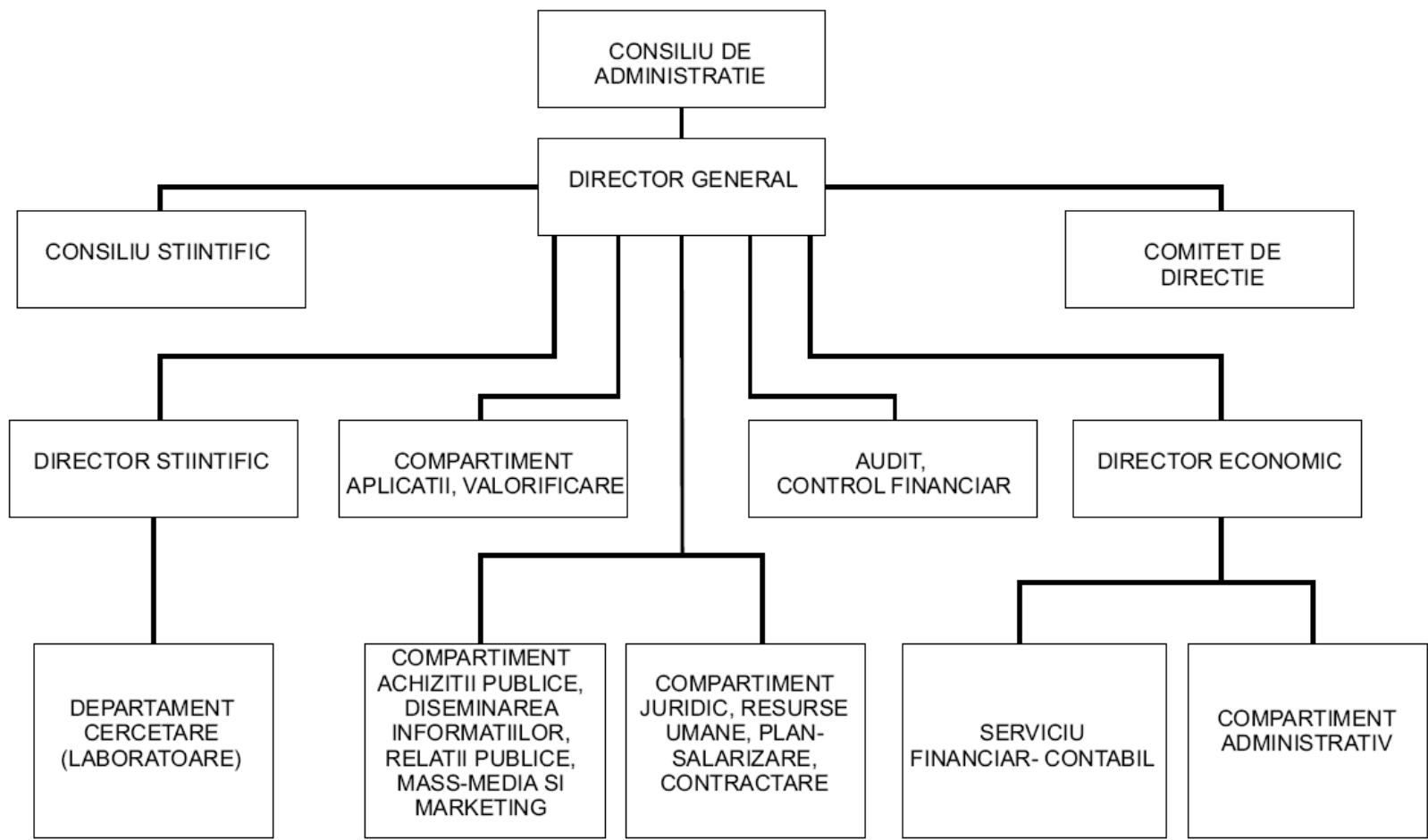


Self-assessment report
(2007-2011)

National Institute of Materials Physics
(NIMP)

STRUCTURA ORGANIZATORICA



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General activity report of NIMP

Period 2007-2011

The National Institute of Materials Physics (NIMP) was founded in 1996 by Government Decision. In 2008 was re-certified as national institute for research and development obtaining the highest score among all the national institutes, 360 points/researcher. NIMP is developing basic and applied research in the field of condensed matter physics with strong implications in materials science, especially regarding advanced (multi)functional materials. The institute had a solid experience in the field of single crystals with semiconductor or optic properties, as well as in the field of bulk ceramics with dielectric, piezoelectric or ferroelectric properties, and in the field of metals or complex compounds with magnetic or superconducting properties. Some thin films were also prepared, mainly using chemical methods or vacuum evaporation.

The research strategy of the institute has shifted markedly towards nanostructures and nanostructured materials in 2006. The main research directions for 2006-2010 were:

- 1. States, processes and phenomena in condensed matter physics.**
- 2. Nanostructured materials and nanocomposites: synthesis, characterization and applications.**
- 3. Advanced materials for special applications: in extreme conditions, for environment protection, biomedical, communications and information technology.**

Consequently, the entire acquisition policy was focused towards purchasing state-of-the-art equipments for fabrication and characterization of thin films, multilayers and nanostructures.

Actually, starting with 2006-2007 almost the entire institute was involved in a big, common research project aimed to transfer the expertise gained on bulk samples to low dimension/dimensionality samples, a project that can be called “**Multifunctional materials: from bulk to nanostructures**” (this is presented in more detail in a separate document). New equipments for depositing thin films were acquired, and new methods of fabricating nanostructures were implemented in the institute combining chemistry, electrochemistry, laser ablation or RF sputtering. Also, equipments for structural characterization were purchased allowing now resolution down to atomic scale (the new atomic resolution microscope from JEOL reaches a resolution of 0.08 nm in the STEM mode). The equipments for investigating physical properties were renewed to gain in sensitivity and to match the challenges imposed by the nanometer scale samples. The funds for purchasing new equipments were obtained mainly through the following sources:

- the Core Program, especially in 2007 and 2008;
- the 6 Capacities projects won by competition in 2007;
- the project “THE EURO-REGIONAL CENTRE FOR THE STUDY OF ADVANCED MATERIALS SURFFACES AND INTERFACES” won by competition in 2008 in the frame of structural funds (about 10 million euros of which 75 % where from EU structural funds). The project started in March 2009 and successfully ended in March 2011.

In total, around 15 million euros were invested in new equipments during the 2007-2011 period.

In parallel with the equipment acquisitions, the research teams were encouraged to shift their research interests towards low dimension systems such as thin films, multilayers, heterostructures, nanocomposites and nano-objects with various shapes. During the years 2007, 2008 and 2010 an important number of projects were obtained by competitions. Some of them ended in 2010, some of them are still funded in 2011, as follows: 80 projects were funded through the Executive Unit for Funding High Education, Research and Innovation (UEFISCDI) among which were 3 Ideas complex research projects (1 coordinated and 2 as partner), 22 Ideas research projects, 11 Human Resources projects and 44 Partnership projects (9 as coordinator and 35 as partner); 2 IFA (Institute of Atomic Physics-Romania) -CEA (France) projects; 5 Euratom-EFDA projects. 20 of the above projects were

won at the national competition organized in 2011 for Ideas and Human Resources programs. Besides the projects won at various national competitions NIMP has benefited also from the funding through the Core Program. The 3 projects funded through this type of program were designated to sustain the implementation of the scientific research strategy of the institute, elaborated for the period 2006-2010.

NIMP has benefited also, to some extent, from funding through various international programs. Currently, NIMP is involved in 1 FP7 large collaborative project, 4 COST actions, 2 SCOPES (funded from Switzerland) projects, 1 EUROCORE project. The institute is also involved in many bilateral cooperation, some of them in the frame of inter-governmental agreements, with research institutions from all over the world (Germany, Italy, Spain, France, United Kingdom, Belgium, Hungary, the Netherlands, Norway, Greece, Austria, Japan, China, India, Ukraine, USA, Turkey, etc.). The average turnover was around 43 million lei in the last 4 years (approximately 10 million euros at the current exchange rate), with a peak in 2008 and a minimum in 2009 when the economic crisis has made its presence in Romania. However, the consistent portfolio of projects allowed NIMP honorably facing the crisis despite the severe cuts in project funding.

The maintenance of a decent financial stability corroborated with the new equipments arrived in the institute made NIMP attractive for young students and researchers. Over 30 young scientists were employed in the last years and the fact that should be noticed is that none of these young people left the institute in these years of crisis. Many of them have finished also their PhD studies, many of them are PhD students at this moment. At present, NIMP has 111 scientists with PhD degree and 25 PhD students. Due to this policy in the field of human resources NIMP has now a balanced distribution of personnel in term of age, with over 40 peoples below 40 years and some 20 experienced senior researchers over 60 years.

A change in the management structure occurred in December 2008, when Dr. Stefan Frunza has left the position of General Director after a successful leadership of NIMP started in 1997, and Dr. Lucian Pintilie has taken the position of General Director after winning the competition organized by the National Authority for Scientific Research in November 2008. The laboratory structure of the Research Department has changed during the year 2009 so that at present NIMP has 5 laboratories, as follows:

Laboratory 10- *Multifunctional Materials and Structures*, head of laboratory: Dr. Ionut Enculescu (2 research teams)

Laboratory 20-*Magnetism and Superconductivity*, head of laboratory: Dr. Victor Kuncser (2 research teams)

Laboratory 30-*Physics of Condensed Matter at Nanoscale*, head of laboratory: Dr. Valeriu Moldoveanu (3 research teams)

Laboratory 40-*Optical Processes in Nanostructured Materials*, head of laboratory: Dr. Mihaela Baibarac

Laboratory 50-*Atomic Structure and Defects in Advanced Materials*, head of laboratory: Dr. Corneliu Ghica

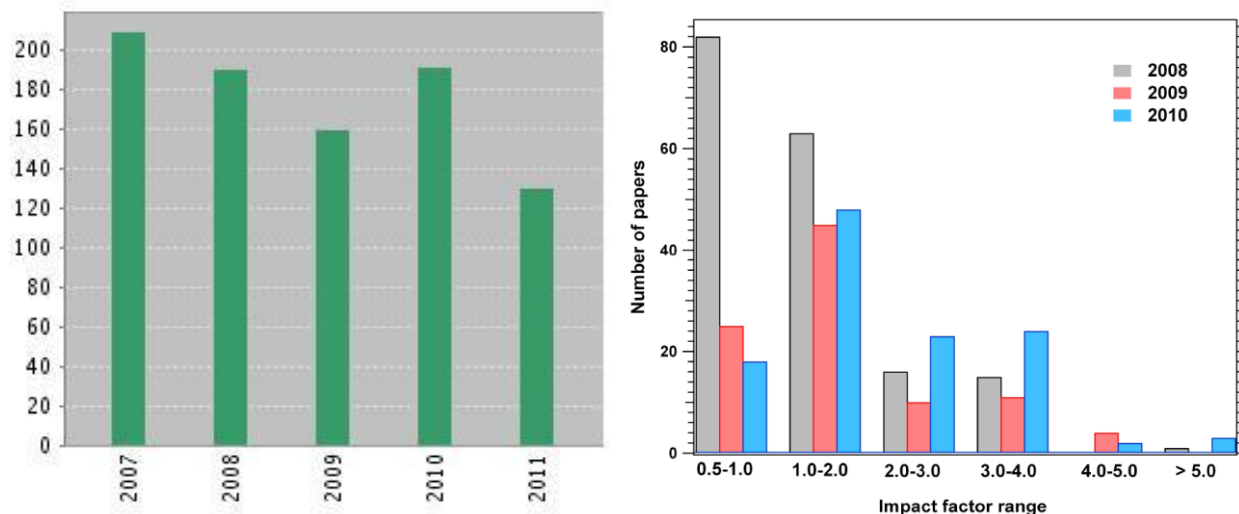
NIMP has also 2 certified laboratories, INDETIR and MAAS.

A new Scientific Council was elected in 2010 and some changes in the composition of the Administration Council took place in 2011 when new representatives of NIMP were nominated by Minister Order.

As the strategic plan for 2006-2010 has ended last year, a new development plan was discussed and approved in the newly elected Scientific Council, as well as in the Administrative Council. This development for 2012-2016 is presented in detail in a separate document.

In the 2007-2011 period the institute has published around 960 papers registered on ISI Thompson Web of Science. Around 800 of the papers are in journals with non-zero article influence score. NIMP has succeeded to maintain a high rate of publication of about 160 to 180 papers per year (see

the graph below). It has to be noticed also that an important number of these papers are published in journals with impact factor over 1.5, the weight of publications in journals with high impact factor increasing constantly in the last 3 years (see the graph below).



The good results obtained by NIMP in term of publications, projects, citations have reflected in very good positions obtained by the institute in different rankings at international and national levels. For example, the report “SCImago Institutions Rankings 2009 World Report”, made public by the portal SCImago Journal & Country Rank and using the information contained in the Scopus® database (Elsevier B.V.), has placed NIMP among the only three National Institutes ranked from Romania (see the following table).

Rank	Organization	Country	Sector	Output	CxD	Int. Coll.	Norm. SJR	Norm. Cit.
879	Universitatea Politehnica din Bucuresti	Romania	Higher educ.	2396	0.98	31.80	0.88	0.37
1034	Universitatea din Bucuresti	Romania	Higher educ.	1904	3.32	50.37	0.99	0.74
1485	Universitatea Babes-Bolyai din Cluj-Napoca	Romania	Higher educ.	950	2.38	49.37	0.95	0.75
1492	National Institute for Laser, Plasma and Radiation Physics	Romania	Government	943	3.17	67.76	0.99	0.80
1585	National Institute of Materials Physics	Romania	Government	809	2.66	64.03	1.01	0.72
1655	Horia Hulubei National Institute of Physics and Nuclear Engineering	Romania	Government	736	3.73	78.40	0.99	0.74
1916	Universitatea din Craiova	Romania	Higher educ.	507	1.32	29.39	0.85	0.48
2067	Universitatea Tehnica din Cluj-Napoca	Romania	Higher educ.	379	0.95	38.52	0.64	0.58

A recent classification, entitled Ranking Web of World Research Centers (elaborated by CSIC-Spain) (<http://research.webometrics.info>), section Research Centers, was published in July 2010. The classification of the Top 4,000 institutions ranked according to their activities and visibility on the Web which is an indicator of their impact and prestige shows that NIMP (position 1120) occupies, amongst Romanian research institutions, the second place after the "Horia Hulubei" National Institute of Nuclear Physics and Engineering (position 946) and before the prestigious Institute of Mathematics of the Romanian Academy (position 1722) and of the Romanian Academy (position 2078). This ranking shows that the NIMP web page has been often consulted and found attractive, in

close connection with the scientific performance indicators such as the number of publications and citations.

At national level NIMP is constantly in the top places in the rankings of Ad-Astra Association. For example, although the year 2011 is not yet ended, NIMP is currently on the first position in the Physics domain, considering the cumulated SRII (individual relative influence score)- (see the table below).

Nr.	Instituție	Localitate	SRII	Contribuția procentuală	SRI	Număr articole	Lista articolelor
1	INCD pentru Fizica Materialelor (INCDFM)	București	46.237	10.17%	97.697	87	Articole
2	INCD pentru Fizica Laserilor, Plasmei și a Radiației (INFLPR)	București	44.378	9.76%	133.785	134	Articole
3	Universitatea Politehnica București	București	40.800	8.97%	127.993	103	Articole
4	Universitatea Babeș-Bolyai	Cluj Napoca	39.651	8.72%	92.500	78	Articole
5	INCD pentru Fizică și Inginerie Nucleară Horia Hulubei (IFIN-HH)	București	36.482	8.02%	279.111	174	Articole
6	Universitatea București	București	36.438	8.01%	92.739	115	Articole
7	Universitatea Alexandru Ioan Cuza	Iași	33.594	7.39%	64.815	60	Articole
8	Universitatea de Vest	Timișoara	17.097	3.76%	90.261	42	Articole
9	Institutul de Chimie Macromoleculară Petru Poni (Academia Română)	Iași	13.023	2.86%	19.377	27	Articole
10	Institutul de Matematică Simion Stoilow (Academia Română)	București	11.280	2.48%	16.194	14	Articole

The institute got also an important number of awards in the last 4 years among which: the best research institute in 2008; the best manager of a research institute in 2008; first place in the top small and medium companies working in the research field in 2008 (top realized by the Chamber of Commerce Ilfov) and in 2011 (top realized by www.ListaFirme.ro); award for the best young scientist in 2008 and 2010; award for the Romanian journal with the highest impact factor in 2010 (for the Digest Journal of Nanomaterials and Biostructures, impact factor 2,079); numerous awards of the Romanian Academy; numerous awards and diplomas at various exhibitions and fairs (gold medal at Proinvent 2009, Cluj-Napoca, diploma at Geneva 2008, diploma of excellence at the Research Fair in 2011, etc.).

NIMP has constantly tried to strengthen its ties with the economy. Several contracts were signed with some important companies such as Turbomecanica, Honeywell, Zentiva, etc. These were service contracts in which the expertise and infrastructure of the institute was used to prepare or characterize some materials of interest for the above mentioned companies. Also, in the last two years the institute has organized a day of “open doors” when visitors from outside, including from companies, had the opportunity to make contact with the experts from the institute and to be informed about the institute’s capabilities. Though, the lack of high-tech Romanian companies is an obstacle towards a more successful relation with the economy. More attention must be given in establishing contacts with companies from European Union which can be interested to transfer some of the research results obtained by NIMP. A first try was with a medium company from Hungary, interested in the materials developed at NIMP for microwave applications, but nothing concrete was concluded until now except successfully testing of the materials included in the products of the Hungarian company.

NIMP has also important educational activities, in collaboration with different universities from Bucharest and from the country. The 15 certified PhD supervisors are associated professors at the Faculty of Physics, University of Bucharest, and many students from this Faculty, as well as from the Polytechnica University Bucharest, are coming to NIMP for license or master diplomas. In the last

five years a number of 27 PhD Thesis have been defended by our researchers, among them 17 being supervised by our PhD student's supervisors. The PhD students working in the institute are enrolled at above mentioned Universities. On the other-hand, post-docs from different universities are coming to work on projects at NIMP. In the last year, some PhD students from abroad came to work in the institute, for periods from 2 weeks to 3 months (e.g. from Turkey, Latvia, France). Postdocs are also expected to come and work at NIMP in the near future in the frame of national or international projects (e.g. one confirmed 1 year workstage will start in 2012 for a postdoc from UK in the frame of the IFOX project).

NIMP has received also the visits of some important political persons from the country and from abroad such as Presidents and Directors from the National Authority for Scientific Research, the cultural attaché of the French Embassy and, just recently, the visit of the German Ambassador. The last visit was intended to mark an important donation from the Alexander von Humboldt Foundation. The visit was also an opportunity for the Ambassador to meet the 5 Humboldt fellows working in the institute.

Another important activity of NIMP in the last 4 years was to invite prestigious researchers from abroad for presenting seminars on research topics of common interests and to visit the institute. New collaborations emerged after such visits. Also, NIMP was organizing or was co-organizers of some important scientific events, as for example:

- The International Romanian Conference on Advanced Materials, editions 2006 and 2009
- The International Conference on Amorphous and Nanostructured Chalcogenides, editions in 2007, 2009 and 2011
- WODEAN workshop in 2010, related to the RD-50 project coordinated by CERN
- The workshop "Micro and nanostructured multifunctional materials: from research to applications" organized in 2010 as part of 2nd Conference with Romanian Diaspora
- An international workshop dedicated to TEM analysis, organized in 2011 with the occasion of inauguration of the new JEOL JEM ARM 200F microscope
- The National Symposium "Radu Grigorovici Centenary", organized in 2011 with the exceptional participation of the EMRS President, Prof. Rodrigo Martins

NIMP is editor or co-editor to three scientific journals, all of the having ISI impact factor:

- Digest Journal of Nanomaterials and Biostructures
- Journal of Optoelectronics and Advanced Materials
- Optoelectronics and Advanced Materials-Rapid Communications

NIMP is part of the consortium designated to commission the ELI-NP (Extreme Light Infrastructure-Nuclear Physics) at Magurele, as one of the 3 (three) pillars of the ELI pan-european structure (the other two pillars will be commissioned near Prague, in the Czech Republic, and in Szeged, Hungary). Also, NIMP was designated as Partner Center to represent Romania in the working group established to organize another pan-European distributed research infrastructure, provisionally named CERIC (Central European Research Infrastructure Consortium). The other members of the CERIC working group are from Austria, Hungary, Italy, Croatia, Slovenia, Serbia, the Czech Republic and Poland. Another important achievement of the last years was the initiation, together with "Horia Hulubei" foundation, of a project aimed to establish a category II UNESCO institute as a legally independent unit in the structure of NIMP. The project was just approved by the executive committee of UNESCO and will get the final approval during the UNESCO General Assembly in November 2011. The new unit of NIMP will be dedicated to advanced studies in Physics and will closely collaborate with the theoretical center ICTP Trieste, Italy.

The conclusion of this short and general report is that NIMP is an excellent research institution at national level and started to be a well appreciated partner at international level, mainly in Europe. It is a dynamic institute, with an enthusiastic and young human resource, and with a significant potential to become one of Romania's representative research institution in the world.

E1-Group of functional nanostructures.

The group led by dr. Ionut Enculescu is comprised of 6 senior researchers (Dr. Daniela Predoi, Dr. Silviu Polosan, Dr. Monica Enculescu, Dr. Nicoleta Preda, Dr. Elena Matei), 4 PhD students (Drd. Florica Camelia, Drd. Carmen Ciobanu, Drd. Simona Iconaru, Drd. Corina Radu) and 2 technicians.

Main research directions

The group aims at an interdisciplinary approach of materials, activating in both preparation of nanomaterials and nanostructures for a wide range of applications but also in characterization, covering several important techniques.

1. Nanowires and nanotubes preparation by template replication.

The template method is one of the most convenient in order to fabricate nanowires or nanotubes. By replicating a nanoporous membrane with cylindrical pores with controlled dimensions, such as polymer ion track membranes or anodic alumina, we were able to obtain nanowires with well controlled morphology and extremely high aspect ratio.

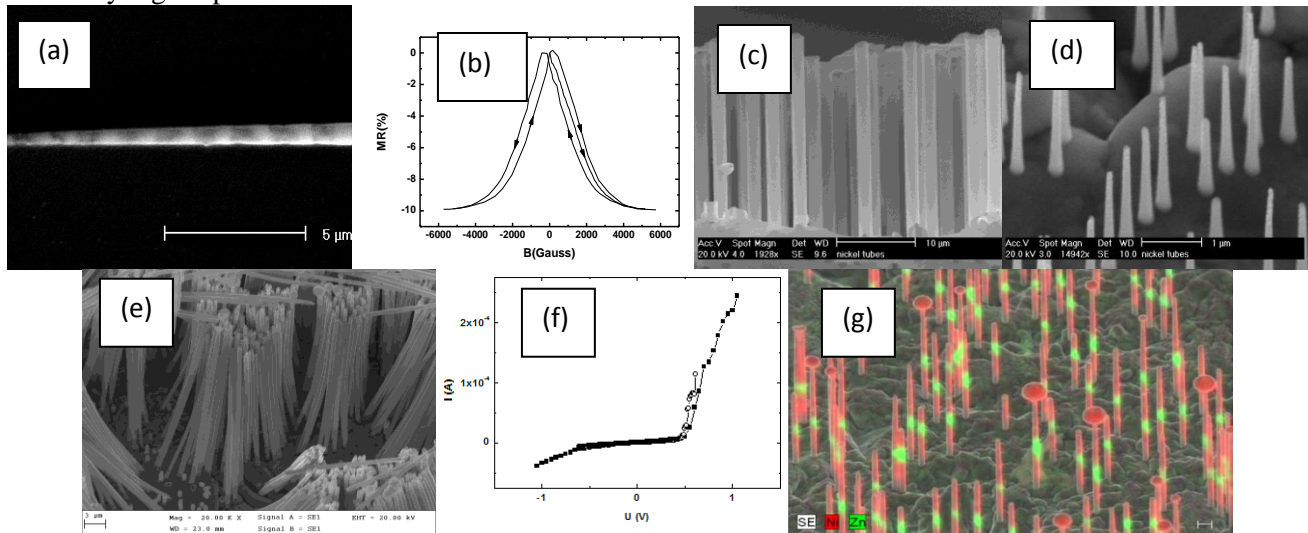


Figure 1. Structures fabricated by template replication in the group of functional nanostructures: (a) multilayered metallic nanowire with giant magnetoresistance; (b) giant magnetoresistance effect in multilayered nanowires; (c) nickel cylindrical tubules fabricated by electroless deposition; (d) nickel conical tubules fabricated by electroless deposition; (e) cadmium teluride nanowires; (f) current voltage characteristics of a CdTe photodiode; (g) multisegment Ni-ZnO-Ni nanowires

Usually the replication of the nanoporous membranes is performed using electrochemical and chemical deposition due to the fact that is more difficult to fill such low diameter pores by employing physical methods. Using this approach metal and semiconductor nanowires were obtained. Further, complex structure nanowires such as multilayered magnetic nanowires with current perpendicular to plane giant magnetoresistance were prepared by a simple electrochemical pulsed deposition. Semiconductor electrodeposition was also employed opening the possibility that by template replication to fabricate high quality pure or doped nanowires. Moreover, the next logical step was to prepare more complex hetrostructures, either by pulsed deposition when the electrochemical properties of the system make it possible or in a more complicated manner namely by a sequential approach where the deposition bath is changed as a function of the desired results. The focus is towards functionality and we succeeded to obtain such nanostructures as a GMR sensor with 10% response at room temperature and a nanowire homojunction diode of CdTe with photovoltaic properties.

The aim at this moment is to integrate nanowires in more complex functional devices, the focus being in using lithographical techniques for providing nanowires with electrical contacts such as for example a field effect transistor.

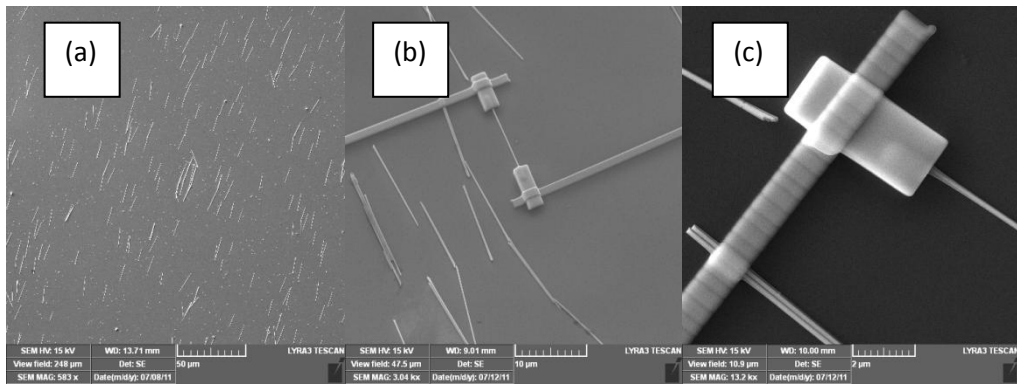


Figure 2. (a) Nanowires aligned by magnetic field; (b) nanowire contacted by focused ion beam induced metallization; (c) details of focused ion beam induced metallization contact to nanowires

The contacts were provided by means of focused ion beam induced metallization technique promising results being already obtained. For the future in this direction we aim at developing new templates, to develop new methods of self assembly of the nanostructures in devices and to develop new functionalities for such nanostructures with tailored properties.

Selected references: Multisegment CdTe nanowire homojunction photodiode, Matei, E., Ion, L., Antohe, S., Neumann, R., Enculescu, I., Nanotechnology 21 (10), art. no. 105202, 2010; Preparation and properties of cobalt doped ZnO nanowires, Enculescu, I., Matei, E., Sima, M., Neumann, R., Granville, S., Ansermet, J.-P., 2008 IEEE Transactions on Magnetics 44 (11 PART 2), pp. 2678-2680; Current perpendicular to plane single-nanowire GMR sensor Enculescu, I., Toimil-Molares, M.E., Zet, C., Daub, M., Westerberg, L., Neumann, R., Spohr, R., 2007, Applied Physics A: Materials Science and Processing 86 (1), pp. 43-47

2. Light emitting materials for applications; photonics

Light emitting materials with properties such as intense photoluminescence, scintillating behaviour or electroluminescence are employed in a wide range of applications from lasers or light emitting diodes to scintillating particle detectors. There are several subdirections which were pursued in our group for such materials.

Wide band gap scintillators, crystals, glasses or glass-ceramic materials, play an important role nowadays, for detection of photons with high energy (like X or gamma rays), charged particles or neutrons. Both preparation and characterization of materials from this class of materials were pursued. From classic BGO crystals to BGO glasses or glass ceramics were prepared and investigated, the experimental conditions necessary for obtaining high quality materials being found. In this range of materials pure and doped inorganic crystals were also prepared and investigated. The optical active color centers were investigated from both a fundamental point of view or for applications.

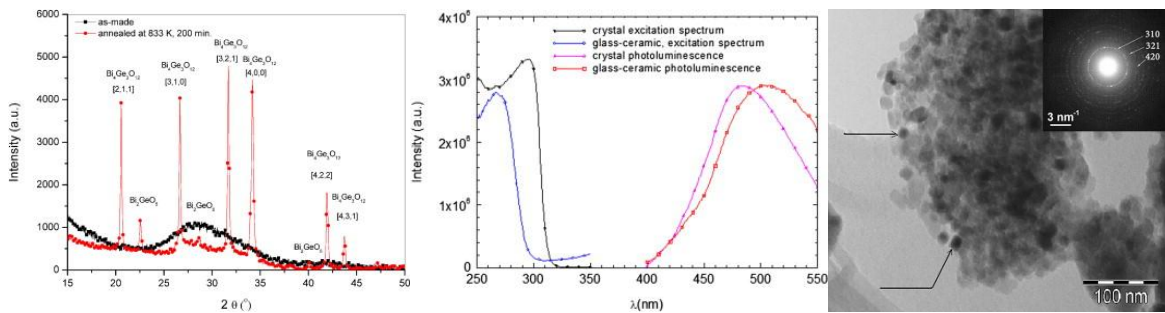


Figure 3. (a) X ray diffraction plots for glass and glass ceramic BGO; (b) excitation and emission photoluminescence spectra of BGO crystal and glass ceramic photoluminescence; (c) transmission electron microscopy and selected area electron diffraction for BGO ceramic glass.

Pure and doped semiorganic crystals with intense photoluminescence and up-conversion properties were prepared either in macroscopic form or as nanorods by template replication. These crystals present a combination of intense luminescence due to organic dyes doping and second harmonic generation of the host (e.g. potassium acid phthalate).

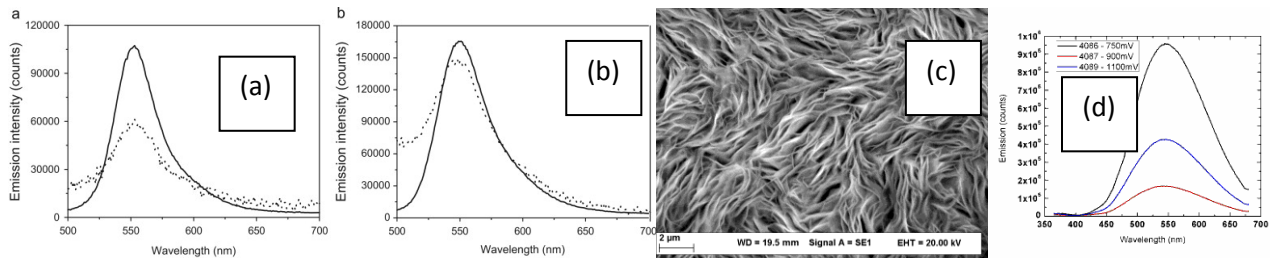


Figure 4. (a) and (b) Emission spectra excited with 480 nm (solid lines) and with 890 nm (dotted lines) for doped potassium acid phthalate crystals, (c) top view of a self assembled ZnO/Sm₂O₃ bilayer with intense luminescence, (d) photoluminescence emission of ZnO/Sm₂O₃ bilayers

Thin film light emitting layers were prepared by various means such as electrochemical deposition, spin coating or vacuum evaporation. The main purpose is to fabricate functional devices as light emitting diodes or organic light emitting diodes with increased functionality and lower fabrication costs.

Templateless fabrication of polymer colloids or of semiconductor nanoparticles with controlled morphology were also a goal for our research during the last few years.

Selected references: Electrodeposited ZnO films with high UV emission properties, Matei, E., Enculescu, I., Materials Research Bulletin 46 (11), pp. 2147-2154, 2011; Luminescence of dye-doped KAP and KDP nanorods, Enculescu, M., Trautmann, C., Radiation Measurements 45 (3-6), pp. 602-604, 2010; Polymer-assisted crystallization of low-dimensional lead sulfide particles, Preda, N., Rusen, E., Enculescu, M., Matei, E., Marculescu, B., Enculescu, I., Physica E: Low-Dimensional Systems and Nanostructures 43 (10), pp. 1826-1832, 2011; Structural changes during the crystallization of the Bi₄Ge₃O₁₂ glasses Polosan, S., Nastase, F., Secu, M., 2011 Journal of Non-Crystalline Solids 357 (3), pp. 1110-1113; Dynamics of energy absorption versus crystallization in Bi₄Ge₃O₁₂ (BGO) amorphous materials, Polosan, S., 2010, Materials Research Bulletin 45 (10), pp. 1492-1495

3. Materials and devices for bio-applications

In this research direction most important results were in the direction of preparing a range of new materials with increased biocompatibility. The preparation methods are mostly sol-gel, chemical bath deposition or other synthesis techniques. Thus the results range from sol-gel prepared thin films of pure and doped hydroxiapatite to the synthesis of biocompatible or environmental friendly polymers. The materials were prepared and characterized by a wide range of techniques.

Research is in development for this field, a device based on odor binding proteins for odor sensing being developed. Also, new methods of protein crystallization inside membrane nanopores are developed during this time for fabricating protein crystals with tailored morphology. Environmental friendly polymers with controlled morphology such as spheres or fibers are prepared for bio applications.

Selected references: Characterization of sucrose thin films for biomedical applications Predoi, D., Iconaru, S.L., Ungureanu, F., Costescu, A., Costache, M., Dinischiotu, A., 2011, Journal of Nanomaterials 2011, art. no. 291512, Synthesis and characterization of bio-compatible maghemite nanoparticles Predoi, D., Andronescu, E., Radu, M., Munteanu, M.C., Dinischiotu, A., 2010 Digest Journal of Nanomaterials and Biostructures 5 (3), pp. 779-786

The group is involved in numerous internal and international collaborations for achieving its research goals. Thus, traditional national partners are: University of Bucharest (Faculty of Physics) on projects related to energy generation in photovoltaic structures, on the study of light emitting materials and structures, Politechnical University of Bucharest, studies related to biocompatible materials, Technical University of Iasi on developing devices for fabricating nanostructures or to employ sensors based on nanostructures, National Institute of Lasers Plasma and Radiation Devices in developing new biocompatible materials. The group performs characterization of materials for national partners, main techniques being scanning electron microscopy and energy dispersive X ray spectroscopy, photoluminescence (both far field and near field spectroscopy), cathodoluminescence, optical transmission spectroscopy, circular dichroism and magnetic circular dichroism spectroscopy.

The group is also part of numerous international collaborations with groups from Great Britain, Austria, Switzerland, Germany, France and Japan. There are several international projects where the group is part, as follows: SCOPES project financed by Swiss National Science Foundation (Project leader Prof. Jean-Philippe Ansermet from EPFL), EUROCORE project (a financing scheme of European Science Foundation), lead by Prof. Wolfgang Knoll, Austrian Institute of Technology, Royal Society project led by Prof. Walther Schwarzacher University of Bristol.

E2-Group of Complex Heterostructures and Perovskite Oxides

Head: dr. Ioana Pintilie, CS1

Main research directions. The Group of Complex Heterostructures and Perovskite Oxides is part of Laboratory 10- Multifunctional Materials and Structures. The main research directions of the group are:

- Deposition and electric/ferroelectric/photoelectric characterization of ferroelectric thin films, multiferroic thin films, artificial multiferroic structures and any other complex heterostructures involving ferroelectric or multiferroic materials such as Pb(Zr,Ti)O₃ (PZT), BaTiO₃, BiFeO₃, etc.
- Investigation of electrically active defects in complex heterostructures such as MOS-like devices, but also in diode-like structures based on semiconductor materials
- Fabrication and characterization of bulk ceramic and thin films for applications in wireless communications (microwave and millimeter wave domains). Among the studied materials are: BaX_{1/3}Ta_{2/3}O₃ (X=Zn or Mg), Ba_{1-x}Sr_xTiO₃ (x=0.25 – 0.90), (Zr_{0.8}, Sn_{0.2})TiO₄ and Ba_{1-x}Pb_xNd₂Ti₅O₁₄.
- Fabrication and characterization of bulk ceramics and thin films with piezoelectric properties such as doped Pb(Zr,Ti)O₃ or lead-free materials as for example (1-x) (Bi_{0.5}Na_{0.5}) TiO_{3-x}BaTiO₃
- Fabrication and characterization of oxide semiconductors with applications in temperature sensing or on water photo-electrolysis
- Investigation of optical and dielectric properties at high frequencies by using spectroscopic methods such as spectroscopic ellipsometry for optical wavelengths and THz time-domain spectroscopy for the THz domain up to 7 THz.

Main scientific achievements. In the reported period the group has obtained some important results, materialized in publications in important journals as follows:

- The transport properties in epitaxial PZT films were investigated on a wide range of temperatures, from 4 K up to 400 K. By correlation with hysteresis measurements, it was shown that the height of the potential barrier at the electrode-ferroelectric interface is affected by the presence of the bound polarization charge localized just near the interface. In the high quality ferroelectric films the spontaneous polarization can be large, reaching values close to 1 C/m², thus the effect on the potential barriers can be significant lowering of its height (around 0.5 eV). The work was made in collaboration with Max Planck Institute from Halle, Germany, was published in PHYSICAL REVIEW B, 75, 104103, (2007), and has already 40 citations on Web of Science.
- A coherent model was developed for the metal-ferroelectric-metal (MFM) structures based on epitaxial films. The model allows explaining the behavior of the dielectric constant with frequency and with the thickness of the ferroelectric layer. It was shown that the intrinsic dielectric constant of PZT is about 40, much lower than the values extracted from capacitance measurements. This fact suggests that the equivalent dielectric constant of the MFM structures is dominated by extrinsic contributions coming from electrode interfaces and structural defects. Results published in PHYSICAL REVIEW B, 75, 224113, (2007), 18 citations.
- Other important results obtained in the field of ferroelectric/multiferroic films and multilayers, as well as in the field of ferroelectric-based heterostructures were published in: JOURNAL OF APPLIED PHYSICS, 101, 064109, 2007 (23 citations); PHYSICAL REVIEW B, 82, 085319, 2010 (4 citations); APPLIED PHYSICS LETTERS, 96, 012903, 2010 (2 citations); APPLIED PHYSICS LETTERS, 94, 232902, 2009 (14 citations); JOURNAL OF APPLIED PHYSICS, 104, 114101, 2008 (10 citations); JOURNAL OF APPLIED PHYSICS, 103, 024101, 2008 (10 citations); NEW JOURNAL OF PHYSICS, 10, 013003, 2008 (8 citations).
- Important results were obtained in the field of radiation induced defects in Si detectors used for LHC experiments at CERN. The work was done in the frame of the RD-50 project, in close collaboration with the Institute of Experimental Physics, University of Hamburg, Germany. Other important results were obtained in the field of defect investigation in MOS structures based on SiC, in close collaboration with University of Oslo. These results were published in: JOURNAL OF APPLIED PHYSICS, 108, 024503, 2010 (4 citations); PHYSICAL REVIEW B, 77, 073206, 2008 (3 citations); APPLIED PHYSICS LETTERS, 92, 024101, 2008 (6 citations); NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT, 583, 58, 2007 (13 citations); NUCLEAR

INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT, 570, 322, 2007 (6 citations).

- $\text{BaX}_{1/3}\text{Ta}_{2/3}\text{O}_3$ (X=Zn, Mg) complex perovskites were prepared for microwave application. The obtained dielectric constant and dielectric loss are: $\epsilon_r \sim 28$ and $Q \times f \sim 120\,000$ GHz for $\text{Ba}(\text{Zn}_{1/3}\text{Ta}_{2/3})\text{O}_3$ and $\epsilon_r \sim 24$ and $Q \times f \sim 220\,000$ GHz for $\text{Ba}(\text{Mg}_{1/3}\text{Ta}_{2/3})\text{O}_3$. Preliminary research on $\text{Ba}_{1-x}\text{Sr}_x\text{TiO}_3$ ($x=0.25 - 0.90$) showed that the increase in Sr content reduces considerably the ferroelectric cubic to tetragonal transition temperature, decreases substantially the microwave dielectric permittivity and losses, decreases the unit cell volume and the effect of grain segregation. Among important publications are: JOURNAL OF ALLOYS AND COMPOUNDS, 509, 477, 2011 (2 citations); APPLIED SURFACE SCIENCE, 256, 6526, 2010 (2 citations); THIN SOLID FILMS, 516, 8210, 2008 (9 citations); THIN SOLID FILMS, 516, 1558, 2008 (6 citations); PROGRESS IN SOLID STATE CHEMISTRY, 35, 513, 2007 (12 citations).
- Development of some applications based on semiconductor oxides or piezoelectric ceramics. A patent was obtained for “piezoelectric ultrasonic transducer for prevention of depositions on the walls inside in heat exchangers”. Some papers were also published in the field of piezoceramics: JOURNAL OF THE EUROPEAN CERAMIC SOCIETY, 27, 4055, 2007 (6 citations); FERROELECTRICS, 350, 38, 2007 (1 citation).
- The ellipsometry proved to be a valuable tool in characterization of thin films and multilayers. Several publications were produced in the reported period, among which: SOLID STATE SCIENCES, 13, 49, 2011 (2 citations); APPLIED SURFACE SCIENCE, 256, 6526, 2010 (2 citations); THIN SOLID FILMS, 518, 4603, 2010 (6 citations).

Facilities and expertise. The group has a valuable expertise in the preparation of bulk ceramics by standard technology, or combining chemical methods with standard technology. It has also expertise in deposition of thin films and multilayers by chemical and physical methods. In the field of characterization, the group has expertise in electrical measurements, piezoelectric measurements (coupled with AFM), trap investigation, photoelectric measurements. The main infrastructures are:

- Pulsed Laser Deposition (PLD) system based on a KrF excimer laser with a wavelength of 248 nm, maximum energy of 700 mJ and repetition rate of maximum 10 Hz. The deposition chamber has a 4 targets carousel and a substrate heater up to 1000 °C. The PLD is equipped also with a high-pressure RHEED system for in-situ monitoring of the crystalline structure and thickness during deposition.
- A RF-sputtering system model GAMMA γ 1000C™ with 4 targets and 3 working gases (Ar, N₂, O₂).
- A complete set-up for complex electric/ferroelectric/photoelectric investigation of the prepared thin films and heterostructures. The set-up contains: a cryogenic probe station from LakeShore, model CPX-VF, working between LHe temperature and 400 K, with 4 manipulating arms, optical window and magnetic vertical field up to 2.5 Tesla; a closed cycle He cryostat working between 10 and 475 K, with optical window; a high temperature cryostat working between 77 K and 800 K; a ferroelectric tester model TF Analyser 2000; a ferroelectric tester from Radiant Technology, model Precision Premier II; several capacitance bridges and multimeters/picoameters; a grating monochromator for 200-3000 nm wavelength range, model SM257 from Oriel.
- An AFM/PFM machine from Asylum Research, model MFM-3D-SA
- A SPM system from NT-MDT model NtegraAura, working in various modes among which AFM, MFM, EFM, SKM, SCM, STM.
- A complete line for characterization of materials and devices in the microwave domain, including: a set of network analysers from Agilent covering a frequency domain from 10 MHz to 500 GHz; a probe station from Cascade allowing contacting microstrip lines at room temperatures; a cryostation from LakeShore, model CPX-HF with two manipulator arms, working in the temperature range from 4.2 K to 400 K, with horizontal magnetic field up to 1 Tesla.
- A state-of-the-art DLTS system which can detect trap concentrations as low as 10^{-8} cm⁻³.
- A broadband time domain THz spectrometer working up to 7 THz.

Funding, projects and collaborations. The group has benefited of funding through several national projects in the frame of CEEX, Ideas, Human Resources and Partnership programs. Currently, the group has 2 Partnership project in coordination and is involved in 4 projects as partner, 2 reintegration grants, 1 IFA-CEA project and 1 Capacities-CORINT project. At the last competition organized in 2011 the group has won 2 Ideas projects, 1

project for Young Team and 1 Post-Doc project. Beside this, the group is involved in 1 FP7 large collaborative project with acronym IFOX (started in 2010), is associated to another FP7 project-Marie Curie Training Network, is member of the RD-50 collaboration lead by CERN, and is involved in 1 COST action SIMUFER. The group is collaborating with research teams Romania (e.g. INFLPR, INOE 2000, IMT, ICPE-CA, University of Bucharest, UAIC, etc.) and with research teams from countries such as Germany, the Netherlands, Italy, Norway, France, Turkey, Japan, Australia, USA, etc. In 2011 the group leader has received a donation from Alexander von Humboldt Foundation, in value of about 20,000 EUR. The Ambassador of Germany has visited the group with this occasion. The close collaboration with different groups from abroad materialized also in several exchanges of peoples. Some researchers from the group went to work abroad (e.g. Dragoi Cristina at MPI-Halle, Germany; C. F. Miclea to LANL, USA; A. C. Galca to CNRS, Rennes, France; M. Cernea to Faenza, Italy; I. Pintilie to Hamburg University, Germany and Oslo University, Norway). On the other hand some researchers from abroad came to work in the group (e.g. H. Khassaf from Sabanci University, Turkey; A. LeFebvrier from CNRS Rennes, France).

Dynamic of the research topic and new directions. The group is connected to the international trends in research on the topic of multifunctional oxide materials and related heterostructures. It was a gradual shift from bulk ceramics, used for applications like pyroelectric detection, thermistors, piezoelectric transducers, dielectric substrates for microwave applications, etc. towards thin films, heterostructures and nanostructures. The group strategy was to combine the expertise of the group members on various oxide materials in order to obtain heterostructures with optimized or new functionalities. Now, most of the group is working on thin films and multilayers, although the expertise on bulk ceramics was not abandoned being very useful in preparing the targets for thin film deposition. For the near and medium term the envisaged research directions will be focused towards:

- Role of interfaces in artificial multiferroics obtained by successive deposition of ferroelectric and ferromagnetic materials
- In depth study of formation of electrode-ferroelectric interface, role of polarization charges in interface construction and charge compensation at the interface
- Tuning of various properties by engineering the interfaces and the defect structure in thin films and multilayers
- Developing left-handed metamaterials for applications in microwave and THz devices
- Study on dielectric thin films and multilayers with high dielectric constant and low losses for microwave applications
- Developing diode-like and field effect devices based on all-oxide structures or on combinations of materials with different functionalities: ferroelectric-magnetic semiconductor; ferroelectric-superconductor; high-k dielectrics-oxide semiconductors.
- Investigation of trapping level in relation with the macroscopic electric properties.

Evolution of human resources. The group has emerged in the present form through a coagulation process taking place a few years. The common interest on oxide materials with perovskite structure, with emphasis on dielectric, ferroelectric, piezoelectric properties and on defect engineering has facilitated the merge of three smaller groups from laboratory 10 in one but stronger group. Currently the group has 22 researchers, among which 5 senior researchers rank 1. However, it has to consider that 1 of the senior researchers rank 1 just retired and another one will retire in the next few months. This is not a matter of concern because the group has other senior researchers, 2 of rank 2 and 6 of rank 3, able to replace the retired and to preserve their expertise. The group has also many young researchers hired in the last 4-5 years. Among them are: dr. Dragos Lucian Filip, who got his PhD in UK and came into the institute with a reintegration grant funded by UEFISCDI; researcher Cristina Dragoi, who just got his PhD in 2011; other two researchers who are in the final year with the PhD thesis, Lucian Trupina and Marius Cioangher; assistant research Adrian Filimon who will get his PhD in Germany this year and will work on the FP7 project; assistant researchers Busuioc Cristina, PhD student in Romania, Roxana Radu, PhD student common supervising in Romania and Germany, and Augustin Dutu, PhD student in Belgium; the last hired were Georgia Ibanescu, Liliana Trinca and Dragos Geambasu (master student). Therefore, the group proved to be attractive for young researchers due to its scientific topics and results, collaboration abroad and state-of-the-art facilities.

E3- “Electronic Correlations and Magnetism”

As one of the two research teams belonging to Laboratory 20 –Magnetism and Superconductivity, at NIMP, the group called “*Electronic Correlations and Magnetism*” has a focused interest in investigation of the electronic phenomena and magnetic properties in materials and especially in nano-size structures.

Actually, the group is composed by 11 senior researchers and 10 young scientists (6 are assistant researchers) plus one highly specialized engineer and 5 technicians for practical activities and for maintenance of the complex measuring systems. Two of the young assistant researchers were employed in the last two years. In average, two PhD students among the members of the group defend their PhD thesis yearly (there are still 5 PhD students, two of them going to defend their PhD thesis by the next 6 months). For research/educational purposes, among the senior researchers there are also 3 PhD certified promoters and advisers, as associated professors to Faculty of Physics.

The experienced senior researchers have a highly national and international recognized expertise, being also promoters of national projects (5 PCE-Ideas, with 2 projects winners at 2011 competition, 12 Partnership projects with 3 as coordinators, 4 Euroatom-EFDA projects, etc.) as well as of many bilateral cooperations (with institutions from Germany, Spain, Italy, France, United Kingdom, Greece, Poland, Russia), just to mention active projects launched after 2008. An FP6 Network of excellence (Magmanet) project, with the group as co-promoting partner, ended in 2009. With an average output of about 25 papers per year registered in ISI Thompson Web of Science and a mean Hirsch Index of about 10 per high senior researcher, the group takes also the advantage of interdisciplinary topics and large possibilities to cover different aspects of materials science, from their preparation to a deep characterization.

The group has a high expertise concerning both preparation/processing of nanostructures (nanopowders, nanocomposites, thin films and multilayers) and in their complex characterization. The magnetic nanophases are prepared by various technologies, like mechanical attrition, melt spinning, microwave annealing, spark plasma & hot press sintering, radiofrequency sputtering, chemical routes, etc. Subsequent processing via thermal treatments (assisted or not by applied magnetic fields) or via gas reaction control can be also applied.

Structural and morphological characterization of the samples and a large field of magnetic, thermodynamic and transport properties are studied by Physical Properties and Magnetic Properties Measurement systems (PPMS, MPMS-SQUID), Vibrating Sample and Magneto-Optic Kerr effect magnetometry (VSM and MOKE), DSC/DTA as well as Laser Flash Calorimetry. The declared purpose of understanding and controlling the electronic phenomena and spin configurations benefit also by the whole range of Mössbauer spectroscopies (the only institute in Romania), from temperature /field dependent Mossbauer spectroscopy, to the surface/ interface sensitive Conversion Electron Mössbauer Spectroscopy (CEMS). In many respects, all the above mentioned devices present state of art performances, being acquired or upgraded along the last 3 years.

According to internationally recognized group abilities and following the general research trend in the NIMP, the focusing of the group activity was shifted along the last years from studying the electron phenomena and correlations in bulky like materials to the investigation of the electronic and magnetic peculiarities induced by size effects (decreased dimension and dimensionality) and surface and interfacial interactions. Three main research directions have to be mentioned:

1. *Size effects and interactions in nanoparticulate systems and nanocomposites*
2. *Interfacial interactions and surface electronic/spin configurations in layered nanosystems*
3. *Phase transitions and electron correlations in functional materials*

1. In the larger frame of magnetic materials with specific properties arising from their nanometer size and multiple phase structure, we have investigated exchange bias effects and reversible phase transformations in Fe / Fe₃O₄ mixed nanopowders (J. Alloys & Compounds 509 (2011) 6522). Other studies concern advanced hybrid nanostructures made of core-shell nanoparticles (Nanotechnology 19 (2008) 505602) that exhibit giant magnetoresistance effects, engineered by self-assembly into regularly dispersed 2D arrays onto lithographically pre-patterned substrates. These researches were funded by 2 national projects and supported by access to international facilities at ESRF-Grenoble and EPFL-Lausanne, as well as by a scientific bilateral agreements with Aristotle University of Thessaloniki.

Exchange coupling effects responsible for the magnetic hardening in Nd₂Fe₁₄B/□-Fe or FePt(NbB) based exchange spring magnets have been also considered. Investigations of the crystallisation process of the metastable amorphous matrix, the relationship between microstructure and magnetic properties, the local magnetic interactions and spin configurations or of the influence of micro-alloying elements in optimizing the microstructure have been reported (3 papers and 2 patents have to be mentioned). Also FePt-based nanocomposite magnets were investigated (J. Appl. Phys. 108 (2010) 093910) since they are highly corrosion resistant and have operating temperatures higher than classical Nd-Fe-B. We have shown (J. Phys. D: Appl. Phys. 44 (2011) 365002) that in Ag-substituted FePtB nanocomposite ribbons, the hard magnetic L1₀ phase can be directly obtained in the as-cast state, without need of post-synthesis annealing and with beneficial influence on magnetic properties. These results were backed out by national projects and international cooperations with Universities from Le Mans, Rostock and DESY-HASYLAB.

Of high interest along the last years was devoted to the study of magnetic relaxation and spin configuration in ferrofluids (obtained by chemical routes) and nanopowders (obtained by both chemical routes and laser pyrolysis), in order to optimize the systems for various applications. The influence of surfactants and type of magnetic nanoparticles on the magnetic relaxation mechanisms in ferrofluids was considered (e.g. J.Phys.:Condens. Matter 19 016205, 2007). Nanopowders obtained by laser pyrolysis, as composite materials containing various phases (oxides, carbides, metals) depending on processing conditions, giving rise also to core-shell structures were studied. Main outputs (8 papers) are related to peculiarities of interactions, dimensionality (e.g. J. Nanosci. Nanotech. 10 1223 2010), catalytic effect (Int. J. Photoenergy 604181 2008), or multi-metal presence (Appl. Surf. Sci. 257 5460–5464, 2011).

Unusual phenomena were revealed in a large number of molecular crystals. The most relevant results evidenced unquenched orbital moment in FePc [Phys. Rev. B 81(2010)195405] and the first tetranuclear compounds [Phys. Rev. B 80(2009)014430, Polyhedron 28(2009)3017] showing spin blocking at 3 K and AF arrangement per molecule. Other novelty data revealed both intra- and inter-molecular AF couplings in oxalates [J.M.M.M. 310(2007)1452 and 323 (2011) 1044] with induced low and intermediate spin state via specific ligands and also intermixing spin state and single molecule magnet behavior in most of new 4f + 3d complexes [J. Amer. Chem. Soc. 129(2007)9248]. The output (8 publications) was realized inside three national projects and an European FP-6 one.

2. Interfacial interactions, spin configuration and atomic inter-diffusion at the interface in bilayer systems presenting exchange bias and exchange spring behavior have been studied in various ferromagnetic/antiferromagnetic and soft magnetic/hard magnetic systems, respectively. Methodological aspects suitable to provide both the angular spin distribution at surface and interface as well as the interfacial atomic diffusion were developed (J.Magn.Magn.Mater 323 2196-2201, 2011, Thin Solid Films 518 5981-5985, 2010, Phys.Rev. B 78 224402, 2008). Multilayer type and

nanoglobular thin film type spin valve structures were approached with respect to the complex correlations between structural, morphologic and magnetic aspects and giant magnetoresistance (GMR)/tunneling magnetoresistance (TMR) effects. Multilayer spin valve structures with different parameters extending in a well controlled way over a convenient range of values have been obtained by combinatorial processing methods (e.g. thermoionic vacuum arc -TVA- or rf sputtering) and subsequently characterized. The Fe phase distribution and local spin configuration was analyzed at the ferromagnetic/conductor and ferromagnetic/dielectric interface as well as at different depths away from the interface via CEMS, within the ^{57}Fe tracer layer technique (e.g. J Alloys Comp. 499, 23-29, 2010, J.Magn.Magn.Mater 320 E226-E230, 2008). The magnetization reversal in the ferromagnetic layers, observed via magnetometry and MOKE was correlated with magnetoresistive effects. The theoretical and experimental study envisaged the optimization of such structures in relation to their magnetic and magneto-conduction behavior. This research, funded by 2 national projects, was done in collaboration with partners from Germany and Spain and provided more than 15 papers output, in the mentioned period.

3. Additional research was conducted in recent years in order to improve the understanding of the structural packing, the specific microstructure, the magnetic properties and their changes during the first order (structural) and second order (magnetic) phase transitions in ferromagnetic as well as non-magnetic shape memory alloys (SMA) prepared by non-conventional techniques like rapid quenching or mechanical alloying. Results concerning the microstructure changes induced by different aging treatments correlated with the variation of thermal hysteresis of the martensitic transformation as well as the magnetic behavior and magnitude of SMA were reported (e.g. J.Appl.Phys. 107 113905, 2010 or J.Alloys and Comp. 509 4495-4498, 2011). The activity in this field was funded by national projects with an output of 6 papers, in the mentioned period.

Using the new infrastructure for materials synthesis at extreme conditions (SPS, HPS, MWS) and various material characterization equipments we were involved in 4 EFDA/Euratom projects. Good results have been obtained concerning the synthesis of functional gradient and composite materials related to the first wall and with respect to the intermixing of W,B and C in multilayers.

The experimental study of strongly correlated electron systems (also funded by national projects, 20 papers output) we are now focused on both fundamental problems like quantum phase transitions or new emergent states and possible applications like thermoelectric materials. Some current points of interest are related to anisotropy and reduced dimensionality effects on ground state stability in Ce(Ag,Ni)Sb₂ system, a new ferromagnetic Kondo system found by our group (Physica B 403, 937-939, 2008). Nano-structuring techniques are applied to rare-earth filled Skutterudite compounds in order to increase their thermoelectric figure of merit above 300 K. Oxides and ceramics as well as hydrogen storage materials are also under our investigation.

A part of the activity was also devoted to understanding the basic interaction mechanisms at the microscopic level, by using first principles atomistic modeling and simulation of materials within the Density Functional Theory (DFT) framework. In this respect the knowledge of various DFT methods and approximations was extended by performing first principle electronic structure on: i) exchange interactions, conductivity and optical properties in defective transition metal oxides, ii) defect structure and magnetism in rare earth doped oxides and iii) in intermetallic borides. The publications are in preparation as this activity is new in the laboratory.

E4- “Superconductivity”

The Group “Superconductivity” is involved in fundamental and technological research for a better understanding of superconductivity and related phenomena, as well as for the optimization of critical parameters of superconductors for practical applications, going through basic structural, electronic transport and magnetic characterization, and covering the main steps for preparation of bulk materials, thin films and nanostructures.

The group is formed by 8 senior researchers, 2 young scientists (1 assistant researcher), and 1 technician for sample preparation. One senior researcher received a Marie Curie Excellence Grant (MEXT-06-041111/2007-2011) at University of Birmingham (U.K.). At present, our group is coordinated by a PhD certified supervisor (associated professor at Faculty of Physics, University of Bucharest). One young scientist is PhD student and the second one is a Master student. A senior researcher has joined the team as a collaborative staff.

The experienced senior researchers with a well-recognized expertise, are promoters of national projects (1 PCE-Ideas, 3 Partnership projects with 1 as coordinator, 1 Euratom-EFDA-ITER project, etc.) and bilateral co-operations (with institutions from the USA, Japan, China, Germany, Italy, United Kingdom, and Singapore) being awarded in some cases (within 2007-2011) by international prestigious fellowships such as Marie Curie, Alexander von Humboldt, JSPS, MANA or invited as visiting researchers/professors. The group has an output of about 23 papers per year (works registered in the ISI Thompson Web of Science) and an average Hirsch Index of about 8 per senior researcher.

The group has significant expertise in both preparation/processing of superconducting materials and of others advanced ceramics and in their subsequent characterization.

The superconducting materials are prepared by various technologies, like mechanical attrition, microwave annealing, spark plasma & hot press sintering, PLD, chemical routes, etc. Subsequent processing via thermal treatments in the presence/absence of applied magnetic fields are also applied. Structural and morphological characterization of the samples as well as magnetic, thermodynamic, and transport properties are studied in our group, similar to the twin group of the laboratory, by Physical Properties and Magnetic Properties Measurement systems (PPMS, MPMS-SQUID), Vibrating Sample (VSM), TG/DSC/DTA as well as Laser Flash Calorimetry. The mentioned devices have facilities and options of high performances, being acquired or upgraded during the last 3 years.

The group activity was shifted along the last years from studying the superconducting phenomena and correlations in bulk materials to the investigation of single crystals, thin films, structures with reduced dimensionality, and the use of self-assembling nanotechnologies for strong vortex pinning centers in superconducting (thin and thick) films and coated conductors. Four main research directions have to be mentioned:

- 1. Vortex dynamics in high- T_c superconductors***
- 2. MgB₂ for practical applications***
- 3. Composite superconductors***
- 4. Exotic superconductors (iron-based pnictides, non-centro-symmetric superconductors)***

Some of the main achievements in the last few years are listed below:

1. We investigated the “pre-formed Cooper pair” scenario for the transition in high- T_c superconductors by determining the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature T_{KT} at the superconducting Cu-O layer level and the mean-field critical temperature T_{c0} in oxygen deficient YBa₂Cu₃O_y films ($y \sim 6.5, 6.55, \text{ and } 6.65$) (Phys.Rev.B 75 214504, 2007), paper selected for the APS Virtual Journal of Applications of Superconductivity, 12(12), June 15, 2007. We used the T dependence of the quasi-2D current-voltage (I - V) exponent for $T < T_{KT}$, and the analysis of the

resistive transition in the framework of the Ginzburg-Landau 2D Coulomb gas model for $T > T_{KT}$. Both procedures give essentially the same results, with T_{c0} remaining in the domain of the electrical resistivity drop, well below the pseudo-gap temperature.

2. The T dependence of the normalized magnetization relaxation rate S in optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$ (Y-123) films exhibits the well-known plateau in the intermediate T range. The disappearance of the $S(T)$ plateau in the high magnetic field H domain ($H > 20$ kOe) is not yet understood. We showed that in the case of high-temperature superconductors with significant quenched disorder the $S(T)$ plateau is directly related to a crossover in the vortex-creep process generated by the macroscopic currents induced in the sample (Phys.Rev.B 78 2121508, 2008). In DC magnetization measurements the creep-crossover temperature decreases rapidly with increasing H , reaching the low- T region where the magnetization decay is dominated by micro flux jumps. Consequently, at high H no well-defined elastic creep domain is present and the $S(T)$ plateau disappears. The activity (5 publications) was funded by two national projects (in collaboration with NILPRP Bucharest-Magurele and TU Cluj-Napoca), and an international co-operation with Institute of Physics, Mainz University, Germany

3. Difficulties encountered in the growth of epitaxial high-quality single-phase Bi-2223 thin films were discussed in literature from several points of view. In our work we brought to attention the influence of the substrate through substrate-film mismatch (CrystalGrowth&Design 9(1) 391-394, 2009) and some other details. Experimentally, thin films of (001) Bi-2223 with high zero-resistance critical temperature T_{c0} of 75-95.1 K and low roughness up to three half- c -axis unit cells were grown by metal-organic chemical vapor deposition (MOCVD) on substrates with large film-substrate lattice mismatch (from -28.6% to +8.47%) and *different film-substrate lattice mismatch anisotropy*. The highest quality, i.e. low roughness, high uniformity, and high T_{c0} is obtained when mismatch anisotropy, taken as the mismatch ratio, is given only by compressive or only by tensile mismatch stress, and it is around 1. Such condition is fulfilled for the Bi-2223 thin film grown on (001) MgO substrate. From a practical point of view, our results and the properties of MgO substrate recommend MOCVD (001) Bi-2223 thin films on (001) MgO substrate as a suitable candidate for microwave applications. These results (3 publications) were facilitated by a national project and international co-operations with Kanazawa Institute of Technology, Japan.

4. Concerning the activity on MgB_2 for practical applications:

High density (more than 90% of the theoretical density) bulk samples with relatively large size (1.9 cm in diameter) of MgB_2 , pristine and doped with 5 mol% SiC or B_4C were obtained by the field-assisted sintering technique (FAST, also known as Spark Plasma Sintering, SPS) from commercial MgB_2 powder (Supercond.Sci.Technol. 20(8) 836-842, 2007). All our samples have shown higher values of H_{c2} and H_{irr} than the values previously reported for FAST- MgB_2 samples. The performed scaling analyses suggest that both additions of SiC and B_4C stabilize two well defined pinning regimes in FAST-processed MgB_2 . At low temperatures, the pinning occurs at the grain boundaries, whereas at high temperatures, T around 24 K, there is a mixed pinning. The activity (4 publications) was funded by a national project.

It has already been established that moderate impurity doping in MgB_2 is effective in increasing critical current density, J_c , through the introduction of flux pinning centers and/or enhancement of the upper critical magnetic field H_{c2} . We investigated the influence of C_{60} addition on the superconducting parameters of MgB_2 bulk samples obtained by spark plasma sintering (SPS). Therefore, we showed that 1.5 wt% C_{60} addition leads to the reduction of the critical temperature T_c by a few K, whereas the magnetically determined critical current density J_c increases by approximately one order of magnitude in an applied magnetic field $H = 70$ kOe at temperature $T = 10$

K (Supercond.Sci.Technol. 23095002, 2010). The substitution of B by C in C₆₀-added MgB₂ samples processed by SPS leads to the reduction of the coherence length, and hence to an increase of the upper critical magnetic field H_{c2}. This is responsible for the shift of the irreversibility field H_{irr} to higher values after doping. The activity (2 publications) was funded by two national projects and international co-operations with Institute of Physics, Mainz University, Germany (Alexander von Humboldt Fellowship).

In Supercond.Sci.Technol.21, 115017, 2008 we also pioneered application of X-ray tomography (XRT) for the characterization of MgB₂ samples. MgB₂ were prepared by solid state reaction of Mg and B mixed powders, the Powder-In Tube (PIT) standard method and the Pulsed-Laser-Deposition (PLD), respectively. The method allowed observation of the local 3D density patterns of the MgB₂ specimens produced in different conditions, observation of the porosity and macro defects such as macro-cracks as well as of the structural and shape integrity of the composite PIT tapes. These results (3 publications) were facilitated by a national project, cooperation with NILPRP and international cooperations with Institute of Physics, Mainz University, Germany, National Institute for Materials Science, Tsukuba, Institute for Materials Research and Department of Applied Physics, Tohoku University, Sendai, Japan.

5. In our work (Supercond.Sci.Technol. 23105018, 2010) we studied the amplitude and phase fluctuation in non-centrosymmetric Li₂Pd₃B and Li₂(Pd_{0.8}Pt_{0.2})₃B using precise magnetization measurements obtained as a function of T and H. The analysis addressed the existence of phase fluctuations in the vicinity of T_c which are expected to occur if the gap contains line nodes due to the spin triplet state admixture to spin singlet state in the studied systems. These results were facilitated by an international cooperation with Mainz University, Germany (Alexander von Humboldt Fellowship) and Federal University of Rio de Janeiro, Brasil. The work is a continuation of the efforts to understand unconventional superconductivity in the Li₂(Pd_{1-x}Pt_x)₃B, x = 0–1 system. It is worth mentioning that the discovery of superconductivity in this system was done together with 2 Japanese teams from Tohoku Univ, Sendai, Japan and NIMS, Tsukuba (Appl.Phys.Lett. 854433 1–3, 2004; Phys.Rev.Lett. 93247004, 2004, J. Phys. Soc. Jpn. 74 2005).

6. The group is also involved in transferring technological know-how, characterization methodology and analysis of superconductors and other advanced materials (see e.g. review Sci Techno Adv. Mater. 12 013001 2011).

E5-Si- and Ge –based nanomaterials and Nanostructures

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2007 – 2011 ACTIVITY REPORT

I. The most important achievements:

- I.1.** 12 projects from National Plan for Research, Development and Innovation and 3 economical projects
- CEEEX contract No. 6111/2005-2008, Project Responsible Dr. M. L. Ciurea (Coordonator), “Network of scientific services of structuring and characterization at nanometric scale, with applications in the development of convergent technologies”
 - CEEEX contract No. 225/2006-2008, Principal investigator Dr. M. L. Ciurea, “Micro- and nanostructured semiconductor materials for gas and temperature sensors”
 - CEEEX contract No. 13/2006-2008, Principal investigator Dr. M. L. Ciurea, “Quantum phenomena in structures of Si and Ge nanoclusters embedded in SiO₂ matrices”
 - CEEEX 69/2006-2008, Subcontract No. 3/2006, Project Responsible Dr. M. L. Ciurea (Partner 2), “Research and service network for synthesis of nanostructures for textile industry, protective coatings and environment protection”
 - Romanian National University Research Council. Grant Number: GR 28/2007-2008, Principal investigator Dr. S. Lazanu, “Experimental and theoretical investigation of defect formation and evolution, produced in silicon by high energy particles”
 - Capacities contract No. 3/2007-2009, Principal investigator Dr. M. L. Ciurea, “Modernization of the Nanostructured Materials Laboratory by the acquisition of a magnetron sputtering equipment and a thermal treatment equipment”
 - Partnerships contract No. 11009/2007-2010, Project Responsible Dr. M. L. Ciurea (Partner 1), “Nanoelectronic devices for high frequencies based on carbon nanostructures for communications and environment monitoring”
 - Partnerships contract No. 11008/2007-2010, Project Responsible Dr. M. L. Ciurea (Partner 1), “Advanced circuits for microwave, millimeter wave and photonics based on mems technologies”
 - Partnerships contract No. 12081/2008-2011, Project Responsible Dr. M. L. Ciurea (Partner 1), “Biosensors based on carbon nanotubes for the real-time detection of nucleic acids with oncogenic potential”
 - Ideas contract No. 471/2009-2011, Principal investigator Dr. M. L. Ciurea, “Electrical transport in low dimensional Ge-Si-O systems: experiment and modelling”
 - Ideas contract No. 499/2009-2011, Principal investigator Dr. S. Lazanu, “Complex studies of the physics of defects produced by extreme fields of radiation in silicon based materials”
 - Human Resources, Postdoctoral research projects PN-II-RU-PD-2011-3-0094/2011, Postdoctoral advisor Dr. M. L. Ciurea, “Ge nanocrystals embedded in amorphous matrices with photoconductive properties”
 - Economical Contract No. 2273/2007, 5000 lei, Project director Dr. M. L. Ciurea
 - Economical Contract No. 2567/2007, 3000 lei, Project director Dr. M. L. Ciurea
 - Economical Contract No. 2315/2008, 5000 lei, Project director Dr. M. L. Ciurea

I.2. Publications: 37

- M. L. Ciurea, V. Iancu, M. R. Mitroi; *Solid-State Electronics* **51**, 1328 (2007): **1.259 (Impact Factor); 0.552 (Article Influence™ Score)**.
- I. Lazanu, S. Lazanu; *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **572**, 297 (2007): **1.114; 0.401**
- S. Lazanu, I. Lazanu; *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **583**, 165 (2007): **1.114; 0.401**.
- S. Lazanu, I. Lazanu; *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **580**, 46 (2007): **1.114; 0.401**.
- S. Lazanu, I. Lazanu, V. Ciupina, G. Prodan; *Journal of Optoelectronics and Advanced Materials* **9**, 814 (2007): **0.827; 0.161**.

- S. Lazanu, I. Lazanu; *Journal of Optoelectronics and Advanced Materials* **9**, 1839 (2007): **0.827**; **0.161**.
- V. Iancu, M. L. Ciurea, I. Stavarache, V. S. Teodorescu; *Journal of Optoelectronics and Advanced Materials* **9**, 2638 (2007): **0.827**; **0.161**.
- I. Stavarache, M. L. Ciurea; *Journal of Optoelectronics and Advanced Materials* **9**, 2644 (2007): **0.827**; **0.161**.
- T. F. Stoica, M. Gartner, V. S. Teodorescu, T. Stoica; *Journal of Optoelectronics and Advanced Materials* **9**, 3271 (2007): **0.827**; **0.161**.
- V. S. Teodorescu, M. L. Ciurea, V. Iancu, M.-G. Blanchin; *Journal of Materials Research* **23**, 2990 (2008): **1.743**; **0.893**.
- T. F. Stoica, C. Morosanu, A. Slav, T. Stoica, P. Osiceanu, C. Anastasescu, M. Gartner, M. Zaharescu, *Thin Solid Films* **516**, 8112 (2008): **1.884**; **0.640**.
- M. Gartner, P. Osiceanu, M. Anastasescu, T. Stoica, T. F. Stoica, C. Trapalis, T. Glannakopoulou, N. Todorova, A. Lagoyannis, *Thin Solid Films* **516**, 8184 (2008) : **1.884**; **0.640**.
- C. Popa, R. Turcu, I. Craciunescu, A. Nan, M. L. Ciurea, I. Stavarache, V. Iancu; *Journal of Optoelectronics and Advanced Materials* **10**, 2319 (2008): **0.577**; **0.113**.
- M. Gartner, C. Trapalis, N. Todorova, T. Giannakopoulou, G. Dobrescu, M. Anastasescu, P. Osiceanu, A. Ghita, M. Enache, L. Dumitru, T. Stoica, M. Zaharescu, J. Y. Bae, S. -H. Suh; *Bulletin of the Korean Chemical Society* **29**, 1038 (2008): **1.257**; **0.196**.
- M. L. Ciurea, V. Iancu, S. Lazanu, A.-M. Lepadatu, E. Rusnac, I. Stavarache; *Romanian Reports in Physics* **60**, 735 (2008).
- I. Lazanu, S. Lazanu; *Romanian Reports in Physics* **60**, 381 (2008).
- I. Lazanu, S. Lazanu; *Romanian Reports in Physics* **60**, 71 (2008).
- A. Slav, A. Ianculescu, C. Morosanu, A. Saranti, I. Koutselas, S. Agathopoulos, M. A. Karakassides; *Key Engineering Materials*, **361-363 I**, 245 (2008).
- C. Trapalis, N. Todorova, M. Anastasescu, C. Anastasescu, M. Stoica, M. Gartner, M. Zaharescu, T. Stoica; *Thin Solid Films* **517**, 6243 (2009): **1.727**; **0.594**.
- S. Lazanu, M. L. Ciurea, I. Lazanu; *Journal of Optoelectronics and Advanced Materials* **11**, 2150 (2009): **0.433**; **0.115**.
- I. Lazanu, S. Lazanu; *Romanian Reports in Physics* **61**, 689 (2009): **0.458**; -.
- I. Lazanu, M. Chera, R. Iordanescu, C. Nita, S. Lazanu; *Romanian Reports in Physics* **61**, 215 (2009): **0.458**; -.
- S. Lazanu, M. L. Ciurea, I. Lazanu, *Physica Status Solidi (c)* **6**, 1974 (2009).
- A.-M. Lepadatu, I. Stavarache, M. L. Ciurea, V. Iancu; *Journal of Applied Physics* **107**, 033721 (2010): **2.064**; **0.875**.
- I. Lazanu, S. Lazanu; *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **268**, 2241 (2010): **1.042**; **0.334**.
- I. Lazanu, S. Lazanu, *Romanian Reports in Physics* **62**, 309 (2010): **0.494**; -.
- I. Lazanu, S. Lazanu, *Journal of Cosmology and Astroparticle Physics* **07**, 13 (2011), **6.497**; **2.039**.
- M. R. Mitroi, V. Iancu, L. Fara, M. L. Ciurea; *Progress in Photovoltaics* **19**, 301 (2011): **5.627**; **1.752**.
- M. L. Ciurea, S. Lazanu, I. Stavarache, A.-M. Lepadatu, V. Iancu, M. R. Mitroi, R. R. Nigmatullin, C. M. Baleanu; *Journal of Applied Physics* **109**, 013717 (2011): **2.064**; **0.875**.
- I. Stavarache, A.-M. Lepadatu, N. G. Gheorghe, R. M. Costescu, G. E. Stan, D. Marcov, A. Slav, G. Iordache, T. F. Stoica, V. Iancu, V. S. Teodorescu, C. M. Teodorescu, M. L. Ciurea; *Journal of Nanoparticle Research* **13**, 221 (2011): **3.250**; **0.998**.
- V. Iancu, M. R. Mitroi, A.-M. Lepadatu, I. Stavarache, M. L. Ciurea; *Journal of Nanoparticle Research* **13**, 1605 (2011): **3.250**; **0.998**.
- I. Stavarache, A.-M. Lepadatu, V. S. Teodorescu, M. L. Ciurea, V. Iancu, M. Dragoman, G. Konstantinidis, R. Buiculescu; *Nanoscale Research Letters* **6**, 88 (2011): **2.557**; **0.764**.
- S. Lazanu, I. Lazanu, Gh. Ciobanu; *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **269**, 498 (2011): **1.042**; **0.334**.
- A. M. Lepadatu, I. Stavarache, T. F. Stoica, M. L. Ciurea; *Digest Journal of Nanomaterials and Biostructures* **6**, 67 (2011): **2.079**; -.
- I. Stavarache; *Digest Journal of Nanomaterials and Biostructures* **6**, 1073 (2011): **2.079**; -.

- A. Slav; *Digest Journal of Nanomaterials and Biostructures* **6**, 915 (2011): **2.079**; -.
- I. Lazanu, S. Lazanu; *Romanian Reports in Physics* **63**, 707 (2011): **0.494**; -.

I.3. Publications presented at prestigious international conferences and published in conference proceedings: 12 ISI proceedings papers

I.4. Number of citations: 806

I.5. Authored books

- "Trapping phenomena in nanocrystalline semiconductors"; M. L. Ciurea; *Nanoelectronics and Photonics (Nanostructure Science and Technology Series)*, pages 191-222, edited by Federico Rosei, Anatoli Korokin, Springer, New York (2008).

- "Quantum confinement in nanometric structures"; M. L. Ciurea, V. Iancu; *New Trends in Nanotechnology and Fractional Calculus Applications, Part I New trends in nanotechnology*, pages 57-67, edited by D. Baleanu, Z. B. Güvenç, J. A. Tenreiro Machado, Springer, Dordrecht Heidelberg London New York (2010).

Dissemination of scientific results: 20 contributions at international conferences

II. The dynamic of the research subjects and directions

The team is working in the field of nanostructured semiconductors with applications in nanoelectronics, photovoltaics and sensors.

- Films of Si nanodots embedded in amorphous SiO₂ matrix (2007-2011): (i) preparation; (ii) investigation of microstructure, electrical transport, phototransport, and photoluminescence with the aim of evidencing quantum confinement effects; (iii) modelling of nanoparticle energy structure.
- Porous Si – based nanostructures for gas and biosensors (2007-2008).
- GeSiO-based nanostructures (2008-in present): (i) preparation of Ge nanoparticles embedded in a-SiO₂ matrix, by magnetron sputtering and sol-gel methods; (ii) investigation of electrical behaviour and phototransport (experiment and modelling), photoluminescence and Hall effect.
- Carbon nanotubes based structures (2009-2011): electrical processes.
- Percolation phenomena (2007-2011): evidenced in carbon nanotubes based structures, Si nanodots embedded in amorphous SiO₂ matrix and nanocrystalline porous Si.
- Trapping phenomena in Si-based nanostructures (2010-2011): stress-induced traps.
- Materials and phenomena to be used in the search for dark matter (2010-2011).

III. Interdisciplinary or entrepreneurial initiatives (see Project List)

- Interdisciplinary contract CEEX contract No. 225/2006-2008.
- Economic contracts No. 2273/2007, 2567/2007, 2315/2008.

IV. Evolution of the human resources and other aspects significant for the scientific development of the research team

At the present time, the team is formed of 10 members: the research team (8 members) with the average age under 43,6 years, and 2 technicians. The team consists in: team leader Magdalena Lidia Ciurea, Ph.D., Senior Researcher 1st degree; Sorina Lazanu, Ph.D., Senior Researcher 1st degree; Toma Stoica, Ph.D., Senior Researcher 1st degree; Gheorghe Iordache, Ph.D., Senior Researcher 2nd degree; Ionel Stavarache, Ph. D., Researcher 3rd degree; Adrian Slav, Ph. D. student, Researcher; Ana-Maria Lepadatu, Ph. D. Student, Researcher; Catalin Palade, Research Assistant; Emil Ion, Technician I; Elena Stan, Technician II.

In our team are 2 PhD students and 1 M. Sc. Student advised by Dr. Ciurea, PhD supervisor, at the Doctoral School of Physics, University of Bucharest. 2 Bachelor theses and 2 Masters theses were performed in our team. Also, 2 Research Assistants became Researchers and 1 Researcher became Researcher 3rd degree. 1 student done his bachelor thesis in our team and then was employed as Research Assistant.

E6-Surfaces, interfaces, thin films and single crystals. X-ray / electron spectroscopies and diffraction (SITSC-XESD)

Outstanding equipment: from sample preparation to multitechnique characterization

The group utilizes and maintains several widely used installations of NIMP: (i) a surface and interface science cluster (Fig. 1) composed by a molecular beam epitaxy (MBE), a scanning tunneling microscopy (STM) and a spin- and angle-resolved photoelectron spectroscopy (SARPES); the whole setup is about 1,3 M€ worth and was delivered in 2009; (ii) a photoemission and low energy electron microscope (LEEM-PEEM), about 835 k€ worth, delivered in 2010; (iii) a multitechnique surface analysis technique (Fig. 2), with X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), STM (about 600 k€ worth, delivered in 2009), with preparation facilities whose setup is in progress (about 200 k€ worth); (iv) an old-but-still-working VG ESCA Mk II X-ray photoelectron spectroscopy equipment (donated from Belgium in 2000), which was the first XPS installation ever operating in the country, estimated worth 100 k€; (v) two X-ray diffractometers Bruker D8 Advance, one for powders (about 110 k€ worth, delivered in 2007) and another for thin films analysis (about 250 k€ worth, delivered in 2006); (vi) an X-ray absorption fine structure (XAFS) Rigaku spectrometer (Fig. 3), 300 k€ worth, delivered in 2011 (this offers a similar brilliance as a second generation synchrotron radiation facility); (vii) two crystal growth facilities, about 200 k€ worth; (viii) a second harmonic generation laser setup, about 100 k€ worth; (ix) an upgraded Russian magnetron sputtering machine, estimated worth about 100 k€. *All these equipments are operational, most of them working 7/7 and 24/24.* The value represented by all equipments is about 4 M€.

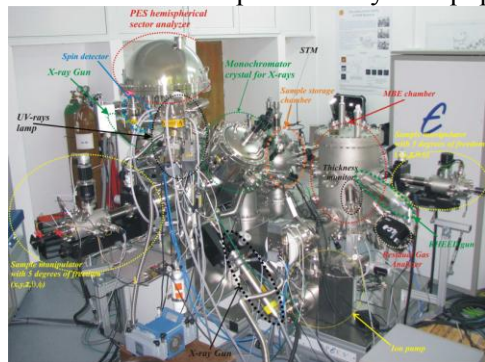


Fig. 1. MBE-STM-SARPES surface science cluster



Fig. 2. Multimethod surface analysis



Fig. 3. X-ray absorption fine structure spectrometer

The group provides unique expertise at national level in two very demanded fields: X-ray diffraction and X-ray photoelectron spectroscopy. Also, this is practically the unique group in the country concentrated on surface and interface science, working in real ultrahigh vacuum (UHV, 10^{-10} to 10^{-11} mbar). This is also the only place in the country where one real MBE setup is installed and works currently. The X-ray diffraction expertise is also boosted by novel developments in the XRD basic theory and data analysis, often implemented in widely used XRD analysis codes, which emerged also from the SITSC-XESD group. The group contains practically the whole expertise in extended X-ray absorption fine structure (EXAFS) at national level. The crystal growth facilities are competing at national level only with another well-known group from Timisoara.

Remarkable manpower

The group leader, Cristian-Mihail Teodorescu, PhD from 1995, Senior Scientist I, 45 years old, has published to date about 90 papers in ISI-ranked journals, has a h-index of 15, about 500 citations, 4 patents. Other Senior Scientists I are: (i) Nicolae C. Popa, 65, PhD from 1988, 50 papers, 500 citations, h-index 12; (ii) Dan Macovei, 65, PhD from 1982, 60 papers, 200 citations, h-index 12; (iii) Mihail Florin Lazarescu, 62, PhD from 1997, 55 papers, 120 citations, h-index 6, 20 patents; (iv) Adrian S. Manea, 67, PhD from 1999, 70 papers, 160 citations, h-index 8, 22 patents. The younger generation is represented by 7 Senior Scientists III: Ruxandra Costescu (PhD 2006), Constantin Logofatu (PhD 2000), Rodica Ghita (PhD 1999), Iuliana Pasuk (PhD 2004), Catalin Negrilă (PhD 2010), George Stan (PhD 2010), Marius A. Husanu (PhD 2011), 3 Researchers: Constantin Cotirlan (PhD 2011), George A. Lungu, Nicoleta G. Gheorghe, and 2 Research

Assistants: Florica Ungureanu (PhD 2011) and Dana G. Popescu. All non-PhD owners are PhD students and expected to defend their theses in 2012-2013. This research staff employs also 4 technicians and 2 workers.

Dr. N.C. Popa, known in the X-ray and neutron diffraction community as the author of the "Popa formalism", has considerably improved diffraction data analysis by Rietveld refinement by adding the effect of anisotropic line broadening caused by strain and size; he also extended the applicability of the Rietveld method to the quantitative texture analysis. These improvements are nowadays widely used in Rietveld refinement computing codes MAUD, GSAS, FULLPROF, TOPAS, MRSA, etc. He has papers cited 200 times and recently published a paper in *Acta Crystallographica A* (impact factor 54.33). Drs. M.F. Lazarescu, A.S. Manea, D. Macovei and C. Logofatu implemented the XPS method in Romania by setting up the donated VG ESCA Mk II installation; this installation was up to 2007 the sole operational XPS system in Romania and therefore was highly demanded; it was included in 2004 on the list of "National Interest Facilities". To date, despite the acquisition of XPS installation in other Institutes or Universities, the main national expertise belongs to the afore mentioned researchers, to whom later Drs. C.M. Teodorescu, R.M. Costescu, C.C. Negrița, C. Cotirlan, M.A. Husanu, F. Ungureanu and PhD students N.G. Gheorghe and G.A. Lungu must be added. Dr. D. Macovei is the pioneer of the EXAFS method in Romania and practically the only scientist in the country able to perform a complete EXAFS data analysis up to the derivation of the structural parameters. Dr. C.M. Teodorescu implemented in Romania the complex surface and interface science, by setting up a complex preparation and analysis technique (about 20 different techniques available in situ) and by forming 5 young researchers on this topic. Drs. M.F. Lazarescu, A.S. Manea and C. Logofatu also are amongst the few people able to grow crystals in Romania.

Unique results

The group has published between 2007-2011 140 papers in ISI-ranked journals, the most outstanding (according to the Journal Impact Factors) being the following 16 papers:

(i) *Acta Crystallographica A* 2011 (IF = 54.33); (ii) *Angewandte Chemie International Edition* 2010 (IF = 12.73); (iii) *Journal of the American Chemical Society* 2010 (IF = 9.02); (iv) *Green Chemistry* 2010 (IF = 5.47); (v) *Langmuir* 2009 (IF = 4.27); (vi-vii) *Journal of Applied Crystallography* 2008 and 2010 (IF = 3.79); (viii) *Acta Materialia* (IF = 3.79); (ix) *Physical Review B* (IF = 3.77); (x-xi) *Electrochimica Acta* 2009 and 2011 (IF = 3.65); (xii-xiv) *Physical Chemistry Chemical Physics*, 1 paper in 2008 and 2 papers in 2011 (IF = 3.45); (xv) *Journal of Biomedical Materials Research A* (IF = 3.04); (xvi) *Catalysis Today* (IF = 3.00).

The group has also elaborated 7 patents during the same period. Dr. C.M. Teodorescu gave invited talks to 7 international conferences. There were two books published in Romania by Dr. M.F. Lazarescu et al. and one book chapter: Dr. N.C. Popa in *Powder Diffraction: Theory and Practice* (eds. R.E. Dinnebier and S.J.L. Billinge), Royal Society of Chemistry Publishing, Cambridge 2008. The group was involved in non-budgetary contracts of about 185 000 lei between 2007-2011.

A wide range of activities, from theoretical studies to application-oriented research

As it may be seen from the publication list, the group comprises theoreticians (Dr. N.C. Popa), experimentalists that have also theoretical skills (Drs. M.A. Husanu, C.M. Teodorescu and D. Macovei), while the main activities are centred on the development and complex studies of new materials, heterostructures, surfaces and interfaces. A non-negligible amount of activity is dedicated to the development of analysis methods, starting from the theory of quantitative assessment to the adjustment of the experimental conditions. Outstanding recent fundamental results in surface science are (i) achievement of ultraclean semiconductor surfaces (contamination level below 10^{-4} of a single atomic layer); (ii) the synthesis and characterization of room temperature ferromagnetic Sm/Si(001) and Mn/Ge(001) systems, together with their complex characterization by XPS, XAFS, MOKE; (iii) a complete photoemission study (XPS and ARUPS, including band structure) of Pb(Zr,Ti)O₃ films; (iv) evidence that catalysts with strong activity in menthol synthesis are composed by AuCl₄ instead of Au nanoparticles (by XPS and EXAFS); (v) Complex studies of molecular adsorbates on GaAs surfaces. Dr. M.A. Husanu is also amongst the few quantum computing specialists in the Institute. Drs. M.F. Lazarescu, A.S. Manea, C. Logofatu, C.C. Negrița and C. Cotirlan are also well known in the experimental community as an innovative group in the field of new measurement methods, particularly they set up the new system of Second Harmonic Generation characterization of semiconducting surfaces.

Interdisciplinarity

Surface science, X-ray photoelectron spectroscopy, X-ray diffraction and X-ray absorption are techniques widely used in chemistry, biophysics, biochemistry. Long date collaborations with several organizations from chemical sciences are currently running, mainly with the Institute of Chemical Physics "I.G. Murgulescu" Bucharest and the Faculty of Chemistry from the University of Bucharest. Dr. C.M. Teodorescu is the leader of a national interdisciplinary project PCCE ID_76 *Surface and interface science: physics, chemistry, biology, applications*, granted in 2010 (7 Mlei). As seen from the publication list, there are numerous publications in chemistry journals. It is also to mention that the 30-year old Dr. G.E. Stan developed during the last years solid research in biocompatible materials, synthesized by magnetron sputtering and characterized by physical and chemical methods, and *in vitro* and *in vivo* tested. Other collaborations with groups from the National Institute of Lasers, Plasma and Radiation Physics centred on biomaterials and with the National Institute of Isotopic and Molecular Technologies centred on nanoparticles for targeted drug delivery and magnetic hyperthermia are running to date. There are also strong application-oriented research activities, in collaboration with the National Institute of Optoelectronics, "Politehnica" University of Bucharest, Zentiva, Honeywell, etc.

European collaborations

One may notice strong collaborations with the following European research entities:

- University of Nottingham (UK), through FENIKS FP5-FP6 Project 2001-2005 (Dr. A.S. Manea);
- Commissariat a l'Energie Atomique Saclay (France), through an IFA-CEA Project (2010-2013), possibly also through an ANCS-ANR Project (Dr. C.M. Teodorescu);
- Universität Ulm, Institute of Theoretical Chemistry (Germany) (Dr. M.F. Lazarescu);
- Istituto di Struttura della Materia, Roma (Italy) (Dr. C.M. Teodorescu);
- Universidad de Aveiro, Dept. de Engenharia Cerâmica e do Vidro (Portugal) (Dr. G.E. Stan);
- synchrotron radiation facilities: Hasylab Hamburg (Germany), Soleil Saclay (France), Elettra Trieste (Italy) (Dr. C.M. Teodorescu).

Entrepreneurial initiatives

Members of the group were involved in several initiatives concerning the future of NIMP and of Romanian Physics. Dr. M.F. Lazarescu managed the "National Interest Facility" XPS system and is also the leader of the national XPS network of National Interest Installations, comprising all XPS setups of Romania. Also, Drs. M.F. Lazarescu, C. Logofatu, C.C. Negriila A.S. Manea and C. Cotirlan promoted and are following the Accredited Laboratory MAAS by the Romanian Accreditation Authority RENAR. Dr. D. Macovei was in charge (2010-2011) with the NIMP participation at the ELI-NP Project. Dr. C.M. Teodorescu was the leader of the 2009-2011 Infrastructure Project (funded by the EC) POS-CCE *Euro-Regional Centre of Advanced Materials, Surfaces and Interfaces*, about 10 M€, where 24 large scale equipments were purchased in the Institute.

Evolution of human resources

Dr. F. Ungureanu was hired in 2004, Drs. I. Pasuk and C. Cotirlan came in NIMP from other Institutes in 2005, Dr. G.E. Stan was hired in 2005, Dr. M.A. Husanu joined the group from another laboratory in 2008, N.G. Gheorghe was hired in 2009, D.G. Popescu was hired in 2011. The most important hiring during the last years was Dr. R.M. Costescu in 2010, who won a Reintegration Grant and the Prize "In hoc signo vinces" (Dr. R.M. Costescu graduated at the University of Urbana Illinois, US, and is the first author of a paper in Science, 2004). *Therefore, the group acts as an 'attractor' for young talents.* Examples of career evolution are the 26-years old N.G. Gheorghe, who published in less than 3 years 14 papers (featuring J. Nanopart. Res., Top. Catal., Green Chemistry and Phys. Rev. B), the 30-years old Dr. G.E. Stan whose publications list accounts for 18 papers (including J. Nanopart. Res., J. Biomed. Mater. Res. A and J. Mater. Sci. - Mater. Med.), or the 33-years old Dr. C.C. Negriila who published to date 40 papers (Phys. Chem. Chem. Phys., Catal. Today). These evolutions, together with a solid financial status of the group during the last decade based on own research and multiple collaborations, make us highly confident in the group's future for the next five years.

E7- Theoretical Physics Group

(2007-2011)

Team Leader: Dr. Valeriu Moldoveanu

I. Activity and research topics. The Theoretical Physics Group traditionally studies quantum transport phenomena in mesoscopic systems and provides phenomenological models and reliable descriptions of various effects observed in transport measurements. The research activity in the last 5 years aimed at:

- i) extending the expertise of the group beyond the Landauer single-particle scattering approach to electronic transport in order to investigate non-trivial correlation (i.e. many-body) effects like mesoscopic Kondo effect, measurement-induced decoherence, Coulomb drag etc.
- ii) developing appropriate theoretical tools for modeling the time-dependent transport phenomena in open quantum systems.

The main research topics of the group cover several timely and challenging issues of mesoscopic transport, both at the level of theoretical formulation and of the numerical implementation in view of advanced simulations. The considered topics were roughly the following:

1. Modeling the transient transport regime in nano-devices.
2. The mesoscopic Kondo and Fano-Kondo effects.
3. Controlled and intrinsic dephasing in mesoscopic interferometers.
4. Coulomb drag and quantum ratchet effects in parallel quantum dots.
5. Spin interference in Rashba rings.
6. Mathematical aspects of mesoscopic transport.

The group's research efforts were mainly motivated by recent intriguing experimental results with quantum dot systems and mesoscopic interferometers but also by some fundamental open problems in theoretical solid state. The team leader established long-standing fruitful collaborations with the group of Prof. Vidar Gudmundsson at the Science Institute, University of Iceland and with Prof. Bilal Tanatar from the Science Faculty, University of Bilkent, Turkey.

II. Achievements. The results of the group were regularly published in prestigious ISI journals and received a fast international recognition through citations in journals with good visibility. On quantitative level the group has published 32 papers in the period 2007-2011 (21 Physical Review B (impact factor IF=3.77), 3 New Journal of Physics (IF=3.89), 1 Europhysics Letters (IF=2.2)) etc. (the full publication list is available on the groups' web page: <http://lab30.infim.ro/html/groups.html>) These papers were cited times in New J. of Physics, Phys. Rev. B, Phys. Rev. Lett., Journal of Chemical Physics, Applied Physics Lett. etc. It has to be pointed out that the group members are usually 1st authors of these papers. On scientific level one can single out several important results:

- extension and numerical implementation of the non-equilibrium Greens functions formalism (NEGF) in view of transient current calculations in quantum dot (QD) systems submitted to time-dependent signals (Phys. Rev. B 76, 085330 (2007) - cited 23 times , Phys. Rev. B 76, 165308 (2007) - cited 16 times).

- a suitable version of the Generalized Master Equation (GME) method for transient transport in interacting and non-interacting systems (New J. Physics 11, 073019 (2009) cited 14 times, Phys. Rev. B 80, 205325 (2009) cited 4 times, New J. Phys. 11, 113007 (2009) - cited 7 times, Phys. Rev. B 81, 155442 (2010)- cited 4 times, New J. Phys. 13 013014 (2011)).
- prediction of a dynamical charge sensing effect in parallel quantum dots (Phys. Rev. B 82, 085311 (2010)).
- specific aspects of the Fano-Kondo regime (Phys. Rev. B 75, 125301 (2007)- cited 3 times, Phys. Rev. B 76, 113302 (2007) - cited 10 times, Phys. Rev. B 79, 033306 (2009), Phys. Rev. B 83, 245317 (2011)).
- theoretical description of the measurement-induced decoherence in Aharonov-Bohm interferometers with an embedded quantum dot (Phys. Rev. B 75, 045309 (2007) - cited 10 times, Phys. Rev. B 77, 195302 (2008) - cited 7 times).
- prediction of a Coulomb drag effect in parallel QDs, emphasizing the role of Coulomb-mediated inelastic transitions. (EPL (Europhysics Letters) 86, 67004 (2009)) and the 1st description of the role of Coulomb-mediated inelastic transitions in mesoscopic quantum ratchets (Phys. Rev. B 82, 205312 (2010)).
- theoretical calculation of spin filter and spin splitter transport regimes in mesoscopic Rashba rings (Phys. Rev. B 81, 035326 (2010), Physics Letters A 375, 187 (2010)).
- the 1st rigorous formulation of the cotunneling effect (J. Phys. A: Math. Theor. 44, 305002 (2011)).
- a mathematically sound proof of the existence of nonequilibrium steady-states (NESS) in interacting open systems (Phys. Rev. B 84, 075464 (2011)).

It should be mentioned that most of the theoretical results enumerated above are supported by involved numerical simulations which qualitatively agree with the experimental findings.

III. Funding and infrastructure. The group received continuous funding both within the Core Funding scheme but also through NP2 research grants:

-2008-2011: Control and optimization of quantum interference in charge and spin transport in mesoscopic systems (PI: V. Moldoveanu, Amount: 936000 RON). The research infrastructure of the theoretical physics group was recently up-dated with 3 powerful computers (Intel Processor Core™ i7 990X, 3.46GHz). A substantial collection of textbook and monographs is available as well.

Recently two more ANCS grants have been awarded to the group:

- Young Research Teams Grant (2012-2014): "Theoretical studies on the open questions in the mesoscopic phase measurement problem" (PI- M. Tolea, Amount: 750000 RON).

- Exploratory Research Projects (PCE) Ideas Grant (2012-2014): "Exciton dynamics and time-dependent transport in optically active quantum dots" (PI V. Moldoveanu, Amount: 1.350.000 RON).

IV. Dynamics of research subjects and new directions. The group is quite flexible in switching between two or more research topics at a time, as proved by the variety of problems addressed in the period 2007-2011. The publication list shows that any research direction tackled by the groups ends up in sound publications. As suggested by the title of the recent grants the group naturally extended its expertise and research interests to mesoscopic quantum optics, while continuing the investigation of quantum interference effects at the nanoscale.

The short and mid-term strategy of the group is to implement the research plans of the two grants mentioned above and to successfully achieve the foreseen objectives. At quantitative level one expect to report at least 5 ISI papers per year. A long-term goal is to further extend the group expertise with advanced many-body theoretical methods (e. g. functional renormalization group theory, full counting statistics).

V. Evolution of the human resource. At present the group is composed of 9 persons: 3 Scientific Researcher 1st degree (SRI), 1 SR II, 3 SR III, 1 Scientific Researcher and 1 Researcher Assistant (also a Master student). The Master student (Bogdan Ostahie) joined the group in 2011 and rapidly integrated within the group. He already co-authored two papers (see the preprints at <http://arxiv.org/>). Two members of the group (I. V. Dinu and M. Tolea) defended their PhD. theses in 2010. The team leader was promoted as SR II in 2010 and should defend his "Habilitation" and therefore obtain the right to supervise PhD students in 2012.

E8- “Optical Processes in Nanostructured Materials”

The team named “Optical Processes in Nanostructured Materials” (OPNM) has **35 persons** from which 31 researchers and 4 technicians. In the last four years, the activity of the OPNM team has been focused on nanostructured materials and nanocomposites – synthesis, study of optical properties and targeting some applications at laboratory level like: i) the conversion and the storage of energy, ii) sensors and iii) optoelectronics. The main achievements obtained in the period 2007-2011 of OPNM team are: i) **218 articles** published in journals registered on ISI Thompson Web of Science which summarize a total relative influence score of **210** and **337 citations**; ii) **3 papers included in ScienceDirect Top 25 Hottest Articles** (Composite Science and Technology, 67, 2556-2563, (2007), Electrochemistry Communications 9, 2121-2127, (2007), Chemical Physics Letters 473, 299-304, (2009)) and **1 paper** selected by American Physics Society as frontier research for the **Virtual Journal in Science & Technology – Nanoscale Science & Technology** (J. Mater. Chem. 19, 5690, (2009)); iii) **7 book chapters from which** 5 are published abroad (John Wiley & Sons, American Scientific Publishers, Nova Publisher, etc.) and 2 published in Romania; iv) **69 papers published as conference proceedings**: 54 abroad and 15 in Romania; v) **2 popular press articles** in Market Watch; vi) **6 patents**: 5 patents in Derwent Innovations Index database of WEB of Knowledge and 1 OSIM patent; vii) **12 patent requests** were deposited for the analysis period; viii) **29 national projects under direct coordination of the team members**: 15 CEEEX projects from which 14 finalized in 2008, 3 IDEI projects, 6 Partnership projects and 1 Capacity project, all these won by competition in 2007 and 2008. Budget allocated to the 25 national projects was of 5.918.689 lei. Other 4 PCE-IDEI projects were won by competition in 2011 having provided for the period 2011-2014 a total budget of 6.000.000 lei. In the analyzed period, other **9 national projects**, with a total budget of 1.216.931 lei, were finalized in which National Institut of Materials Physics (NIMP) acted as **partner**; ix) **5 international projects**: 1 reintegration NATO project finalized in February 2008 (with budget of 25.000 euros), 1 Brancusi Romania-France project finalized in 2010, 1 Romania-China project won by competition in 2010 and 1 Institutional Partnerships Scopes Project (cooperation between Switzerland-Romania-Ukraine) which has been won by competition in 2011. For the latter project, the Swiss National Science Foundation allocated to NIMP, for the period 2012-2015, a budget of 74.000 CHF; 1 COST Action CM1006; x) **6** of the team **members** were engaged in the **organizing committees** of 5 national conferences and 4 international conferences; xi) **82 contributions at conferences and meetings**: 9 oral conferences, 6 invited lectures and 67 posters; xii) **5 oral dissemination activities** – 2 at National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj Napoca, Romania, 1 at the Workshop “Excellence in Romanian Science”, 2 at the “National seminar of nanoscience and nanotechnology – 9nd edition”; xiii) **4 awards**: 1 Romanian Academy Prize “Constantin Miculescu”, 1 Romanian Academy Prize “I. G. Murgulescu”, 1 prize awarded by the National Authority for Scientific Research for the best achievements of a young researcher, 1 Diploma of Excellence and Gold Medal PROINVENT 2009; xiv) finalization of **4 master thesis**; xv) finalization in the last two years of **5 PhD thesis** and preparation for finalization in 2012 and 2013 of **4 PhD thesis**; xvi) **10 agreements** of bilateral collaborations signed with research institutions from France, Spain, Germany, Switzerland, Ukraine, Italy and Morocco. xvii) a **collaboration agreement for 5 years** with **Texas Institute of Science** signed in 2008. In this context we note as a result a **whitepaper** written at the request of Oceanering International. xviii) Beginning with 2006, the team has been constantly engaged to **modernizing the infrastructure**. Thus, on the base of the projects gained by competition, in the period 2007-2011 were purchased: 1) up-grades to FT Raman spectrophotometer RFS 100S Bruker, UV-VIS-NIR spectrophotometer, Lambda 950 and FTIR spectrometer Vertex 80 model, Bruker; 2) a Fluorolog-3 spectrophotometer FL3-22 model Horiba Jobin Yvone; 3) 2 ion lasers, with Ar and Kr; 4) a DSA 100 drop shape analysis system from Kruss, DMA 4500 densitometer from Anton Pan, 5) two broadband dielectric spectrometers, Novocontrol, 6) a Spotlight 400 FTIR imaging microscope, Perkin Elmer; 7) a photoconduction and I-V characteristics measurement system; 8) Sputtering system Hummer 6, 9) a vacuum deposition equipment with turbo-molecular pump, 10) thin film evaporation system for organic materials research “SPECTROS”, 11) a Multiview 4000 Nanonics SNOM/SPM system, 12) 2 Langmuir Blodgett KSV 2000 system, 13) up-grades to the potentiostat/galvanostat

VoltaLab 80, Radiometer Analytical and Grove Box System MBraun and 14) a solar simulator for testing solar cells. According with to the strategy of NIMP to purchase state of the art equipments, in the frame of a POS-CCE project (project director: Dr. C. M. Teodorescu, 2010) was acquired a Raman spectrophotometer T64000, Horiba Jobin Yvone, which is devoted to Raman studies using excitation wavelengths in VIS range.

In the period 2007-2011, the **main research direction of the OPNM team** has been oriented towards the **synthesis and optical properties of nanostructured materials destined to be used in different applications** such as the conversion and the energy storage, bioscience and biotechnology, catalysis, information technology and optoelectronic. The main research topics developed by OPNM team were: 1) development of the synthesis procedures and optical characterization of inorganic micro and nanoparticles of different shapes destined to be used in different applications; 2) development of the synthesis procedures and optical characterization of composite materials based on carbon nanoparticles (carbon nanotubes, fullerene, etc.) and polymers for applications in energy storage and biotechnology; 3) production of chalcogenide and soft materials for applications in the field of sensors, information technology and optoelectronics. A briefly review of the dynamics of these research topics in the period 2007-2011 is shown in the following.

Research topic no. 1 – Development of the synthesis procedures and optical characterization of inorganic, micro and nanoparticles, of different shapes destined to be used in different applications.

Some significant results: a) development of new strategies for synthesis of semiconducting micro- and nanoparticles such as ZnO, PbI₂, CdS, Bi₂Te₃, etc. with different shapes: wires, rods, plates and dots (OPTICAL MATERIALS 30, 72, 2007; J. PHYS. CONDENS MATER. 21, 025507, 2009; SUPPERLATTICES AND MICROSTRUCTURES 46, 833, 2009). As main synthesis routes were used the template method, hydrothermal procedure, wet chemistry method, chemical-electrochemical synthesis method and pulsed laser deposition; b) some applications of these particles were reported in the field of : i) preparation of indium-doped zinc oxide thin films for solar cells (THIN SOLID FILMS 519, 573, 2010); ii) solar cells, using as photo-anode an eosin Y sensitized ZnO nanorod to the assembling of the dye-sensitized solar cells (THIN SOLID FILMS, 2011); iii) the synthesis of carbon nanotubes using ZnO nanoparticles as supported catalyst (CHEMICAL PHYSICS LETTERS 473, 299, 2009); iv) synthesis of composite materials for the use in the field of: iv.1) energy storage, ZnO/SWNTs composites used as active material in lithium rechargeable batteries for which were reported high discharge capacities values (J. PHYS. CONDENS MATER. 21, 025507, 2009); iv.2) as charges collector, an example in this sense being polyaniline/PbI₂ composite (JOURNAL OF SOLID STATE CHEMISTRY 182, 827, 2009); v) CdS dots evidenced as mesoscopic media in which can be generated a nonlinear optical process that behaves as Anderson localization of light (JOURNAL OF APPLIED PHYSICS 110, 053106, 2011); vi) evidencing of some catalytic processes (CATAL. TODAY 141, 361-366, 2009 ; APPL. CATAL B: ENVIRONMENTAL 96, 548, 2010) and water confinement (J. PHYS. CHEM A 111, 5166, 2007; J. EUR. PHYS. E 26, 379, 2008) in the presence of nanostructured oxides.

Research topic no. 2 – Development of the synthesis procedures and optical characterization of composite materials based on carbon nanotubes and polymers for applications in the energy storage and biotechnology.

Some significant results: a) the elucidation of mechanisms concerning functionalization of single-walled carbon nanotubes (SWNTs) with different conjugated polymers such as poly(N-vinyl carbazole) (POLYMER 48, 5279-5288, 2007), polybithiophene (CARBON, 47, 1389-1398, 2009), poly(3,4-ethylenedioxythiophene) (J. MATER. CHEMISTRY 19, 5690, 2009), etc. using investigation techniques such as Raman/surface enhanced Raman scattering (SERS), photoluminescence, FTIR and UV-VIS-NIR spectroscopy; b) anti-Stokes/Stokes Raman scattering manifesting as a non-linear optical process is evidenced in poly(3,4-ethylenedioxy thiophene)/ SWNTs composite (JOURNAL OF RAMAN SPECTROSCOPY 42, 3030-312, 2011); c) using composites of the type poly(3,4-ethylenedioxy thiophene)/SWNTs (JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY 9, 6204-6209) and polydiphenylamine/ SWNTs (MAT. SCIENCE ENGINEERING B – ADVANCED FUNCTIONAL SOLID-STATE MATERIALS 985, 211, 2011) as active materials for electrodes of rechargeable lithium batteries, high dischargeable capacities were reported; d) surface enhanced infrared

absorption (SEIRA) spectroscopy is reported in 2011 as a new method for the optical characterization of composite materials (SYNTHETIC METALS, 2011, DOI [10.1016/j.synthmet.2011.09.001](https://doi.org/10.1016/j.synthmet.2011.09.001)); e) one used the carbon nanotubes functionalized with barium stearate in producing of the sensors based on ammonium nitrate (OSIM Patent Request No. A/01014/26.10.2010). Strong collaborations with research groups from France and Spain were established.

Research topic no. 3 – Production of chalcogenide and soft materials for applications in the field sensors, information technology and optoelectronics. Significant results: a) development of new synthesis method for chalcogenide materials for luminescent devices (CHALCOGENIDE LETTERS 7, 621, 2011); b) the creation of devices for producing chalcogenide micro-lenses used in surgery (PATENT nr.: RO122979-B1, 2010); c) development of 2D photonic structures for applications in the field of optoelectronic devices (OSIM PATENT REQUEST No A/01135/19.12.2010); d) the specific interaction of liquid crystals with the substrates depending on the aerosil type or molecular sieves (PHYS. REV. E 78, 051701, 2008, SPECTROCHEM. ACTA A 72, 248, 2009); e) new evidences for charge transfer in organic heterostructures for electronic and photovoltaic applications (THIN SOLID FILMS 515, 8733, 2007; APPLIED PHYSICS A – MATERIALS SCIENCE & PROCESSING 104, 921, 2011); f) evidence of emission properties of doped organic semiconductor crystals (J. CRYST. GROWTH 310, 1765, 2008).

For the period 2007-2011, the entrepreneurial initiatives of the OPNM team are quantified by the coordination in partnership of 21 projects. A recent interdisciplinary initiative developed in 2011 consists in sensitive detection of endocrine disrupters using ionic liquid-single walled carbon nanotubes modified screen-printed based biosensors (TALANTA 85, 2007-2013, 2011).

At present, in the OPNM team work 6 Ist degree senior researchers, 2 IInd degree senior researchers, 10 IIIrd degree senior researchers, 4 researchers and 6 assistant researchers. Four members of the OPNM team are certified as PhD supervisors. Three of them are associated as professors at the Faculty of Physics, University of Bucharest and one is associated to the Romanian Academy-Institute of Physical- Chemistry “Ilie Murgulescu”. Academic degrees for other members are: 12 PhD, 5 Physicists, one Engineer, 5 PhD students and one person is a Master student. In addition, another result regarding the educational activity of the OPNM PhD supervisors consists in the finalization of other five PhD thesis whose authors are not in the OPNM team. The distribution of personnel in terms of age is: 10 peoples below 40 years and 8 experienced senior researchers over 60 years. Concerning the evolution of the human resources, in the period 2007-2011, 9 researchers have been promoted by exam as follows: i) in 2009 - one has been accredited as Ist degree senior researcher, two were certified as IInd degree senior researchers and one person was promoted as IIIrd degree senior researcher; and ii) in 2011 - 2 persons were promoted as IIIrd degree senior researchers and 4 persons as researchers. The 8 researcher assistants were employed in the OPNM team in the period 2007-2011.

The conclusion of this activity report is that the OPNM team has an adequate infrastructure and expertise in the field of: i) synthesis of novel energy-oriented nanomaterials; ii) evidence of new optical process of nanostructured materials; iii) development of applications in the field of sensors and optoelectronics. All these are very attractive for the young who wish to make a carrier in the research and academic field. The future perspective consists in developing new optical methods for the characterization of nanomaterials (for example: SEIRA, anti-Stokes photoluminescence of organic materials, etc.) and new applications of nanomaterials in the field of energy, sensors and optoelectronics.

E9- Structures and Defects in Advanced Materials (2007-2011)

The *Laboratory of Atomic Structures and Defects in Advanced Materials* (<http://lab50.infim.ro>) has been created on January 1-st 2010 after the internal re-organization of NIMP, by the unification of two smaller laboratories with related research subjects: Laboratory of Structure and Dynamics of Condensed Matter and Laboratory of Microstructure of Defects in Solid Materials. In the first place, I would like to mention that, although our lab has been created by unifying 2 smaller labs, one of our main concerns was to build up a *strong unique research group in our lab*, by encouraging the participation in variable staff formulas in all the projects and activities developed in our newly created lab, regardless of the former affiliation to one or the other lab.

At this moment, our lab counts 31 personnel, out of which 24 are research personnel and 7 represent technical graduate and undergraduate personnel. The research personnel includes 11 senior researchers 1-st degree out of which 3 are also PhD supervisors, 3 senior researchers 2-nd degree, 3 senior researchers 3-rd degree and 7 young researchers (MSc students, PhD students, post-doc). During the previous 4 years, 3 young researchers of our lab have defended their PhD thesis at the University of Bucharest (2 PhD students) and Claude-Bernard University in Lyon (1 PhD student). 1 (one) young researcher has obtained the MSc degree working in our laboratory. 5 (five) graduate students (physics and chemistry) have been recruited as young researchers during the last 4 years. Among the young researchers, 3 (three) are currently PhD students (2 physics, 1 chemistry) and 1 (one) is MSc student (physics) in the final year. Based on the valuable results published in highly ranked ISI journals, 2 prizes of the Romanian Academy have been obtained by two members of our team in 2008 and 2009.

Our research activity concerns mainly the physical properties (structure, optical, electrical properties) in advanced materials, resulting either as size effects (nanostructures, thin films) or by structural defects engineering. Therefore, we assume as our mission to discover, investigate and manipulate the physical properties at nanometric and atomic scale for the development and characterization of new materials (dielectrics, semiconductors, alloys, ceramics) to be used in various applications (semiconductor technology, gas sensing, radiation detectors, telecommunications). Our lab groups scientists with common fields of interest and expertise in solid state physics and materials science, covering several complementary techniques of materials preparation and characterization such as:

Structural methods

- Analytical Transmission Electron Microscopy (TEM/HRTEM, STEM, EFTEM, EELS, EDS).
- Analytical Scanning Electron Microscopy and Focused Ion Beam (SEM-FIB, EDS, EBSD).
- Powder, thin film and single crystal X-ray diffraction (XRD).

Spectroscopic methods

- Multifrequency Electron Spin/Paramagnetic Resonance (ESR/EPR) spectroscopy.
- Mössbauer spectroscopy (^{57}Fe , ^{151}Eu , ^{119}Sn , TMS, SMS and CEMS) techniques.
- Optical spectroscopy (absorption and emission).

Gas-sensing measurements

- Complex electrical measurements under controlled gas atmosphere for gas sensing
- Catalytic investigations (Photo-acoustic gas analyzer).
- Relative work function investigations (Kelvin Probe).

Materials synthesis

- Single-crystal growth from melt (Czochralski, Bridgman).
- Preparation of nanocrystalline materials by co-precipitation, solvothermal method and high-energy ball milling.

State-of-the-art equipments have been acquired during the last 2 years in the frame of infrastructure projects (“PN II - Capacities” and “POS-CCE”), such as: i. ultra-high resolution analytical transmission electron microscope JEOL ARM 200F (0.08 nm resolution in STEM HAADF

mode), the first sub-Angstrom resolution TEM at 200 kV in Eastern Europe; ii. Bruker ELEXSYS E500Q CW Q-band ESR spectrometer with E560 ENDOR accessory, Bruker ELEXSYS E580 Pulse/CW X-band ESR spectrometer with E560 DICE II pulse ENDOR and E580-400 pulse ELDOR accessories; iii. Tescan Lyra III XMU SEM-FIB dual system; WissEL Mössbauer spectrometer with ICEoxford cryogenic superconducting magnet system, and so on. We mention that these are extremely powerful instruments, unique in Romania and even in Eastern Europe, which makes that our lab has the opportunity to become a very attractive partner in national and international research projects.

As *research directions*, we mention:

- Investigations down to atomic scale by structural (TEM/HRTEM/STEM, XRD), spectroscopic (EPR, Mossbauer spectroscopy, EELS, EDS) and optical methods of native and induced defects in bulk and nanostructured solid materials.
- Investigations of material properties by using paramagnetic point defects as atomic probes.
- Synthesis of oxide semiconducting or magnetic nanostructures for applications in gas sensing, catalysis and photocatalysis.

A rather wide range of materials has made the subject of our researches in the frame of the funded projects, such as: doped II-VI semiconductor nanoparticles (e.g. ZnS, ZnO - synthesis and characterization), oxide nanoparticles for gas sensing (e.g. WO_3 , $\alpha\text{-Fe}_2\text{O}_3$ - synthesis and characterization), high-k and TCO thin films (e.g. ZnO, $\text{SnO}_2\text{:Sb}$, HfO_2 – sol-gel or PLD growth and characterization), laser and plasma processing of thin films and surfaces (e.g. Si, $\text{SnO}_2\text{:Sb}$), doped TiO_2 nanoparticles for photocatalysis, ceramic nanocomposites for applications in solid oxide fuel cells (e.g. $\text{Y}_2\text{O}_3\text{:ZrO}_2$, $\text{Sc}_2\text{O}_3\text{:Y}_2\text{O}_3$), dilute magnetic semiconductors (e.g. Co:ZnO, Mn:ZnO – PLD growth, ion implantation, complex characterization)

We mention only a few of the *most important achievements* of our research team:

1. *Synthesis and characterization of doped nanoparticles of II-VI semiconductors of interest for opto-electronic applications (ZnS, ZnO).*

We have demonstrated from correlated multifrequency EPR and HRTEM investigations of Mn-doped cubic ZnS small nanocrystals (2 nm), that substitutional Mn^{2+} impurities are localized at cation sites subjected to an axial distortion, which is attributed to the presence of a neighbouring extended planar lattice defect, such as stacking fault or twin. The obtained results have been published in highly ranked ISI journals such as *Physical Review B*, *Journal of Nanoparticle Research*, *Crystal Growth and Design*, *Journal of Nanoscience and Nanotechnology*, *Applied Magnetic Resonance*, *Journal of Physics-Condensed Matter*.

2. *H-plasma and laser processing of Si wafers for the development of the SOI (silicon-on-insulator) technology based on the smart-cut method*

Our studies included thorough investigations by various TEM techniques of the structural defects induced in Si by RF-plasma treatment showing the specificity of the induced defects. We have demonstrated that the laser processing of the H-plasma treated Si wafers results in the formation of structural defects at a precise depth below surface, favouring the smart cut of layers thinner than 50 nm. The obtained results allowed us to apply for a national patent on this matter and to publish 5 papers in important ISI journals like *Journal of Applied Physics*, *Plasma Processes and Polymers*, *Applied Physics A*, *Journal of Physics D: Applied Physics*.

3. *Synthesis and characterization of doped oxide nanoparticles (WO_3 , $\alpha\text{-Fe}_2\text{O}_3$, CuO, Cr_2O_3) for gas sensors*

Several types of oxide nanoparticles have been synthesized via hydrothermal method followed by deposition onto ceramic substrates provided with specially designed electrodes. The gas sensing (NO_2 , CO) properties have been demonstrated using a gas mixing station and a McAllister Kelvin Probe setup. The obtained results have been published in important ISI journals like *Sensors and Actuators B-Chemical*, *Materials Chemistry and Physics*

4. *Hydrothermal synthesis and complex characterization of (Fe, Eu)-doped TiO₂ photocatalyst.* With the aim to extend the spectral response of TiO₂ photocatalyst to the visible light region, we have synthesized Fe and Eu codoped TiO₂ by a hydrothermal route. The structure, morphology and optical peculiarities were investigated by XRD, TEM, EXAFS, Mössbauer and UV–VIS spectroscopy. The photocatalytic properties were analyzed in the photodegradation reaction of phenol and salicylic acid. The obtained results have been published in high impact factor journals such as *Materials Chemistry and Physics*, *Topics in Catalysis*.

Given the complexity of the tackled research subjects, involving a highly interdisciplinary approach, the senior researchers of our lab have initiated and coordinated numerous large scale research projects in the frame of the national research programs such as CEEEX, Ideas, Partnerships Program I and II. 19 projects have been developed by our team members since 2007 till present. In 4 projects, members of our team have had the role of Project Coordinator, while for the other 15, our colleagues had responsibilities of team leader. Moreover, at the recently closed projects competition, 2 (two) Ideas type projects and 1 (one) post-doc project have been accepted for funding. The research projects have been developed in collaboration with high-performance research institutes and universities in Romania, such as NILPR, NIPNE-HH, ICF Ilie Murgulescu, IMT, University of Bucharest, Polytechnic University of Bucharest. Members of our lab are currently involved in large scale European projects such as EURATOM and ELI-NP. Our research team includes researchers with *high international visibility* achieved by participating in international projects, bilateral cooperation projects (Belgium, France, Greece, Turkey), long working periods abroad in famous research institutions (University of Antwerp, Claude Bernard University in Lyon, IPCMS Strasbourg, IPTC Tuebingen). The collaboration with these institutions allowed us to get access to high-performance scientific equipments, to train our young researchers in advanced scientific techniques (PhD, post-doc) and to publish the obtained results in journals with high impact factor. It is worth mentioning, however, that following the recent acquisition of state-of-the-art scientific equipment in our lab, an important number of publications in highly ranked ISI journals (impact factor > 3) started to emerge from our lab, involving mostly or even exclusively Romanian authors. It proves the high scientific level of the senior scientists in our lab, which guarantees, on one hand, the efficient exploitation of the newly acquired scientific instruments and, on the other hand, the solid instruction that the young researchers in our lab have the chance to receive during their PhD and post-doc periods.

As a proof of the *international visibility* of our team, we mention the organizing along 2007-2011 of 4 international workshops with reputed invited lecturers: i. International roundtable on Advanced Wide Band Gap Materials for Radiation Detection – MATRAD 2007, 17-20 June, 2007, Sinaia; ii. “Local disorder at nanoscale”, Satellite Workshop at the Fifth Conference PIM 2007, September 20-22, 2007, Cluj-Napoca; iii. International workshop “Performed nanomaterials for a new generation of IT-SOFC” June 8-15, 2008, Bucharest; iv. International workshop on the inauguration of the first sub-Angstrom resolution 200 kV TEM in Romania and Eastern Europe, May 6, 2011, Magurele. Highly reputed professors and researchers from West European institutions have given invited lessons at the invitation of the senior researchers in our team: Prof. Gustaaf Van Tendeloo from EMAT-University of Antwerp, Prof. Udo Weimar from IPTC Tübingen, Dr. Marie Genevieve Blanchin, Claude Bernard University in Lyon, Prof. Florian Banhart from the Institute of Physics and Chemistry in Strasbourg, Dr. Oleg Lebedev from University of Caen, Prof. Peter D. Townsend from University of Sussex, Brighton, Prof. Anna Vedda from University of Milan-Bicocca, Prof. Dr. Miguel Moreno from University of Cantabria, Santander.

Representative project

Multifunctional materials: from bulk to nanostructures

The multifunctional materials present physical properties which make them very attractive for a large number of applications in high-tech industry. However, the vast majority of these applications are subject (implying important efforts) to miniaturization. Moreover, by decreasing the size and/or dimensionality of the systems, new specific and unexpected properties appear. Therefore, the study of physical properties at micro and nanoscale has become a very important topic at international level. Our institute noticed the trend and decided, some 5 years ago, that the main strategic objective is to shift the weight of the scientific activities, in the field of multifunctional materials, from bulk samples to thin films and nanostructures.

Considering this, a coherent plan was set up consisting in:

- Developing suitable processing methods for fabrication of nanostructured samples, whether these are thin films, nanocomposites or nano-objects of various forms (nanowires, nanotubes, nanoribbons, nanoparticles, etc.);
- Developing suitable techniques and methods for structural and physical characterization, by taking into account that measurements on small size samples and/or on phenomena and mechanisms specific to nanometer or molecular/atomic range, are more demanding in terms of precision, location, noise, vibrations, temperature stability, etc. than the measurements performed on bulk samples;
- Acquiring the necessary equipment for preparation of thin films and nanostructures, as well the equipment for structural and physical characterization with precision going down to atomic level;
- Training the research personnel to learn the methods for preparation and characterization of thin films, nanostructures and nanostructured materials. This goal was achieved by collaboration with research institutions from abroad and by encouraging colleagues from diaspora to return and work into the institute.
- Encouraging the submission of project proposals with research subjects related to nanostructures, nanomaterials and nanoscience in general. Starting with the CEEEX competitions over 75 % of the successful projects were studying topics in these fields. Only some of projects were dealing with bulk samples in ceramic forms but even in these cases, the samples were nanostructured by using various fabrication techniques.

The first step for a successful transition from bulk to nanostructures was to acquire the necessary equipments and to develop the appropriate methods for the fabrication and characterization of nanostructured multifunctional materials, thin films and nanostructures. This was achieved by using the funding through the Capacities Program, the Operational Program for Enhancing the Economic Competitiveness, the Core Program and the Partnership Program. At this moment, the NIMP has:

- Capabilities for depositing thin films, multilayers and heterostructures, as well to fabricate nanostructures by using various techniques, such as: wet chemical methods, electrochemistry, molecular beam epitaxy (MBE), pulsed laser deposition (PLD), magnetron RF sputtering, electron beam lithography, focused ion beam (FIB) cutting. It worth mentioning that the expertise gained on fabricating bulk samples is now used to prepare the necessary targets for PLD or RF sputtering depositions, under the form of nanostructured, dense ceramics obtained by spark plasma sintering or microwave annealing.
- A comprehensive set of equipments for structural characterization including: X-ray diffraction (XRD); scanning electron microscopy combined with EDS and cathodoluminescence; atomic resolution transmission electron microscopy with analytical capabilities; various forms of scanning probe microscopes; a well equipped laboratory for electron paramagnetic resonance studies; several Moessbauer spectrometers working at various temperatures and applied magnetic fields, in both scattering (surface sensitive CEMS) or transmission geometry; state of the art

equipments for XPS/UPS analysis; a PEEM/LEEM microscope; a X-ray absorption spectrometer, etc.

- Set-ups for complete physical characterization from the point of view of electric, magnetic and optic properties, many of them including state of the art equipments as for example broad band dielectric spectrometer, THz spectrometer, PPMS system, deep level transient spectroscopy system, SQUID, VSM and MOKE magnetometers, etc.

The research activities were focused mainly on the following topics:

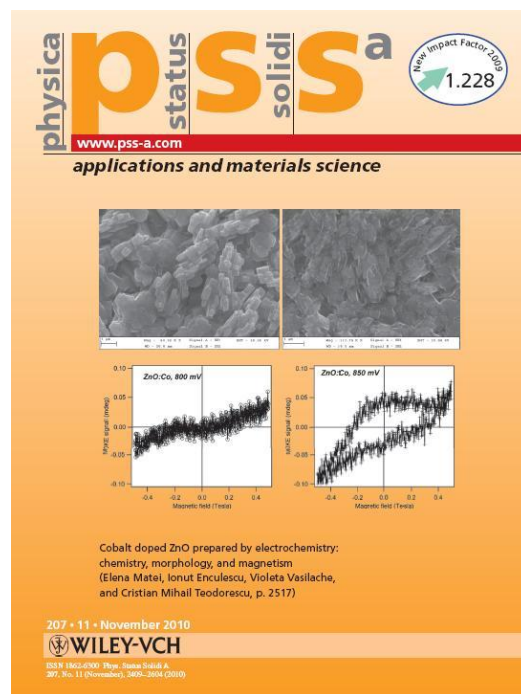
- Fabrication and characterization of semiconductor or metallic nanowires and nanotubes with applications in solar energy conversion and sensing devices (e.g. photodiodes or magnetic field sensors)
- Thin films and heterostructures based on oxide materials with perovskite structures, having dielectric, ferroelectric, piezoelectric, multiferroic properties and with applications in telecommunications, processing and storage of information, infrared sensing, ultrasound devices, etc.
- Complex multilayers and nanostructures including magnetic materials for applications in spintronics, information storage, sensors, etc., as well as magnetic nanopowders and nanocomposites with biomedical applications.
- Nanocomposites based on carbon nanotubes and various types of polymers with potential of applications in energy storage
- Doped nanocrystals for applications in electroluminescence or in photo-catalysis
- Surface and interface phenomena in various systems including both oxide and non-oxide (metallic) thin films
- Development of new theoretical models to explain the physical properties at meso and nanoscale, with special emphasis on transport properties

The convergent efforts in terms of funding the research activities related to investigation of physical phenomena in nanostructures, correlated with the purchasing of the suitable equipments and training of the personnel in the field of nanosciences have been repaid by recent significant results, very well appreciated and with significant impact at international level. Some of these results are mentioned below.

1. Nanowires and nanotubes. The template methods combined with electrochemistry was successfully used to produce nanowires and nanotubes of various semiconductor and metal materials. However, two of the results worth to be mentioned:
 - Growth of CdTe nanowires. It was found that by a careful control of the electrochemical parameters it is possible to grow CdTe nanowires with either a slight deficit of Cd or a slight deficit of Te. This fact allows obtaining, during the same growth process, segments of CdTe wires with n or p type doping. Therefore, it is possible to obtain CdTe p-n homojunctions under the form of nanowires. The photosensitivity of this photodiodes in the visible range was also demonstrated. The CdTe nanowires proved to be also useful as sensitizing element in hybrid solar cell. A paper was published in Nanotechnology in 2010, with one of the pictures selected for the front cover of the respective issue (see figure 1a).
 - The template method was also used to grow ZnO nanowires doped with elements having magnetic properties. This is a kind of diluted magnetic semiconductor (DMS), with potential applications in spintronics (e.g. in field effect devices for controlling the spin currents). The presence of magnetic properties was demonstrated by measuring a magnetization hysteresis at room temperature. The article published based on these results made the front cover in Physica Status Solidi-Applications and Materials Science (see figure 1b).



a)



b)

Fig. 1 Front covers for a) Nanotechnology and b) Physica Status Solidi-applications and materials science.

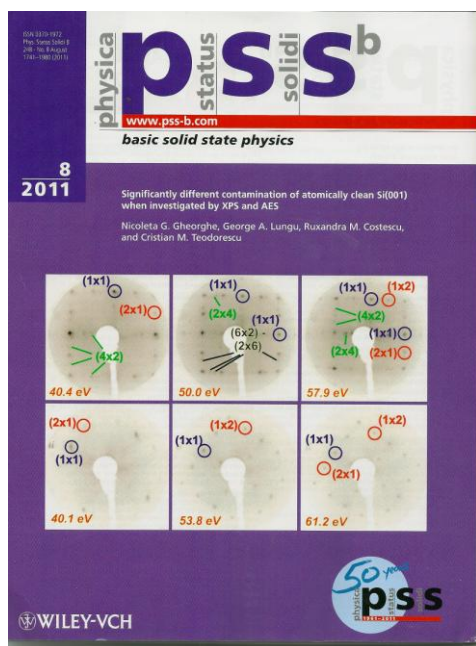
- Thin films and heterostructures based on oxide materials with perovskite structure. Important results were obtained mainly in the case of ferroelectric materials as for example PZT. The newly acquired PLD system allowed growing epitaxial films and the electric measurements performed on such films have shown that a strong interaction is present between ferroelectric polarization and the metal electrode with consequences on the electronic properties of the interface between electrode and ferroelectric materials. This fact impacts the transport properties in epitaxial ferroelectric films, as well as the hysteretic behavior not only in metal-ferroelectric-metal (MFM) structures but also in metal-ferroelectric-semiconductor (MFS) structures. For example, recently was shown that the hysteretic behavior of the capacitance of a MFS structure based on PZT-ZnO combination changes its orientation with increasing temperature and that the temperature of change depends on the structural quality of the interface. It worth noting that, due to the expertise gained in NIMP, a fruitful collaboration with the Max Planck Institute for Microstructure Physics in Halle, Germany, was established. This was materialized by exchanging peoples and samples, by common publications and by joint participation in a large collaborative project in the frame of FP7-NMP theme (acronym of the project is IFOX, funding started at the end of 2010). Several of the publications dealing with epitaxial ferroelectrics and having as first author peoples from NIMP have collected an important number of citations (see PHYSICAL REVIEW B 75, 104103 from 2007 with 40 citations, or JOURNAL OF APPLIED PHYSICS 101, 064109, also from 2007 with 23 citations, or more recently APPLIED PHYSICS LETTERS 94, 232902, published in 2009 and with 14 citations already).

Important results were obtained also in the field of dielectric thin films with applications in the field of microwave telecommunication devices. Demonstrators of various circuit elements were made, still the methods has to be optimized to obtain the best results.

- Very interesting results were obtained also in the field of nanomagnetism. Magnetic thin films and multilayers, as well as nanocomposite systems presenting interesting effects, like as exchange-bias, exchange-spring, giant and tunneling magnetoresistance, magneto-striction, shape memory, etc., have been prepared by various techniques, including rf sputtering, melt spinning, spark

plasma sintering, etc. Methodological aspects suitable to provide both the angular spin distribution at surface and interface as well as the interfacial atomic diffusion were developed (*J.Magn.Magn.Mater* 323 2196-2201, 2011). Complex studies concerning the influence of geometrical, structural and compositional parameters on the magnetic and magneto-transport properties of multilayer and nanoglobular spin valve structures have been performed (e.g. *J ALLOYS COMP.* 499, 23-29, 2010). Magnetic nanopowders and nanofluids as well as molecular compounds have been considered with respect to magnetic relaxation phenomena and spin configurations (*J.PHYS.-COND MATTER* 19 01625 2007, *PHYS. REV B* 80 014430 2009). Different magnetic alloys were prepared and studied in the form of thin films or ribbons. Some interesting results were obtained, as for example: the martensitic transformation (MT) was studied in Ni-Fe-Ga ferromagnetic shape memory alloys with Co substitutions on Ni and Fe sites, evidencing a variation of the MT's temperature and a field dependent thermomagnetic hysteresis for MT's temperature below room temperature (see *J.Appl Phys* 107, 113905 published in 2010); the magnetic properties of some Fe-Co and Fe-Mn/Fe-Co thin films were studied, evidencing that the composition of the antiferromagnetic films has a sensible influence on the magnetic parameters of the exchange coupled ferromagnetic films (see *JOURNAL OF ALLOYS AND COMPOUNDS* 499, 23-29 published in 2010); the direct formation of the L1(0) FePt phase without the need for post-synthesis annealing procedures in Fe-Pt-based melt-spun ribbons, obtained by a conventional melt spinning method (see *JOURNAL OF PHYSICS D-APPLIED PHYSICS* 44, 365002 published in 2011), etc. Important collaboration were established with research groups from Spain, United Kingdom, Germany, etc. It worth mentioning that the physical properties of magnetic thin films, multilayers and nanocomposites were characterized by using various techniques existent at NIMP, among which vibrating sample magnetometry, different calorimetric methods and Moessbauer spectroscopy.

4. The surface phenomena can now be investigated by using the newly cluster for surface/interface physics. The cluster allows to study the physical phenomena taking place on clean surfaces during the deposition of various metals, as well as the formation of electrode interfaces on various materials as for example ferroelectric oxides with perovskite structures. The first results started to



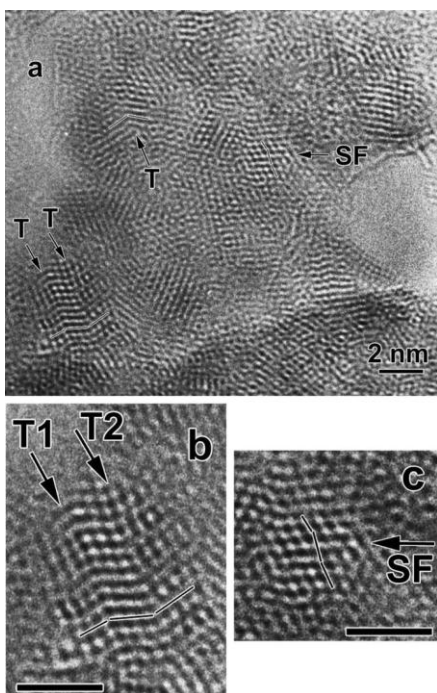
appear in the last 2 years, some of them being published in international journals. For example, it was found that a clean surface can be contaminated during the in-situ analysis of the surface reconstruction by using Auger electron spectroscopy (AES) or X-ray photoelectron spectroscopy (XPS). The AES produced a much more severe contamination of the surface than XPS because of the surface reactions initiated by the electron beam. The results were recently published, making the back cover in *PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS* 248, 1919-1924, published in 2011 (see figure 2).

Figure 2

5. Significant results were obtained in the field of organic-inorganic composites based on carbon nanotubes. Different optical methods existing at NIMP were used to investigate the properties of these nanocomposites with potential applications in energy storage. Some examples: the elucidation of bulk polymerization mechanism of N-vinyl carbazole in the

presence of single-walled carbon nanotubes (SWNTs) using as investigation techniques such as SERS, FTIR, photoluminescence and TEM (see POLYMER 48, 5279-5288, published in 2007, already with 14 citations); using of anti-Stokes/Stokes Raman scattering for characterization of the poly(bithiophene)/SWNTs interface (see CARBON, 47, 1389-1398 published in 2009, already with 11 citations); non-linear optical properties evidenced on poly(3,4-ethylenedioxythiophene)/SWNTs composite, used afterwards as active material for application to rechargeable lithium batteries, when high dischargeable capacities were reported (see JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY 9, 6204-6209 published in 2009, and JOURNAL OF RAMAN SPECTROSCOPY 42, 303-312, published in 2011). Strong collaborations were established with groups from France and Spain.

6. A series of undoped and doped nanocrystals were fabricated by using chemical or hydrothermal methods. For example cubic ZnS nanocrystals doped with 0.2% mol Mn^{2+} , taken from a batch prepared at room temperature by a surfactant-assisted liquid-liquid reaction were investigated by using a combination of EPR and TEM techniques. It was found that Mn ions are localized at Zn^{2+} sites subjected to a local axial lattice distortion and that such distortions are associated to a stacking fault or twin (see figure 3, published in 2010 in PHYSICAL REVIEW B 81, 035336, already with 17 citations).



Good results were obtained also in the field of photo-catalysis. Some undoped TiO_2 nanocrystals, or doped with different rare earth elements, were prepared by hydrothermal method or by high energy ball milling, and successfully tested for decomposition of various contaminants in the water (see MATERIALS CHEMISTRY AND PHYSICS 112, 146-153 published in 2008, with 11 citations, or TOPICS IN CATALYSIS 52, 544-556 published in 2009).

FIG. 3. a) HRTEM image of the $cZnS:Mn$ QDs sample revealing in some crystallites (marked by arrows) planar defects such as twin interfaces (t) and stacking faults (SF). b) and c) enlarged HRTEM images of crystallites oriented along the (110) zone axis showing the atomic structure of these defects. The black lines are drawn to guide the eye. Scale bars: 2 nm.

7. The modeling of physical phenomena at nano and mesoscale had become important in order to confirm the experimental results and to developed realistic theoretical models. The theory group had obtained also some good results in the last years, many of them published in well known international journals, as for example transient regime in nonlinear transport through many-level quantum dots (see PHYSICAL REVIEW B 76, 085330 published in 2007, with 23 citations) or Coulomb effects in open quantum dots within the random-phase approximation (see PHYSICAL REVIEW B 77, 195302 published in 2008, with 7 citations).

In conclusion, the common project to change from bulk to nanostructures has considerably enhanced the infrastructure, is attracting more and more young researchers to work in NIMP, has produced already important results in terms of visibility through publications and citations and made NIMP a valuable and reliable partner for research institutions from abroad reflected in an increased number of bilateral collaborations and projects funded through various international programs.