thin film on a variety of substrates, creating a variety of different strain states. PZT has a high polarization (120 $\mu C/cm^2$), which can be adjusted by varying the stoichiometry. The Curie temperature may also be tuned by the in-plane strain. Furthermore, epitaxial growth on a wide variety of other perovskite oxides is possible, allowing straightforward strain tuning by judicious choice of the substrate. The lattice constant of PZT varies from 3.98 to 4.15 Å according to the Zr stoichiometry. Due to the use of suitable substrates chosen for example from amongst $SrRuO_3$ (SRO), $La_xSr_{1-x}MnO_3$ (LSMO), $SrTiO_3$ (STO), $BaTiO_3$ (BTO) and $DyScO_3$ (DCS), a wide range of compressive and tensile strain states will be available.

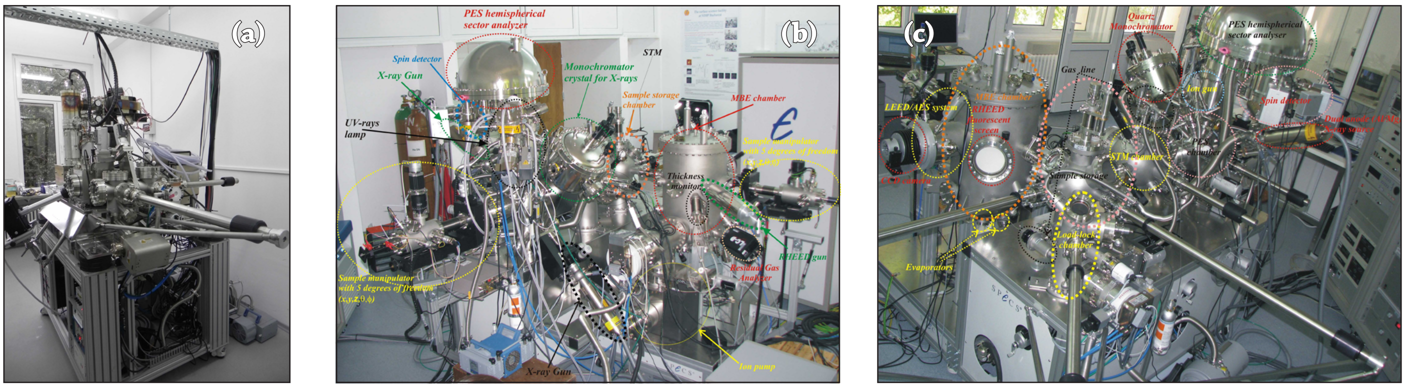

Figure 1. *Experimental facilities in NIMP: (a) Low-energy and photoemission electron microscopy (LEEM-PEEM); (b, c) Surface science cluster, composed by a molecular beam epitaxy (MBE), a scanning tunneling microscope (STM), and a spin- and angle-resolved photoelectron spectroscopy (SARPES) chamber.*

These studies will investigate the quality of the epitaxial layers (in-situ techniques used: low-energy and reflection high energy electron diffraction: LEED, RHEED; X-ray photoelectron spectroscopy XPS, see Fig. 1) as well as their properties, assessed by hysteretic cycles at different temperatures and stresses.

The second idea of this Project is to work on artificial multiferroics which can be obtained by combining ferroelectric materials with diluted magnetic semiconductors (DMS). We estimate that a DMS system containing 1 % magnetic ions with 1 μ_B/atom may generate a field of ~ 100 Oe at the interface. For a conversion factor of 1 V/(cm x Oe) and a 1 mm ferroelectric film, a 10 V potential difference may be generated. The use of an oxide semiconductor for DMS, for example ZnO or TiO_2 will avoid many of the problems occurring at the interface with a ferroelectric or multiferroic oxide such as parasitic oxide phases, interdiffusion, accumulation of oxygen vacancies. The aim of this second part of the project is to produce and characterize such a DMS/FE device, as illustrated in Fig. 2.

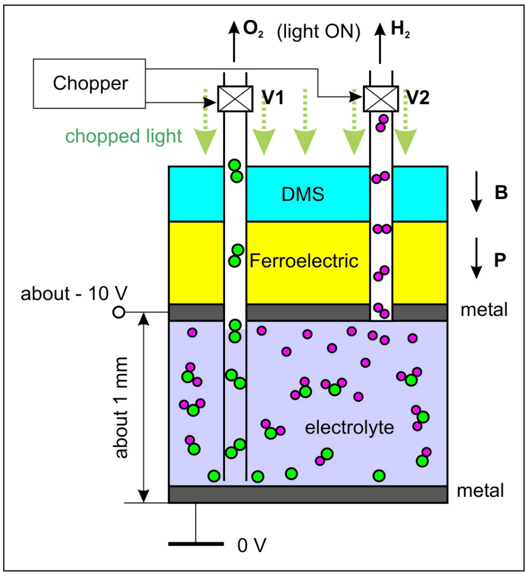

Figure 2. *Schematics of a prototipe photolysis cell driven by the DMS magnetic ordering tnakks to light-induced ferromagnetism.*

The main scientific tasks of the project are: (i) Synthesis of high quality epitaxial layers (combining PLD and molecular beam epitaxy, MBE) and their master strain tuning via the epitaxy parameters (choice of the substrate, growth temperature, excess oxygen, etc.). (ii) Investigation of the chemical reactivity and the alternate photolysis route driven at a ferroelectric interface. (iii) Synthesis of reproducible DMS layers or alternatively 2D Stoner ferromagnets with light-induced ferromagnetism. (iv) DMS layers need to be investigated from the point of view of their magnetostrictive properties. To date, no such study was reported. (v) Fabrication of DMS/ferroelectric multiferroic systems where the electrical polarization may be triggered by light absorption will be produced. Microdevices for collection of hydrogen may then be obtained by nanolitography.

Several levels of impact may be emphasized: (a) *Educational*: as mentioned above, young researchers from both sides will benefit from the expertise and access to facilities of the other side through this partnership. Two or three PhD theses will be defended within the framework of this Project. The clear orientation of the project towards validation of a potential device architecture will provide the young researchers with training adapted to both industry and academia. (b) *Technological*: The Project will end with well-defined laboratory technologies for the synthesis of (i) high quality epitaxial ferroelectric films, with properties adjustable through stress and stoichiometry; (ii) diluted magnetic semiconductors with light control of ferromagnetism; (iii) DMS/ferroelectric multiferroic systems with electrical polarization adjustable by light irradiation; (iv) newly-developed hydrogen microplants. (c) *Fundamental research and excellence*: The Project aims at investigating new phenomena, such as photolysis at ferroelectric interfaces and its triggering by external parameters. We foresee a high impact of the publications that will emerge. (d) *Environmental*: the setup of a novel technology for direct hydrogen production from light absorption creates a very high added value to this Project. The photolytic yield of the proposed heterostructures, and their precise control make the results important for developing materials and effective architectures for new energy technology. (e) *Employment*: The project aims at creating a bridge between ground breaking fundamental research and successful fabrication of basic device architecture. Its success could provide the required core knowledge base for small or medium sized companies to implement the proposed technologies within the high technology poles of both the Magurele and Saclay sites.

Project webpage address: http://www.infim.ro/

Project C1-09

Investigation of metal-ferroelectric interface at macro and nanoscale

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The main objective of the project will be to study the construction of the metal-ferroelectric interface and the dynamic of charge compensation in relation to polarization switching. The results will be compared to the results of the macroscopic electric measurements performed on standard metal-ferroelectric-metal (MFM) capacitors. Also, the metal-ferroelectric interface will be compared with the results reported for the free surface.

The entire project is based on the idea that, in a ferroelectric material with structural quality close to perfection, the polarization ends up with two sheets of surface charges, one negative and the other one positive. In order to have a stable polarization state, these charges should be compensated with charges of opposite sign, otherwise they will generate a depolarization field leading to formation of opposite polarization domains. This fact could have an impact on the formation of the metal-ferroelectric interface.

In the first year the project aims at growing epitaxial PZT films of very good quality and to investigate these films with specific techniques, such as: X-ray diffraction (XRD), high-resolution transmission electron microscopy (HR-TEM) and piezoelectric force microscopy (PFM). Then the electronic properties of surface will be investigated using X-ray photoelectron spectroscopy (XPS) and photoemission electron microscopy (PEEM). Finally, the dynamic of polarization switching and charge compensation at the surface will be studied by combinations of the above mentioned techniques.

In the second year, the formation of the metal-PZT interface will be studied by depositing different metals on the surface of the PZT film. The focus will be on metals with full d-shell, such as Cu, Au, and on metals with almost empty d-shell, such as Ta, or with no d-shell, as for example Al. Thin layers of metals will be deposited in controlled conditions and surface physics techniques (XPS, STM, PEEM, etc.) will be used to extract information about the electronic properties of the interface. Alternately, HR-STEM can be used in order to investigate possible diffusion phenomena at the interface. The aim is to obtain an accurate characterization of the metal-ferroelectric interface and to see how the interface properties are dependent on the polarization orientation. In the end, polarization switching and charge compensation at the metal-PZT interface will be studied using PFM.

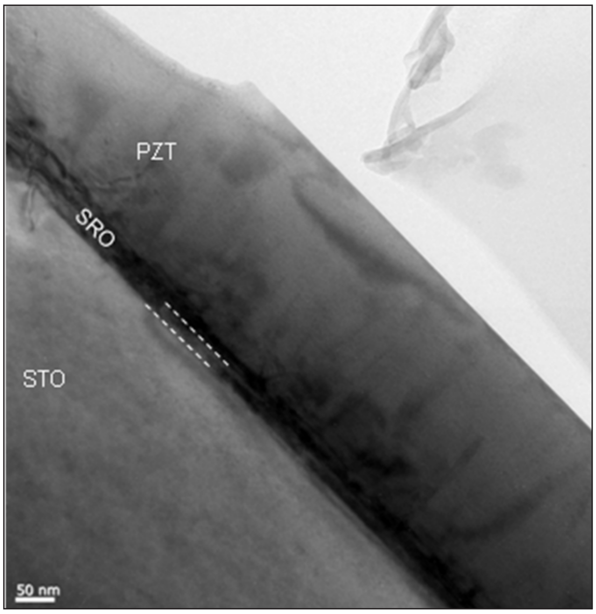
In the third year, the project will focus on the correlation between the characterization of metal-ferroelectric interface at nanoscale and electric characterization at macroscale. Standard electric measurements at different temperatures will be performed in order to extract information about polarization, potential barriers, etc. The results will be compared with the results of measurements performed in previous years using surface/interface investigation techniques. It will be possible to asses the link between macroscopic properties and microscopic formation of the interface, in relation with dynamic of charge compensation during polarization switching.

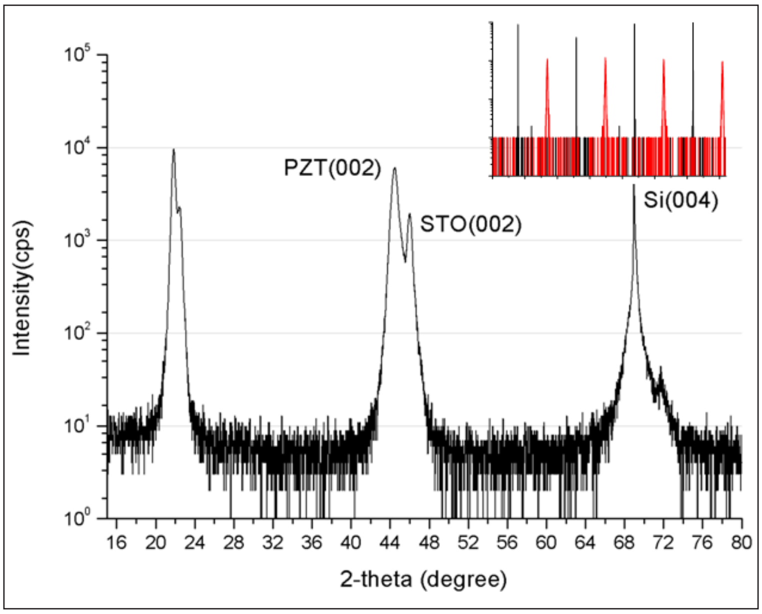
The PZT films will be grown by pulsed laser deposition (PLD) on single crystal SrTiO3 substrate, using the $SrRuO_3$ as bottom contact. The metal electrodes on the surface will be deposited either by e-beam evaporation or by RF-sputtering. The Romanian partner has the access to all the surface/interface characterization techniques mentioned above (XPS, STM, PEEM) as well as to HR-TEM/STEM. The French partner has the necessary expertise in the field of PFM characterization and interpretation. The two teams will complement each other in terms of infrastructure and expertise.

The proposed subject of the project is of very high interest in the community of researchers working in the field of ferroelectrics. Actually, it would be for the first time at international level that a comprehensive and coherent study is to be performed on the formation of the metal-ferroelectric interface, and the first time that the role of interface in the dynamic of charge compensation during polarization switching is to be studied. Traditionally, the electronic properties of the interface were decoupled from the ferroelectric properties of the film, and in many cases the interface was just disregarded, considering that any metal on ferroelectric forms ohmic contacts. In other words, it does not matter what metal we use, the ferroelectric properties should be the same. This view proved to be completely inaccurate, especially in the case of epitaxial films, where it was found that the properties are strongly dependent on the metal-ferroelectric interface.

The project can have a significant impact in the field of ferroelectric capacitors and development of electronic ferroelectric structures, especially ferroelectric diodes (Schottky or p-n diodes). The next step would be to develop performing ferroelectric MOS structures, as well as junction transistors but with ferroelectric properties. The greatest impact will be in the field of non-volatile memories, setting the ways to control the leakage current through the metal-ferroelectric interface engineering.

The results of the project could set the basis for a larger collaboration within the frame of international programs like FP7 or FP8. Other topics of common interest could emerge during the project, that can be valorised by submitting other joint project proposals in the frame of national and international programs in the next five years.





LEFT-TEM image of the PZT films deposited by PLD on $SrRuO_3$/$SrTiO_3$ substrates (preparation done at the Romanian partner). RIGHT-XRD patterns for sol-gel deposited PZT films on $SrTiO_3$ templated Si wafer (preparation done at the French partner).

Project webpage address: http://www.infim.ro/

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