L5: Simulation, Modelling and Computer Aided Design Laboratory

- Mission
- Main areas of expertise
- Research Team
- Specific facilities
- International networks
- Services

Mission: research, simulation and modeling activities oriented to collaborative research projects, education (short courses, hands on training, seminars, workshops), services (offering access to hardware and software tools) and consulting (design/optimization) in the field of micro-nano-bio/info technologies. The lab plays a key role in supporting the research activities of other laboratories of IMT- Bucharest, being also involved in European and national research projects.

Main areas of expertise: **design, development and optimization of MEMS/MOEMS components and devices** (switches, cantilevers, bridges, membranes, microgrippers); mechanical, thermal, electrical and electrostatic, piezoelectric, fluidic, as well as coupled field (static and transient) analysis; modeling and simulation for multi-physics problems; **design, modelling and simulations of microfluidic components and systems for biomedical applications and micro-electronic fluidic systems**

Others expertise of the lab's members include: elastomer based microstructures; optical processing and storage of information; micro-systems applications in the field of energy; manufacturing and characterization of materilas for advanced nanoelectronic devices based on oxidic materials; techiques of chracterizations as cathodoluminescence and photoluminecence

Research Team: The team has a multidisciplinary expertise in: mathematics, physics, electronic and mechanics 4 PhD, 3 physicists, 2 engineers (mechanical and electrotechnical), 3 PhD students.

Specific facilities:

Soft/hard Tools:
• **COVENTOR 2008.2**; • **MATLAB 7**; • **ANSYS Multiphysics 11.0**; • **COMSOL Multiphysics 3.3 and 3.4**; • **Solidworks Office Premium 2008** ; • **Mathematica 7**; • **Origin PRO 8**; • **Visual Studio 2008 Pro**; • **Dual IBM 3750 Server** with 8 quad-core Intel Xeon MP 2.93 GHz processors, 196 GByte RAM and 1 TByte HDD + 876 GByte external storage; • Computer network used for training

Characterization equipments: • **Avantes Fiber Optic Spectrometer - AvaSpec NIR256-2.2**; • **Fluoreecence spectrometer in UV-vis-NIR**; • **Semiconductor Characterization System (4200S/C/Keithely)** with Manual Probe Station (EP6/SüssMicroTec).

International networks and projects:

Partner in international FP6 Projects:

- **MI-Lab on chip**- "Lab-on-a-chip implementation of production processes for new molecular imaging agents- STREP (2005-2008), NMP-No 516984; coordinator University of Liege, Belgium
- **IPMMAN**: Improvement of industrial Production Integrating Macro, Micro And Nanotechnologies for more flexible and efficient manufacturing FP 6 Project (CA, NMP-CT-033205, 2006-2009): Coord. Profactor, Research and Solutions GmbH, Austria
- **ComEd:** Leonardo da Vinci - Life Long Learning Development of competences of educational staff by integrating operational tasks into measures of vocational training and further education" ComEd (2008-2010); Coordinator BWAW Thüringen GmbH, Germany, Contract No: DE/08/LLP-LdV/TO/147174 (2008-2010)

Services: We offer simulation, consulting and training services in micro and nano domains; Application areas: microsensors, microfluidics, MEMS/NEMS, MOEMS, RF MEMS

- **Computer Aided Design** using dedicated software tools: COVENTOR 2008 and ANSYS;
- Mask Design, Process Editor, 3D building and mesh;
- Modeling for technological processes/ optimizations;
- **Computer Aided Engineering and Analysis (using FEM, FVM, BEM tools)**;
- **Microfluidics analysis; Electro-thermo-mechanical and piezoelectric analysis**; **Coupled field simulations**: thermo-electro-mechanical;

Team from left to right:
Rodica Voicu; Victor Moagar-Poladian; Oana Nedelcu; Catalin Tibeica; Florina Ravariu; Gabriel Moagar-Poladian; Rodica Plugaru; Irina Codreanu

Laboratory Head — Dr.Raluca Muller (raluca.muller@imt.ro)

Raluca Müller received the M.Sc and PhD in Electronics and Telecommunications from "Polytehnica" University of Bucharest. From 1978-1994 she was researcher with ICCE Bucharest; since 1994 she is with IMT Bucharest. Currently R. Müller is **Head of Scientific Services Department and Coordinator of the Simulation, Modelling and Computer Aided Design Laboratory**.

Her main scientific interests include design and technological processes for sensor and actuators based on MEMS/ MOEMS techniques, integrated optics, nanolithography. She was involved in teaching activities as associated professor at University "Valahia Targoviste".

Raluca Muller is coordinator of several national research projects and scientist in charge from IMT - Bucharest in international projects as: *FP 6: ASSEMIC- Marie Curie Training Network (2004-2007)- FP6- PATENT (Modelling and Simulation cluster), Leonardo da Vinci- Microteaching (2005-2007) , IPMMAN- CA (2006-2009).*

She is author and co-author of more than 70 scientific papers presented at conferences and published in journals (Sensor & Actuators, J. of Micromechanics and Microengineering, Appl.Optics., Journal of Luminescence etc).

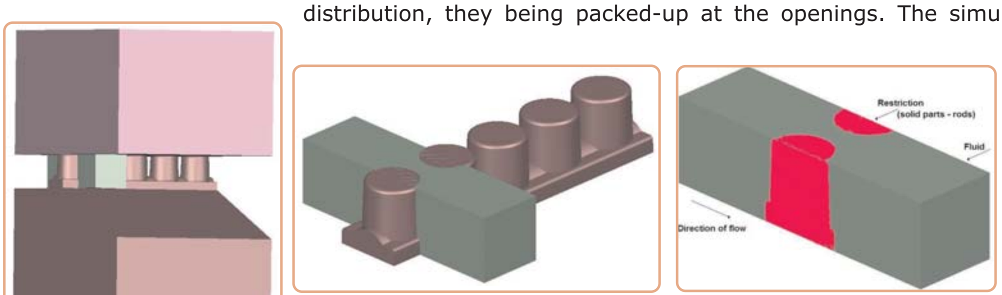
L5: Participation in FP6 projects

Implementation of Production Processes for New Molecular Imaging Agents MI-lab on chip-Lab-On-A-Chip

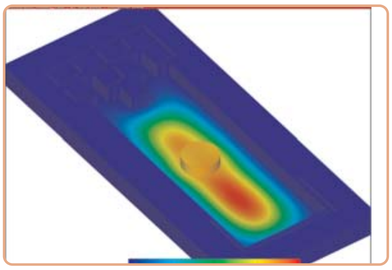
STREP-FP6**,** Priority 3 **NMP,** No 516984, (2005-2008)

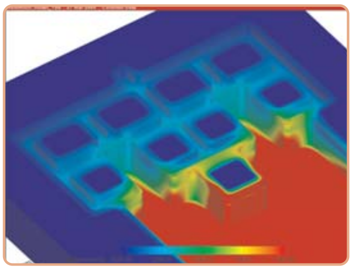
Coordinator: ***University of Liege, Belgium.*** **Partners:** Trasis S.A. Belgium, Bartels Mikrotechnik GmbH Germany, IMT- Bucharest Romania; GG.Tec injection Belgium, Universite Henri Poincare–Nancy France.
IMT- Bucharest (contact person: ***Oana Nedelcu- oana.nedelcu@imt.ro***)

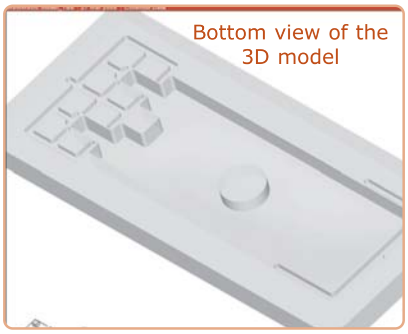
Results: Filter Simulation and Implementation of the filters into the chip - The objective of this work was to design and simulate the filtering system that is required for chemical processing flow into the chip. The filters have to retain the particles of solid phase in the cavity, but still keeping the liquids flow as freely as possible through the solid phase. Also, studies on possible ways to implement the filters into the chip were carried out.
The concept to implement the filter uses a narrow slit rather than any other method involving the structuring of the foils (which require more sophisticated production methods). The different designs that were studied rely upon a series of slits wider than the average diameter of the beads (50 to 70μm). The slits keep the beads in place due to their size distribution, they being packed-up at the openings. The simulations were performed for pressure drop in the range of 5-50 kPa. A problem to be solved was the bulging of the plates due to the pressure in the cavities, which could cause the slit located at each end of the cavity to widen and therefore making possible leakage out of solid phase.

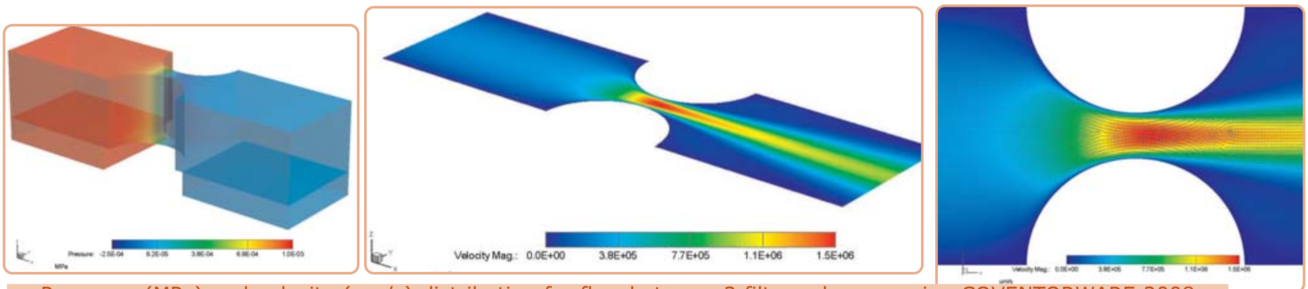


Design of microfilter based on separation columns


Simulation of displacements (bulging) due to internal pressure- view from the bottom size


Displacements distribution: a detailed view on the channel


Bottom view of the 3D model



Pressure (MPa) and velocity (μm/s) distribution for flow between 2 filter columns, using COVENTORWARE 2008

Improvement of Industrial Production Integrating Macro-, Micro- and Nanotechnologies IPMANN

Project coordinator: **Christian Woegerer- PROFACTOR Research and Solutions GmbH, Austria**
IMT-Bucharest partener, contact person Dr. Raluca Müller (raluca.muller@imt.ro);
FP6 NMP2-CT2006-033205; (2006-2009)

Results: Coordination of Disseminarion Workpackage.
Active participation with scientific talks at different IPMMAN/MINAM sections within EU events:
- **SEMINAR on Micro- and Nanotechnologies for Industrial Applications** - organized by MINAM Platform and the ISQ - Instituto de Soldadura, Lisbon, Portugal- March 2008
- **MINAM Special Section** at The **7-th The Coating's** and **the 3-rd ICMEN** International Conference on Manufacturing Engeneering, organized by the Laboratory for Machine Tools and Manufacturing Engineering - Aristoteles University of Thessaloniki- EEDM, Greece, October 2008
- **MANUFACTURING 2008 Conference**, Budapest, Hungary- November 2008
- Contributions to **MINAM Newsletters-MNT Future Vision**.

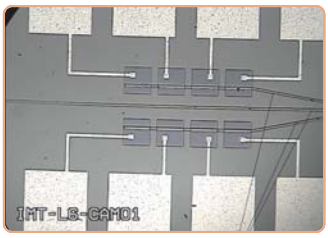
NATIONAL PROJECTS

Sensors and actuators microstructures for microrobotic pozitioning, mechanical and biological manipulation - MEMSAS

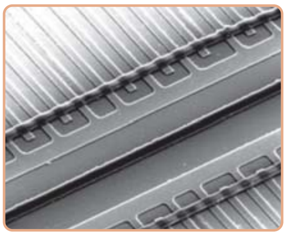
MEMSAS (2005-2008); Project type: CEEX – Contract No. 28/2005- INFOSOC;
Project coordinator: IMT Bucharest; **Project manager: Dr. Raluca Müller (raluca.muller@imt.ro);**
Partners: INCD-SB, INCD-FLPR, Univ. "Politechnica" Bucharest, Univ. "Valahia" Targoviste

The project scope was to develop two kinds of microstructures, using microelectronic and MEMS technologies: optical position sensors, based on different configurations and thermo-actuated microgrippers, using surface micromachining techniques.

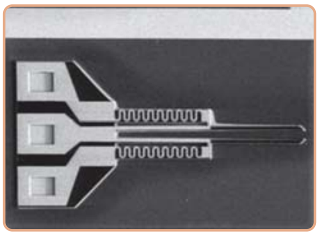
Results: An original configuration was proposed for a microsensor which can function as positioning sensor for detecting the position of an object placed on his axis in 0-300 μm domain and as proximity sensor. In the second case it can find out the presence of very small objects, in a predefined area, without measuring the distance between the sensor and the object.



Optical microscope image of the linear photodetector arrays integrated with SU8 optical waveguides.

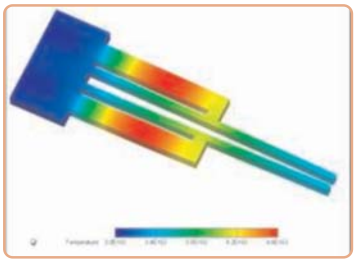


Detail of the MSM photodiode (interdigitated structure integrated with the SU-8 optical guide).

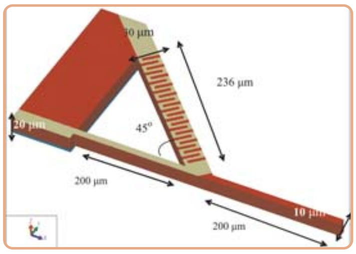


SEM image of the metallic (Cr-Au) resistance of the microgripper

These constructions were composed of two different types of photodetectors: PIN photodiodes and Schottky (MSM) photodiodes both integrated with SU-8 optical waveguides. The optoelectric characterization of the photodiodes has shown a breakdown voltage greater than 90V at 100μA and a dark current less than 0.02 nA at 5 V reverse bias. The device has a very good rectifying characteristic with low absolute leakage current. A responsivity of 0.39A/W for of 630nm wavelength and 20V bias was obtained.



Maximal values of the temperatures in the microgripper when a voltage of 0.25 V is applied-simulation with CoventorWare tool



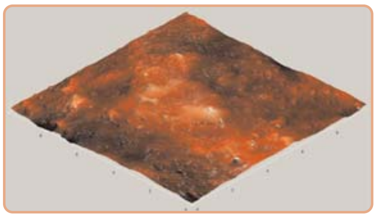
Design of the half of microgripper model without the SU-8 layer on the 0.25 V is applied - simulation with CoventorWare tool (Rodica Voicu – PhD student)

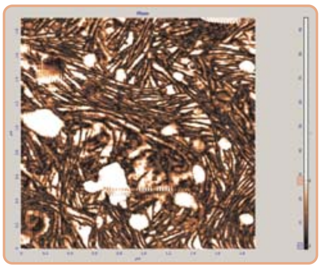
A new design was developed for a **polymeric microgripper**, which can realize a movement of the gripping arms with possibility for positioning and manipulating of the gripped object. Two models of the microgripper, electro-thermo-mechanical actuated, using low actuation voltages, designed for SU-8 polymer fabrication were investigated and compared. Finite-element analyses (**FEM**), using **COVENTOR-WARE 2008** tool, were performed in order to evaluate the relation between the displacement, temperatures and the electrical current passing through the metallic layers. Different thickness of the polymeric layers was considered in order to evaluate the minimum out of plane displacements that can occur in the behaviour of the microgripper. The choice of biocompatible materials, as SU-8, together with the low actuation voltages and large deflection produced at low temperatures, makes this microgripper highly suitable for bio-manipulation experiments in air or in aqueous media. Other potential applications of these devices are micro-relays, assembling and miniature medical instrumentation.

Unconventional Materials for Microtechnology – Research and Experimentation of Elastomer Based Microstructures for Applications in the field of Microsystems

NOELSYS (2005-2008); Project Type: CEEX 15 I 03 / 2005 INFOSOC; Coordinator IMT-Bucharest; Project manager: Dr.Gabriel Moagar-Poladian (gabriel.moagar@imt.ro); Partners: S.C. ICEMENERG S.A., Univ. Bucharest, S.C. IPEE-ATI S.A., S.C. ProOptica S.A., S.C. Optoelectronica – 2001 S.A.

Results: Deposition of elastomeric thin films (policloroprenic, butilic and butadien-styrenic rubbers) with very good adherence to surface and good surface topography. Nano-crystallization of the film as a consequence of its thermal annealing was observed. Extensive characterization of the deposited films, as regards surface topography, structure, spectral properties (by FTIR method) and internal mechanical stress. An improved type of infrared sensor was conceived and will be registered at OSIM. An original method of stress determination in the elastomeric thin film was tested experimentally and compared to measurements made by other means (optical polarimetry). The internal mechanical stress is less than 3,7 kPa. Papers presented at conferences and sent to publication.



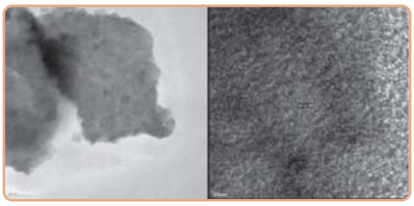


AFM images of the elastomer thin film. a) on a 10 μm x 10 μm scale; b) phase image on a 2 μm x 2 μm scale, a different location.

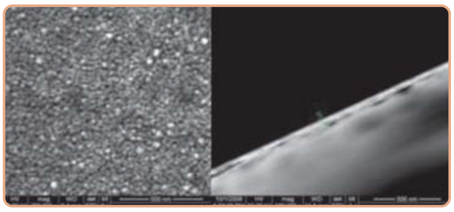
NATIONAL PROJECTS

Electronic Nanodevices Based on Oxidic Materials

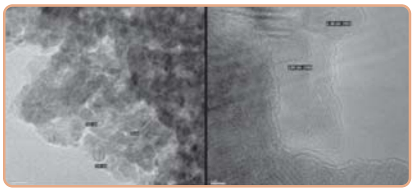
NANOXI (2007-2010); Project Type: PNII- Contract Nr. 11-048; **Coordinator IMT- Bucharest;**
Project manager: Dr. Rodica Plugaru (rodica.plugaru@imt.ro); **Partners:** University Politehnica of Bucharest (UPB-Bucharest), Institute of Physical Chemistry "I.G. Murgulescu" Romanian Academy, National Research and Development Institute for Electrical Engineering- ICPE-CA, S.C. METAV-Research & Development S.A.



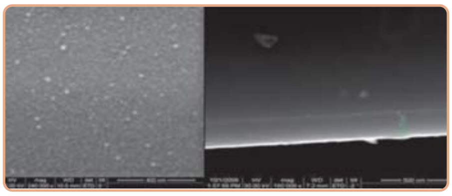
HR-TEM images of ZnO thin film deposited by RF magnetron sputtering from ZnO target. The grains size is less than 50 nm, with (002) oriented nanocrystallites and wurtzite structure.



SEM surface and cross section images of the ZnO (Zn 0,05 M 1) film, formed by 4 successive sol-gel deposited films, annealed in air at 500ºC, 1h.



Bright Field HR-TEM images of ZnO thin film deposited by DC magnetron sputtering from Zn target and further oxidized in air at a temperature of 450ºC for 3h. The nano-crystallites size is less than 20nm, are (100) and (002) oriented, and their structure is wurtzite.



SEM surface and cross section images of the ZnO (Zn 0,05 M 1) film, formed by 4 successive sol-gel deposited films, annealed in air at 500ºC, 1h.

Results:

• **Experimental studies** on thin films semiconductor oxides deposition by sol-gel and DC/RF magnetron sputtering methods, for advanced optoelectronic and magnetic devices. Characterization of morphology, thickness, grains size, texture, structure, refractive index, transmittance, extinction coefficient, fluorescence properties and elemental composition.
1. Sn-Zn-O (Sn/Zn=1) thin films obtained by sol-gel route;
2. ZnO thin films and ZnO:Al doped thin films obtained by sol-gel route;
3. ZnO thin films deposited using DC and RF magnetron sputtering from Zn and ZnO targets;

• **Tunnelling leakage current characterization** of silicon oxide and high-k dielectrics for advanced semiconductor devices. Numerical simulations were performed using ATLAS devices simulator software package from Silvaco. An iterative approximate method was used to calculate the 1D MOS structures main electric parameters without using the Schrödinger-Poisson equations. This method is based on approximation of effective field function of doping parameters. The tunnelling currents can be calculated more rapidly and the study for different gate dielectric stacks can be made.

• **Ab initio study of electronic structure of semiconducting oxides**. Modelling of defects influence on localized states. Ab initio calculations were performed using the FPLO code in order to explore the electronic structure of semiconductor oxides for advanced opto- and magneto-electronic devices. The oxygen deficiency in these materials may be used to tune the material optical and magnetical properties. The computational study was devoted to understand the effect of oxygen vacancies (OVs) on the electronic structure of rutile and anatase TiO_2. Various OVs concentrations and distributions in the supercell permitted to determine the vacancy-induced states localization and structure, the effect of vacancy concentration on the orbital occupation numbers, as well as the vacancy energetics. The present results, reflect the real material behavior.

Unit of Analog Optical Processing of Image Type Information

PROIMAGE (2006-2008), Project Type: CEEX 139 I 03 / 2006 INFOSOC;
Coordinator IMT- Bucharest; Project manager: Dr.Gabriel Moagar-Poladian (gabriel.moagar@imt.ro);
Partners: Univ. Bucharest, S.C. Optoelectronica – 2001 S.A., S.C. RD Concept S.R.L.

Results:
a) The architecture of an analog optical processor was conceived.
b) The emulation software was tested for applications in the field of radiology.
c) Several papers were conceived and are under preparation.

Applications of high technologies based on microsystems and nonlinear optics for the measurement of the electric current parameters on the high voltage lines

Project type: Parteneriate 31-021 / 2007, (2007-2010); Coordinator: IMT-Bucharest,
Project Manager: Dr.Gabriel Moagar-Poladian (gabriel.moagar@imt.ro);
Partners: Bucharest University, S.C. SITEX 45 S.R.L.

We have devised several methods for exciting microsystems used for measuring the electric current parameters on high voltage lines. Because these microsystems work in very harsh conditions, the reading of their displacement is made optically. We have devised several optical methods that can be suited for this purpose. A new method, based on advanced materials, was conceived for the voltage measurement. The method is now subjected to patenting at OSIM.

NATIONAL PROJECTS

Micro-welding systems for microsensors and actuators for micro-joining of circuit elements and packaging

MICROWELD (2007-2008); Project Type: PN II Project.
Coordinator ISIM, IMT-Bucharest partner,
Contact person: Eng. Phys. Victor Moagar-Poladian (victor.moagar@imt.ro)

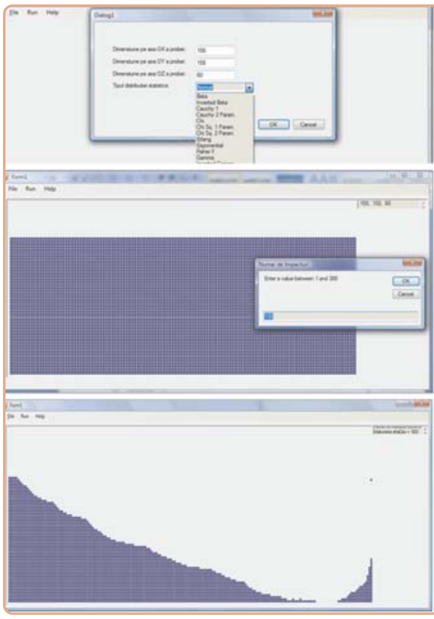
Results: The aim of the project is the development of the knowledge in the field of technologies dedicated to micro-assembling of MEMS components by developing 3 methods of micro-joining of metallic and non-metallic materials that are commonly used in MEMS devices. These welding procedures will respect either one of the following conditions: - to realize a good electrical contact between different components of MEMS; - to enable a good sealing for MEMS devices. *IMT-Bucharest role in the project is the design and simulation of the behavior of the micro-welded components under exploitation conditions and the characterization of the quality and the properties of the welding.*

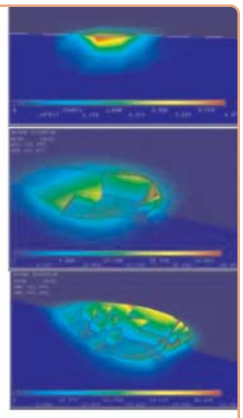
New materials having high anti-corrosive performance with applications across different domains for the use environtments presenting complex and severe loads

INTERMAT (2006-2008); Project Type: CEEX Project;
Coordinator ICEMENERG, IMT-Bucharest partner,
Contact person: Eng. Phys. Victor Moagar-Poladian (victor.moagar@imt.ro)

Results: The project has as expected result the fabrication of new protection materials that have to eliminate the disadvantages of the present protection materials, namely: limited or specialized domains usefulness, toxicity, high number of different types of layers needed to provide enough resilience to aggressive environment. These new materials will have an use in industrial fields by providing protection against harsh environments (high temperature, aggressive chemical agents, abrasion, thermal and mechanical shocks, etc.).

The role of IMT-Bucharest in this project is to provide simulations regarding the protective layer behaviour in contact with different types of aggressive agents. Due to the complexity of the problem, the software used was ANSYS Multiphysics 11.0. The results of several cases of impacts simulated in ANSYS for the previous year were the input for the a home made software, based on Monte Carlo simulation, in order to achieve the protective layer state.





Layer integrity and summed deformation after impact is presented. The numbers above the figures are representing the angle, speed and diameter of the impacting particle.

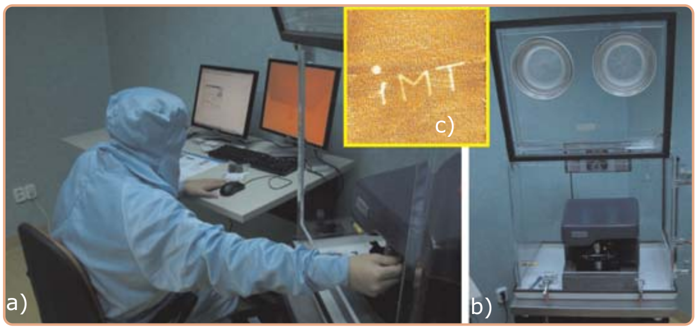
Home made Monte Carlo simulation software (based on ANSYS simulations), providing the number of colision until protective layer penetration

National projects: Capacities

Integrated laboratory of advanced technologies for micro and nanosystems

MICRONANOLAB (2007-2009); Project Type: PN II-Capacities Contract no.13/2007-
Project manager: Dr. Gabriel Moagar-Poladian (gabriel.moagar@imt.ro)

Results:
Dip Pen Nanolithography system (already installed and put into work). This scanning probe lithography technique allows pattering in nanometric range ans is direct writing method that can use molecular and biomolecular "inks" on a variety of substrates. Current activity is that of training and improving work with the system.



Images of:
a- Seting-up the system. Left monitor: used for working with the CAD-like software that controols the system; right monitor (orange): real-time imaging of the cantilever tip; extreme right (blue): the NScriptorTM system. The window of the environmental chamber is open. RiGht"
b- the NScriptorTM system setup with the window of the environmental chamber open.
c- Text written on a gold substrate with MHA (16 – Mercaptohexadecanoic Acid - Image size is of 5 microns x 5 microns, the width of the letters is of 115 nm while the dot on "i" radius is of 180 nm.

National projects: Capacities

LABORATORY FOR MODELING AND SIMULATION OF MICROSYSTEMS

LAMSYS (2007-2009); Project Type: PN II- Capacities; Contract no.7/2007
Coordinator IMT- Bucharest; Project manager: Mat. Oana Tatiana Nedelcu- (oana.nedelcu@imt.ro)

The aim of the project is the development of the knowledge in the field of technologies dedicated to micro-assembling of MEMS components by developing 3 methods of micro-joining of metallic and non-metallic materials that are commonly used in MEMS devices. These welding procedures will respect either one of the following conditions: - to realize a good electrical contact between different components of MEMS; - to enable a good sealing for MEMS devices.

IMT-Bucharest role in the project is the design and simulation of the behavior of the micro-welded components under exploitation conditions and the characterization of the quality and the properties of the welding.
The main objective of the project is the development of the research infrastructure in the field of modeling, simulation and computer aided design for microsystems, improvement of the research capabilities, offering scientific services in a dedicated laboratory, by modernization the existing capabilities.

New facilities: ***Software:*** Coventorware supplementary modules [ARCHITECT - system-level modeling environment, SEMulator3D (semiconductor software), EM3D (Electromagnetic 3D Solver)], SolidWorks (design of complex geometries), Matlab, Mathematica (technical computing software packages), OriginPro8 (tehnical graphics and scientific data processing and interpolation); ***Hardware:*** computers, graphic station for design, workstation for simulations; ***Other:*** Training room for courses and services in MEMS design, modelling and simulation, including presentations / dissemination facilities.

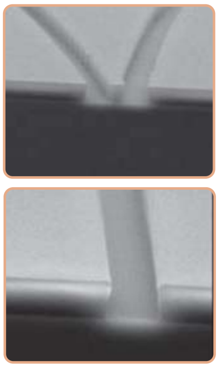
Applications: MEMS (sensors, actuators, accelerometers), Optical MEMS, RF-MEMS, microfluidic microsystems as micropumps, micromixers, microfilters, reaction chambers used in lab-on-chips for pharmaceutical research, medical diagnosis and treatment (medical imaging, drug delivery), genomics, ink-jet devices.

National basic funding projects:

Reserch for integrated photonics and microfluidics structures based on SU-8 and others polymers

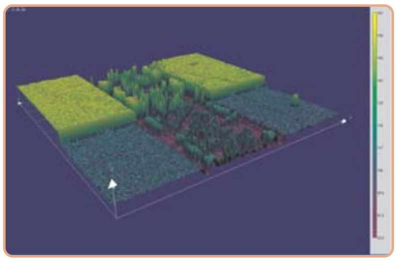
MINASIT PLUS (2006-2008);
Project manager: Dr. Raluca Müller (raluca.muller@imt.ro)

Results: We desined and manufacture different configurations of microchannels to be used in microfluidic applications, obtained in SU-8. Simulations of fluid velocity were performed using COMSOL Multiphysics software. Rectangular and y-shaped microchannels, with vertical walls and high aspect ration wrere obtained. We fabricated a microfluidic device, with an array of Cr/Au electrodes, which control the fluid flow of an aqua solution where have been introduced different nano-particles as: magnetite-Fe_3O_4, magnetite Fe_3O_4-functionalized with silver particles, Fe_3O_4- functionalized with gold particles, and gold nanoparticles. The microfluidic is composed of an inlet, an outlet and a microfluidic channel with a width of 100 μm and a length of 5000 μm. The flow was controlled by applying a small voltage on the electrodes array.



SEM phots of SU8 mirochannels.

Magnetite crystallites Fe_3O_4 + Ag

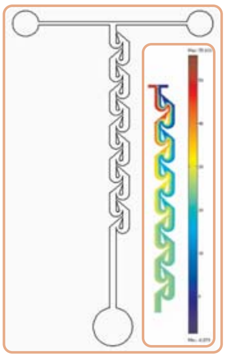


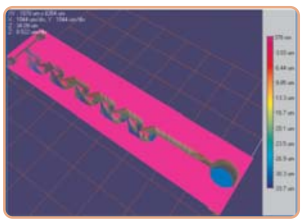
WLI profilometry of the microchannel, with bottom electrodes for a fluid containing nanoparticles

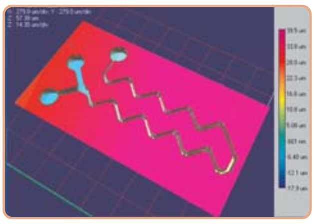
Computer aided design for microfluidic components

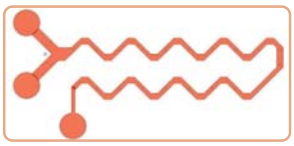
MINASIT PLUS (2006-2008);
Project manager: Mat. Oana Tatiana Nedelcu (oana.nedelcu@imt.ro)

The project scope was to develop new design of microfluidic components, particularly micromixers.
Results: Two concepts of micromixers have been designed, microfabricated in polymer (SU-8) and characterized by simulation and measurements (test structures).









The figures above present different steps related to design, simulation (COMSOL Multiphysics) and characterization using 3D profilometry (WLI) for 2 types of micromixers