



YEARBOOK

2005

**RESEARCH INSTITUTE FOR  
TECHNICAL PHYSICS AND  
MATERIALS SCIENCE**



**HUNGARIAN  
ACADEMY OF  
SCIENCES**

<http://www.mfa.kfki.hu>

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Hungarian Academy of Sciences

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MTA MFA Yearbook 2005

*Editor:* Zoltán Hajnal

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## Director's foreword

Resolutely "follow the way to perfection... against all odds" was the guiding principle of the operation of the Research Institute for Technical Physics and Materials Science - MFA in 2005.

The institute's activities in 2005 were further geared towards nanotechnology – following the restructuring and refocusing of 2004. The research was conducted in the – meanwhile generally accepted – organisational scheme of the previous year. Therefore, the management could concentrate on the intensification of the *development of human resources*.

In acknowledgement of their lifelong achievement, the institute established the title of "*Professor Emeritus Instituti*" for those distinguished scientific advisors (DSc), who reached the retirement age of 70. *The first emeritus professors of MFA, Árpád Barna, Péter Barna, László Bartha, György Gergely, József Gyulai and Péter Varga* obtained their honorary title in January 2006. Three of our colleagues obtained the DSc. degree, i.e. the title Dr. of HAS in 2005. One of our colleagues became Dr. habil. of the University of Western-Hungary and six young MFA researchers successfully defended their PhD thesis. In the supervision and control of the progress of the PhD projects running at MFA, the active role of the Scientific Council is indispensable and much appreciated.

MFA is also being affected by the *unfavourable age composition of the staff* prevalent at academic research institutions in Hungary. We are happy to state that *2005 was the first year, in which a reduction of the average age could be registered* due to the hiring of new, qualified young co-workers. *Twelve new colleagues* joined MFA, corresponding to almost 10% of the whole scientific and research-support staff! The hiring of new co-workers indirectly also served the modernisation of the administrative procedures, but at the same time a considerable improvement in the level of qualification could be achieved, too. In order to *train and position the potential research team-leaders and scientific managers of the future*, we started to encourage the *organised postdoctoral training* of our young PhDs at collaborating leading laboratories abroad. One of our postdoc fellows started his research at Osaka University and two at the National Institute for Materials Science, Tsukuba, Japan last year. Since they can act as personal envoys of the Institute, *they will be instrumental in the extension of co-operation*, too. Also the *co-operation with domestic universities*, our main source of talent supply was enhanced by a more intensive involvement of our leading scientists (a.o. three professors at the University of Veszprém, two at the Budapest Polytechnic, an assistant professor at the Roland Eötvös Science University) in higher education. All our DScs are members of the Doctoral Schools at different universities of the country, and our senior researchers supervise the training of 15 PhD students at MFA.

In the scientific activities we followed the proven strategy of *pursuing a good blend of fundamental and applied research at MFA*. Thereby we were able to properly respond to the *increasing demand* of society and government for *practically exploitable research results*, without endangering the progress of fundamental research projects. The applied research budget, raised from project funding by the National Office for Research and Development, almost equalled the amount of subsidy obtained from the HAS.

Financing of the research at a dynamically growing institute in a year of domestic economic difficulties is a very tough task to master. Generally much delayed payments, subsidy cuts, adverse effects of new VAT regulations, as well as the obligatory formation of budget reserves from institute income at the end of the calendar year (a true "innovation" of the Hungarian fiscus) caused serious liquidity problems, and often made the introduction of severe restrictions necessary. Thanks to the successful efforts of both our scientists and administrators in obtaining project funding, from the economic point of view 2005 was the most successful year so far in the existence of MFA.

The nearly 20% increase in income laid the foundation for the realisation of our plans to improve research infrastructure and working circumstances alike. Beyond the completion of the *laboratory for the adaptation of bio-receptors in nanosensorics*, in 2005 we established a *new clean-room laboratory for electron-beam lithography* and a *student laboratory for STM/AFM training*. Further in 2005 we equipped a.o. the 300keV JEOL TEM with a *new Gatan Imaging Filter unit*, both of our *SEM systems with Energy Dispersive Spectroscopy units*, and the Veeco STM/AFM system with a *tapping-mode drive*. Also *6 working cabinets* could be renovated.

A big step toward the utilisation of the research results as well as the preparatory and analytical capabilities of the institute was the establishment of the first spin-off company of MFA in 2005. In the medium term this 100% owned company, "ANTE Innovative Technologies Ltd" ([www.ante.hu](http://www.ante.hu)) will not only contribute to the financial success of MFA but also be instrumental in offering alternative career opportunities to those young postdocs of the institute who would like to develop their original ideas in the private sector up to product level.

We booked another first success in this regard in 2005. The *fundamental research on nanostructured porous Si* started in 1992 at the predecessor institute of MFA. Using porous Si we developed the *new single sided bulk micromachining technology*, which allowed a.o. the construction of the *suspended-type catalytic gas sensors*, perfected with European support in two international research projects (PORSIS and SAFEGAS). In collaboration with the Hungarian SME, WESZTA-T Ltd, this led to the development of an *electronic nose system for the explosion-proof analysis of combustible gas mixtures*. After passing the necessary safety tests, the electronic system, equipped with MFA sensors, is now *ready to be commercialised*.

By handing over this booklet, we hope to demonstrate to the reader the progress we achieved despite the economic difficulties. Following the MFA Yearbook's tradition, below you will find a compilation of the most important developments and results of the research projects of the Institute. Again we have to stress our readiness for co-operation in any of the fields discussed, hence please do not hesitate to contact the respective colleagues at the given address.

Budapest, March 31 2006

István Bársony

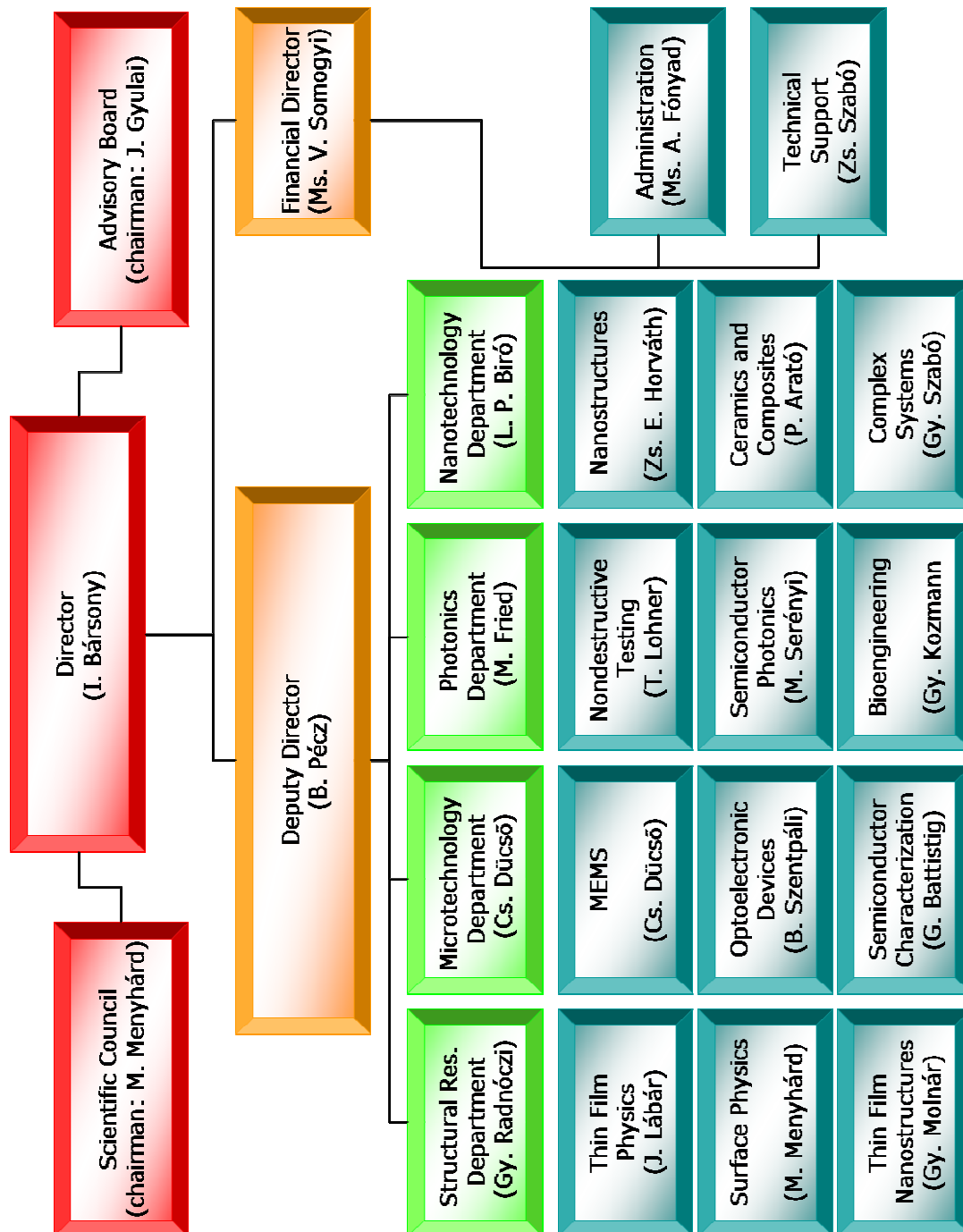


## *General Information*

## Organisation

The Institute is organized in four Departments representing the research fields of our activities. Each Department is divided into three Laboratories, some of which are centered around given technological infrastructure, others are more readily described by their focus of interest.

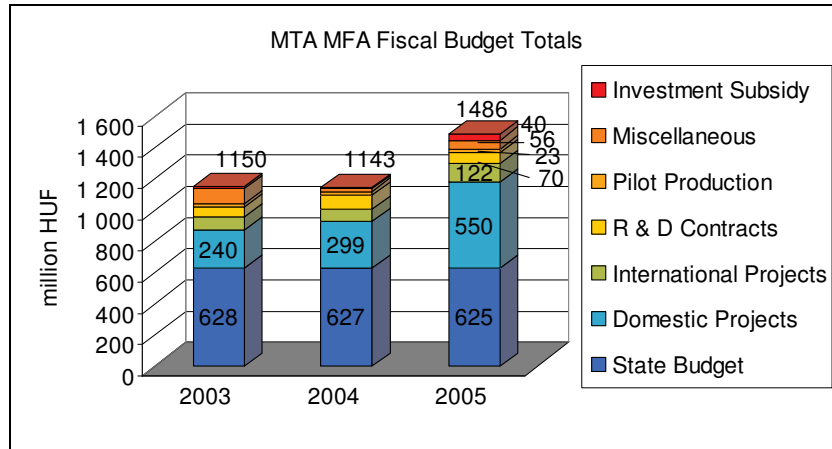
Life of the whole organization is supported by a strong administrative and technical support branch. Top level decision making in scientific and policy issues is assisted by the two boards.



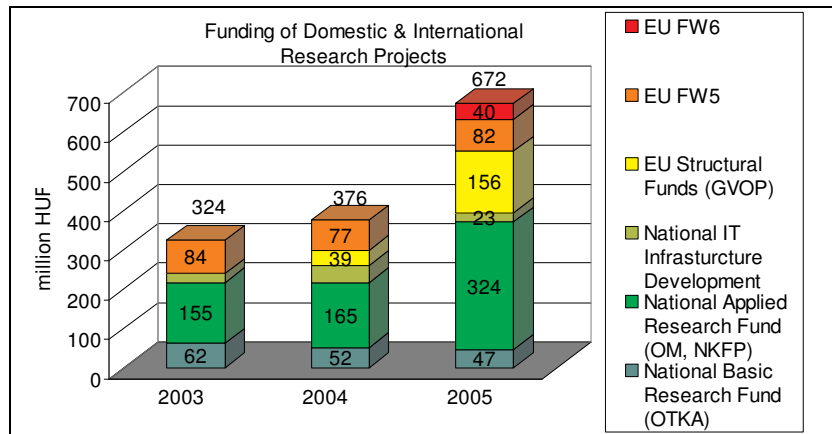


## Key Financial Figures

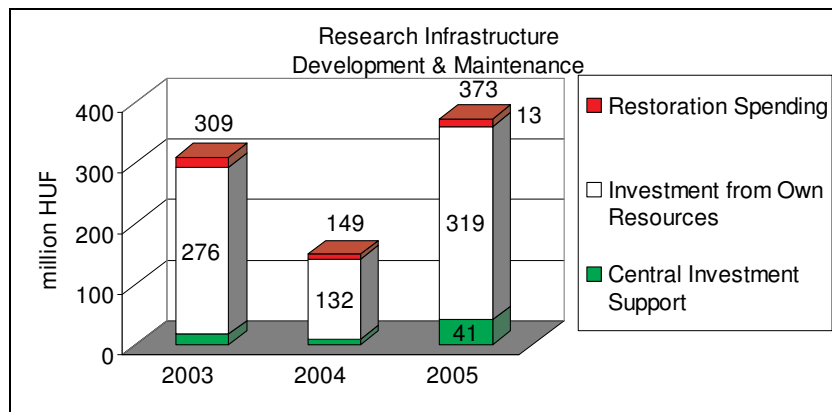
The total budget of MFA has grown over 20% in 2005 and reached € 5.7 million.\*



Funding from research projects provided roughly half of the Institute’s financial resources. This means a doubling of the support obtained for national and international R&D projects with increased societal and economic impact.



This unprecedented growth also enabled more investment in the development of research infrastructure of strategic importance:



\* Figures of this section are stated in millions of Hungarian Forints. 1 million HUF ≈ 3800 EUR

## Prizes and Honours

### *MFA Researcher Prize*

János LÁBÁR, D.Sc.

For his outstanding achievements in the development of the infrastructure of MFA, organisation of collaboration in research and education and for the development of the internationally successful ProcessDiffraction software.

### *MFA Postdoctoral Prize*

Zoltán HAJNAL, Ph.D.

In recognition of his prominent role in editing of the MFA Yearbooks, in the re-organisation of the institute's seminar-series, and his successful initiatives for research project applications.

### *MFA Young Scientist Prize*

György Zoltán RADNÓCZI

For the development of the facilities of the lab for magnetron sputtering, for growing of the "AlInN nanograss", and his excellent collegial support.

### *Jedlik Ányos Prize*

Árpád BARNA, D.Sc.

### *Ferenczi György Memorial Prize*

Péter FÜRJES, Ph.D.

### *Inventor of the Year*

Antal GASPARICS

### *Best Dissertation Prize (Czech and Slovak Society for Microscopy)*

Katarina SEDLACKOVA

### *Pollák-Virág Prize*

Edvárd Bálint KUTHY

For his paper published in the Hungarian Telecommunication Technology Journal (Híradástechnika), January 2004 (title: Crystalline Silicon Solar Cells with Selective Emitter and the Self-doping Contact)

### *Scientific Students' Conference (TDK) 1st prize*

Péter NEUMANN

"Measurements and applications of nano-leads"

### *Scientific Students' Conference (TDK) 1st prize*

István TAKÁCS, undergraduate

## Patents Obtained in 2005

- *Apparatus and measurement procedure for the fast, quantitative, non-contact topographic investigation of semiconductor wafers and other mirror like surfaces.*

Patents: HU0104057, EP1434981, WO03031955, US2004263864:

Europäisches Patentamt GD2	European Patent Office DG2	Office européen des brevets DG2
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Annex to EPO Form 2004, Communication under Rule 51(4) EPC

Bibliographical data of European patent application No. 02 785 145.0

For the intended grant of a European patent, the bibliographical data are set out below, for information:

<b>Title of invention:</b>	<ul style="list-style-type: none"> <li>- VORRICHTUNG ZUR SCHNELLEN, QUANTITATIVEN, KONTAKTLOSEN TOPOGRAFISCHEN UNTERSUCHUNG VON HALBLEITERSCHEIBEN ODER SPIEGELÄHNLICHEN OBERFLÄCHEN</li> <li>- APPARATUS FOR THE FAST, QUANTITATIVE, NON-CONTACT TOPOGRAPHIC INVESTIGATION OF SEMICONDUCTOR WAFERS AND OTHER MIRROR LIKE SURFACES</li> <li>- APPAREIL DESTINE A L'ETUDE RAPIDE, QUANTITATIVE, TOPOGRAPHIQUE EXEMPTÉ DE CONTACT DE PLAQUETTES SEMI-CONDUCTRICES ET D'AUTRES SURFACES SIMILAIRES A DES MIROIRS</li> </ul>
<b>Classification:</b>	G01N21/88, G01B11/30
<b>Date of filing:</b>	01.10.2002
<b>Priority claimed:</b>	HU /02.10.2001 /HUA0104057
<b>Contracting States*</b> for which fees have been paid:	AT BE BG CH CY CZ DE DK EE ES FI FR GB GR IE IT LI LU MC NL PT SE SK TR
<b>Extension States*</b> for which fees have been paid:	
<b>Applicant(s)**:</b>	<p>Hungarian Academy of Sciences Research Institute for Technical Physics and Materials Science Konkoly-Thege ut 29-33 1121 Budapest HU</p> <p>Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V. Leonrodstrasse 54 80636 München DE</p>
<b>Inventor(s):</b>	<p>LUKACS, István, Endre Füredi u. 15/133 H-1144 Budapest HU</p> <p>MAKAI, János Váci u. 71 H-1056 Budapest HU</p> <p>RIESZ, Ferenc Ortorny u. 1. H-2000 Szentendre HU</p> <p>SZENTPALI, Béla Katlona József u. 9/11 H-1137 Budapest HU</p> <p>PFITZNER, Lothar Spardorfer-Strasse 57 91054 Erlangen DE</p>

- *Multiplet Lens of Variable Focal Length* (Patent No. 224577)  
inventors: József GYULAI and András HÁMORI



## Technology Transfer

### ***Electronic nose for explosive gas mixtures***

An almost decade-long R&D work arrived at the verge of economic utilisation when the European FP5 "SAFEGAS" project was concluded in 2004. The project targeted the development of an artificial nose for the analysis of combusive gas-mixtures using appropriate evaluation methods by exploiting the results of various disciplines (physics, informatics, chemistry and microtechnology).

From an early phase of the olfactory research the Hungarian SME, WESZTA-T Ltd. was also involved, defining the final target and taking its share in the development of the electronics. *We have to emphasize that domestic need, well defined targets and participation of a competitive domestic company having sufficient capital and capacity to take part in the long term procedure are all essential prerequisites of the final success.* Besides the final economic benefit, the complex R&D also forms the frame for postgraduate programmes, which results in Ph.D. theses, scientific publications and development of intellectual property by patenting.

Owing to our experience in Si technology of over two-decades we started a fundamental research programme for the investigation of the formation, structure and physical properties of porous Si. In the early nineties this basic research was supported by the grants of the National Scientific Research Fund (OTKA). We soon realised that besides the promising quantum

and optical properties of the *nanoscaled* porous semiconductor, its increased solubility in alkaline solutions and the possibility of its selective formation offers more freedom in 3 dimensional structuring of crystalline Si, too. This opened new routes of micromachining in the manufacturing of MEMS (Micro ElectroMechanical Systems), in particular the preparation of integrated, suspended micro-membranes for various functions.

The first promising results encouraged us to initiate the EU4 Copernicus "PORSIS" project, aimed at the development of a novel processing technology using porous Si. The novel, front-side processed perforated-membrane technique in combination

with appropriate metallization offered the capability to develop locally high temperature in the chip. Thermally isolated micro-hotplates (filaments) could be manufactured on Si-crystal, driven by reduced power and possessing small response time in high temperature applications (typically 18mW and 4ms for heating up to 550°C as shown in Fig.1.).

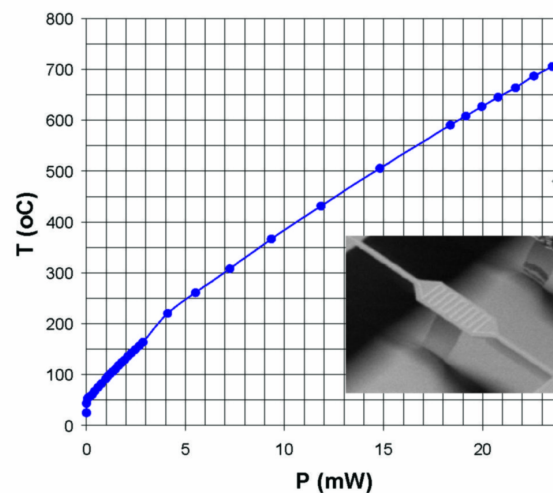


Fig. 1: Input power vs. temperature characteristics of the micro-hotplate manufactured at MFA. Insert shows the SEM image of the the Pt heater on the 100x200  $\mu\text{m}^2$  supported SiN membrane.

This micro-hotplate forms the basis of a gas sensing device known as *micro-pellistor*. A pellistor detects the heat generated by the exotherm catalytic oxidation of combustible gases via the measurement of the change in the resistance of the heater filament. The method requires an efficient oxidation of the gas on the surface of the sensory element. Therefore, the filament is covered with porous ceramic of large specific surface, which is containing the finely dispersed catalytic Pt nano-particles, and the hotplate is heated up to 300-540 °C (Fig.2.). The micro-pellistor is constructed with a chemically active, and an inactive reference element (without Pt catalyst thus) of the very same geometry.

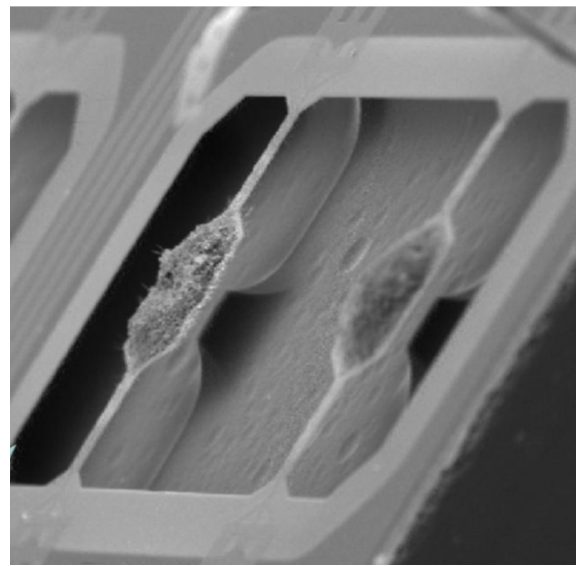


Fig. 2.: Micro-pellistor element manufactured at MFA. The thermal properties of the chemically active (left) and passive (right) components are identical.

In this manner the chemically generated heat is read-out by measuring the difference in the resistance of the two elements, typically in a Wheatstone-bridge configuration. The bridge's error voltage is proportional to the concentration of the combustible gas component. The described measuring method, however, suffers from poor selectivity, i.e. it has a similar sensitivity to all hydrocarbons.

After the successful completion of the "PORSIS" project we were able to initiate a follow-up IST proposal in the Framework 5. The EU5 project, "SAFEGAS" was already aimed at the development of a complex, multi-element olfactory system for identification of selected components in hydrocarbon mixtures. In the multinational consortium, coordinated by the Irish research institute NMRC, besides MFA a German sensor-chip manufacturer (HL-Planartechnik), a French olfactory system specialist (Alphamos), a Hungarian system integrator (WESZTA-T Ltd.) and a Greek research institute (IMEL-Demokritos) cooperated.

When the micro-pellistor contains different catalysts and/or is operated at different temperatures, the individual sensor shows different sensitivity for the same component. Therefore, a parallel operation of several devices offers the possibility of identification of gas mixtures and even a

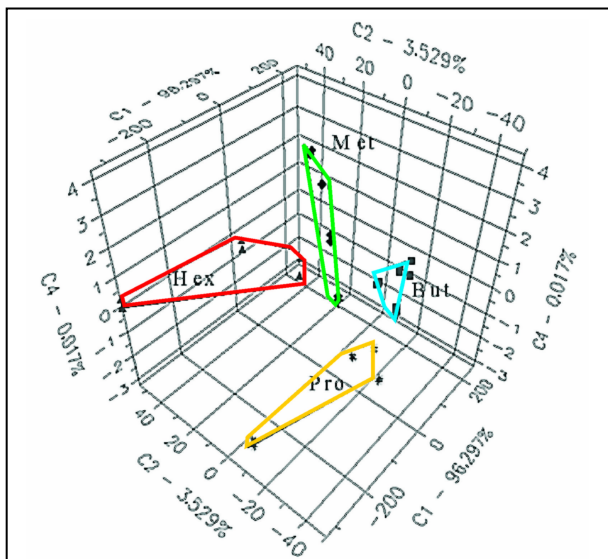


Fig. 3: Classification of explosive gas mixtures by principal component analysis.

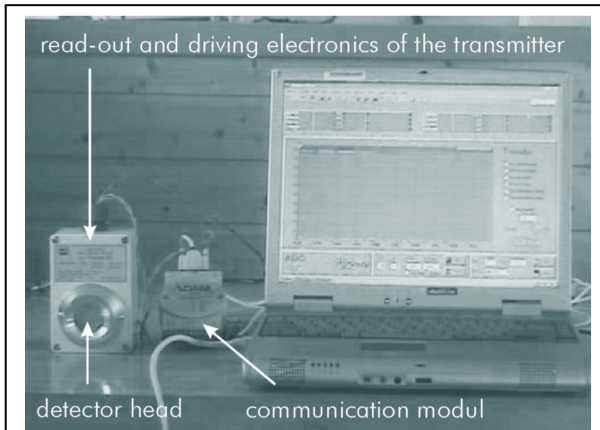


Fig. 4:  
Explosion proof transmitter for olfactory detection of methane, propane, butane and hexane. (WESZTA-T Ltd.)

quantitative determination of gas concentrations. This is done by the evaluation of the readings detected for different compositions by the individual sensors using the *principal component analysis* method or the *neural network principle*. Both methods, however, require a large number of training situations to be taught to the software. This is the basis of the *electronic nose principle*. When the characteristic responses of individual sensors to various gas mixtures undergo "classification" by the principal component analysis or by a properly trained neural network, even the array of sensors of rather poor selectivity can provide a reliable approximation for the concentration of the known components present in the gas mixture. The results of the classification of four components (methane, propane, butane and hexane) are shown in Fig.3.

The task thereby includes the integration of different pellistor elements, the driving, read-out and signal evaluation circuitry. In order to avoid the *risk of explosion* during operation in explosive gas mixtures, the system has to meet the strict safety regulations. The electronics (voltage and current limits) and encapsulation must comply with the European transmitter norms. In "high power" dissipation conventional systems the required robust explosion-proof encapsulation increases the costs significantly, the targeted system has to fulfil both the safety norms and the cost requirements. This was quite a challenge for the consortium.

Fig. 4. shows the transducer system developed by WESZTA -T Ltd. and operates with the integrated sensor chip of MFA. The chip, shown in Fig. 5, contains 3 pellistors and a heat conductivity sensor formed by the same micromachining technique. The high speed and small power dissipation of our sensory elements, however, in combination with their sequential operation, the adequate communication protocols and the fast evaluation algorithm opens the way for the minimization of power consumption of the device. Thereby, the electronics meets the safety norms even without expensive explosion-proof encapsulation, as

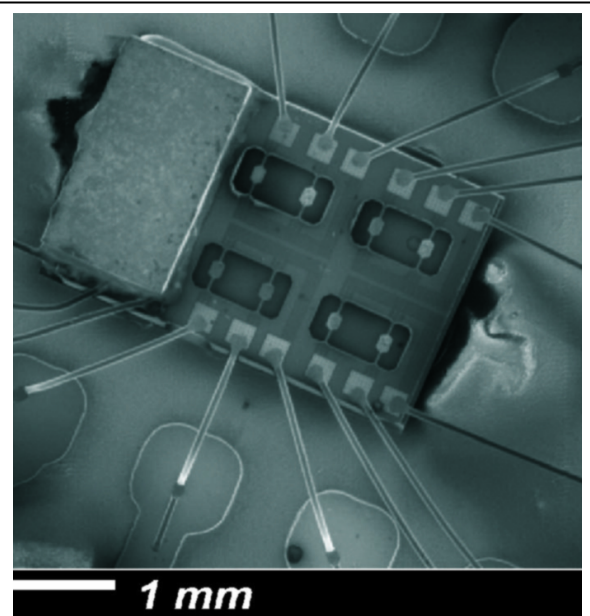


Fig. 5:  
The sensor array chip of the transmitter. (MFA)

was demonstrated in 2004 by the end of the SAFEGAS project.

The development tasks of MFA did not end with the successful demonstration. The partner company intends to introduce the system into the market in 2006. The safety test of the explosion-proof system is being carried out by the responsible authorities, but all the components must further be tested for long term stability and reliability, too.

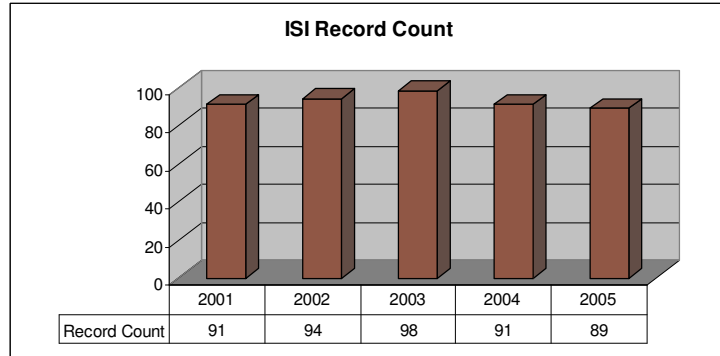
Even after obtaining the permission for marketing of the system, a continuing task of MFA remains the improvement of long term stability and sensitivity of the enabling, crucial element, the integrated micropellistors. The success of the complex attempt across the full innovation chain starting with fundamental research on the nanostructured porous Si, via the innovative bulk-micromachining process, the micro-pellistor development and integration in a wide international and domestic industrial collaboration proves the ability of a research institution of the Hungarian Academy of Sciences to enable the market success of a Hungarian SME not only by the generation of innovative products, but also by the supply of the crucial MEMS parts for their systems.



## Scientometry (International Impact)

International bibliographic services, such as the *Web of Knowledge* (<http://wos.isiknowledge.com>) provide very interesting collections of data on individual researchers' as well as scientific institutions' publication activity. This can be used for independent and (more-or-less) standard assessment of scientific performance. The simplest measure of activity is the

number of publications in refereed international journals. Measured by this record count (see fig. on the right) the MFA has been producing a very stable rate of scientific output. The publication list, closing this year-book, consists of considerably more titles, due to hungarian journal papers

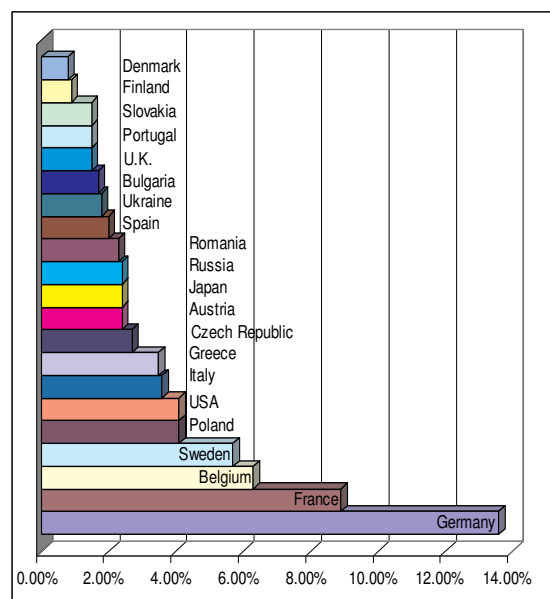
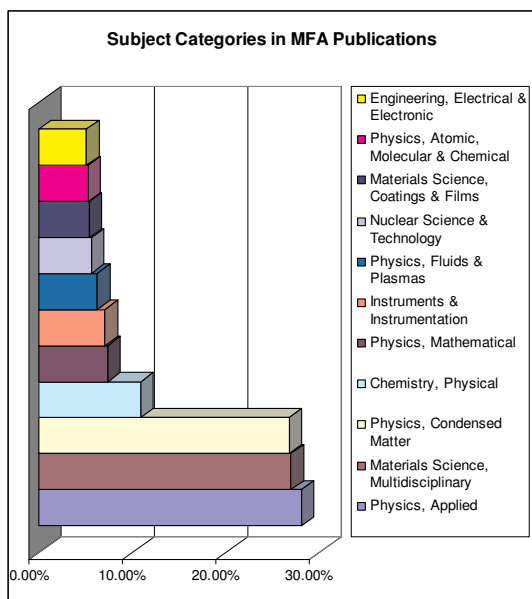


as well as conference proceedings and book chapters which are not in the scope of the refereed periodicals' database.

Taking only the raw data of the *Science Citation Index* into account, the average impact factor of the last 5 years MFA publications is over 3.4 citations per title.

Among other interesting points, two collections may be of general interest. On the left hand side (see below) the chart shows the distribution of subject categories of the publications of MFA, clearly indicating our major fields of interest: condensed matter physics, and applied, multidisciplinary materials science.

To the right hand side, the distribution of co-authors' country of origin is shown. The listed countries and their proportions represent the strength of our scientific ties to the world.



## Visitors

Prof. G. AMSEL, Université Pierre et Marie Curie and French National Research Center, Paris

K. ARSTILA, University of Helsinki, Finland

N. P. BARRADAS, Instituto Tecnológico e Nuclear, Portugal

M. BAUMANN, Gatan/MB Science Service, Slovakia

J. BETKO, Slovakian Academy of Sciences

M. BIANCONI, Istituto per la Microelettronica ei Microsistemi, Bologna, Italy

A. BISHOP, Dept. of Materials Science and Engineering, SUNY, USA

Dr. O. CARNEIRO, Universidade do Minho, Polimer Engineering Dept., Guimarães, Portugal

Dr. L. CENIGA, Slovak Academy of Sciences, Institute for Materials Research, Kosice

Prof. L. A. CHERNOZATONSKII, Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, Russia

Prof. V. CHIKAN, Lawrence Berkeley National Laboratory, USA

N. DYTLEWSKI, International Atomic Energy Agency, Austria

N. L. DMITRUK, Institute of Semiconductor Physics, Kiev, Ukraine

Dr. S. DUB, Ukrainian Academy of Sciences

A. V. DVURECHENSKII, Institute of Semiconductor Physics, Novosibirsk, Russia

Prof. Chr. EISENMENGER-SITTNER, Austria

L. N. EREC, Physical Institute, Athens

Dr. L. FEDÁK, University of Uzhgorod

Dr. G. FROSH, Oxford Instruments Ltd.

P. GRABIEC, Polish Academy of Sciences

V. GORODYNSKY, Institute of Radio Engineering and Electronics, Academy of Sciences of the Czech Republic, Prague

J. GRYM, Institute of Radio Engineering and Electronics, Academy of Sciences of the Czech Republic, Prague

Dr. B. HANEKAMP, Twente University, Netherlands

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Guimarães, Portugal

P. INCZE, Babes-Bolyai University, Romania

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J. P. JAKOVLEV, Ioffe Physical Technical Institute, St. Petersburg, Russia

Ch. JEYNES, University of Surrey, UK

V. I. KANEVSKIJ, Shubnikov Institute of Crystallography, Russian Academy of  
Sciences

J. KNAUP, Universität Paderborn, Germany

Dr J. KRISTOFIK, Academy of Sciences of the Czech Republic, Prague

U. KUERNER, Sopra GmbH, München, Germany

Prof. Ph. LAMBIN, Facultés Universitaires Notre Dame de la Paix (FUNDP),  
Namur, Belgium

T. LAMMERS, Royal Netherlands Academy of Arts and Sciences

Dr. V. LIEDTKE, ARCS Seibersdorf, Austria

V. G. LITOVCHENKO, Institute of Semiconductor Physics, Kiev, Ukraine

S. LUGOMER, Materials Science Department "Ruđer Bošković" Institute,  
Zagreb, Croatia

D. MACHAJDIK, Institute of Electrical Engineering, Slovak Academy of  
Sciences, Bratislava

I. P. MAYER, The Hebrew University of Jerusalem, Israel

M. MAYER, Max-Planck-Institut für Plasmaphysik, Garching, Germany

Dr. J. NEIDHARDT, Department of Physical Metallurgy and Materials Testing,  
University of Leoben, Austria

L. V. ORLOV, Nizhnyj Novgorod, Nizhny Novgorod State University, IPM RAS,  
Nizhny Novgorod, Russia

L. PAPADIMITRIOU, Department of Physics, University of Thessaloniki, Greece

- R. V. PARFENYEV, Ioffe Physical Technical Institute, St. Petersburg, Russia
- E. M. PASHAEV, Shubnikov Institute of Crystallography, Russian Academy of Sciences
- E. PECHEVA, Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia
- G. PETROU, Physical Institute, Athens
- L. D. PRAMATAROVA, Institute of Solid State Physics of the Bulgarian Academy of Sciences, Sofia
- J. RAMSDEN, Cranfield University, UK
- E. RAUHALA, University of Helsinki, Finland
- V. F. SAPEGA, Ioffe Physical Technical Institute, St. Petersburg, Russia
- K. W. B. SCHWARZ, Patmos Nanotechnologies Llc.
- Dr. O. SHIKIMAKA, Moldavian Academy of Sciences
- Prog. J. STOEMENOS, Aristotle University of Thessaloniki
- Vavrinec SZATHMARY, MD, DSc, Institute of Normal and Pathological Physiology, Slovak Academy of Sciences, Bratislava, Slovak Republic
- Ch. THILL, Universität Paderborn, Germany
- M. THOMPSON, Cornell University, USA
- Dr. I. TOMÁŠ, Institute of Physics, Academy of Sciences of Czech Republic
- M. TOSAKI, Osaka University, Japan
- Milan TYSLER PhD, Institute of Measurement Science, Slovak Academy of Sciences, Bratislava, Slovak Republic
- Dr. I. VICKRIDGE, Institute de NanoSciences de Paris, Université Paris 6, Paris France
- F. WAKAYA, Research Center for Materials Science at Extreme Condition, Osaka University
- Dr. Konstantin ZHURAVLEV, Institute of Semiconductor Physics of the RAS, Novosibirsk, Russia

*Scientific Reports*

## Thin Film Structure Research Department

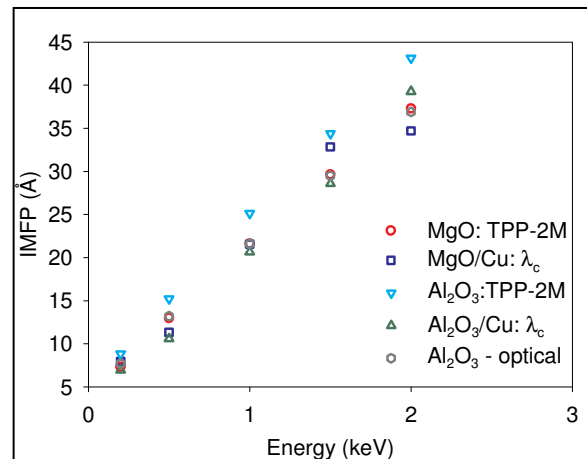
<b>Surface Physics Laboratory</b>	<b>Thin Film Physics Laboratory</b>	<b>Thin Film Nanostructures Laboratory</b>
<p><b>Head:</b> Miklós MENYHÁRD, D.Sc.</p> <p><b>Staff:</b> G. GERGELY, Prof. Emeritus, D.Sc. S. GURBÁN A. SÜLYOK, Ph.D. P. SÜLE, Ph.D.</p> <p><b>PhD Students (Advisor):</b> L. KÓTIS (M. Menyhárd)</p>	<p><b>Head:</b> János L. LÁBÁR, D.Sc.</p> <p><b>Research Staff:</b> Árpád BARNA, Prof. Emeritus, D.Sc. Péter B. BARNA, Prof. Emeritus, D.Sc. Zsolt CZIGÁNY, Ph.D. László DOBOS, Ph.D. Mrs. Olga GESZTI Éva HEGEDŰS, Ph.D. András KOVÁCS, Ph.D. István KOVÁCS Viktória KOVÁCS-KIS Béla PECZ, D.Sc. György RADNOCZI, D.Sc. György SAFRAN, Ph.D. Katarina SEDLACKOVA Lajos TÓTH, Ph.D. Bernadett VEISZ, Ph.D.</p> <p><b>Technical Staff:</b> Mrs. Árpád BARNA Sándor CSEPREGHY Mrs. Ferenc GLÁZER Andrea JAKAB Andor KOVÁCS Mrs. Antal KOVÁCS László PUSKÁS Mrs. András TÓTH</p> <p><b>PhD Students (Advisor):</b> Róbert GRASIN (J. L. Lábár) György J. KOVÁCS (G. Radnóczy) Fanni MISJÁK (B. P. Barna) György Z. RADNÓCZI (B. Pécz) Lajos SZÉKELY (B. P. Barna)</p>	<p><b>Head:</b> György MOLNÁR, Ph.D.</p> <p><b>Staff:</b> Gábor PETŐ, D.Sc. (Head of Lab till 28-02-2005) Tamás HORÁNYI, Ph.D. Albert KARACS György LEHEL</p> <p><b>PhD Students (Advisor):</b> Gergely KOVÁCH (till 30-11-2005) (Gábor Pető)</p>

## Surface Physics Laboratory

### **Determination of surface excitation parameter for various oxides (OTKA T 037709, Hungarian-Polish bilateral agreement PL-11/2002)**

G. GERGELY, S. GURBÁN, M. MENYHÁRD, A. SULYOK, A. JABLONSKI

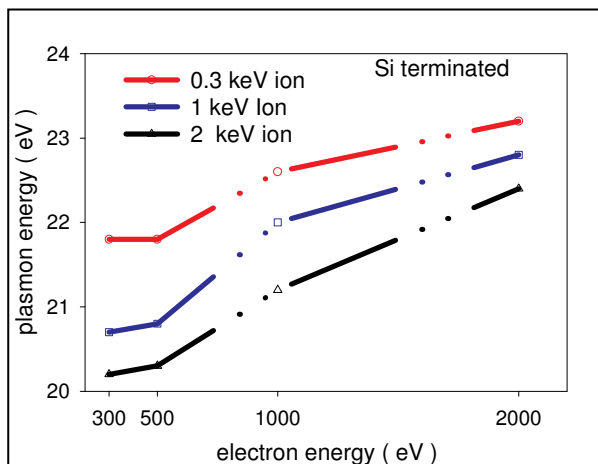
Correction for surface excitation is necessary for determination of the IMFP, which is an important parameter for surface analytical techniques. We have shown that elastic peak electron spectroscopy (EPES) can be applied to determine surface excitation parameter. This year we have determined the surface excitation parameters for various oxides [51]. In the figure we show the corrected IMFP values determined by EPES, and the ones recommended by TPP-2M and optical measurements. It turns out that that the correction is important for higher energies.



It turns out that that the correction is important for higher energies.

### **Ion bombardment induced damage in SiC (OTKA T 043704, DAK-11-03)**

Á. BARNA, L. KÓTIS, S. SULYOK, M. MENYHÁRD, J. MALHERBE



Earlier we have shown by AES analysis that the ion bombardment induced damage is different on the differently terminated faces of SiC single crystal. This work was extended by measuring the plasmon energy of the same faces applying various ion bombardment conditions. In the Fig. we show the apparent plasmon energy as a function of the primary electron energy (probing layers of different thickness measured at various ion bombardment conditions). The found behavior can be explained with a damaged layer exhibiting lower density, with a thickness depending on the ion energy [87].

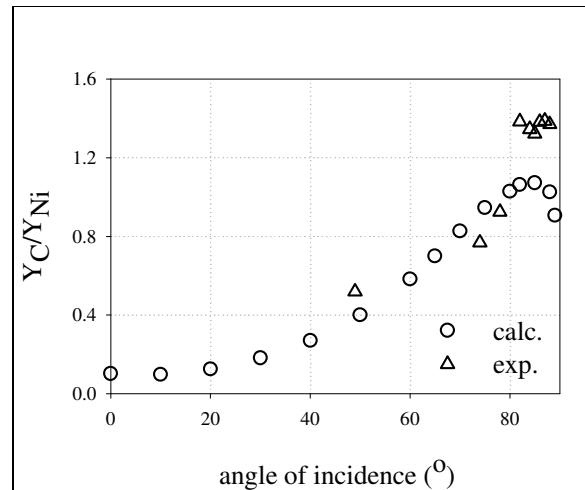
### **Sputtering yield measurements**

(NKFP 3A/071/2004, OTKA T 043704, SLO 14/03)

Á. BARNA, L. KÓTIS, M. MENYHÁRD, A. ZALAR, P. PANJAN

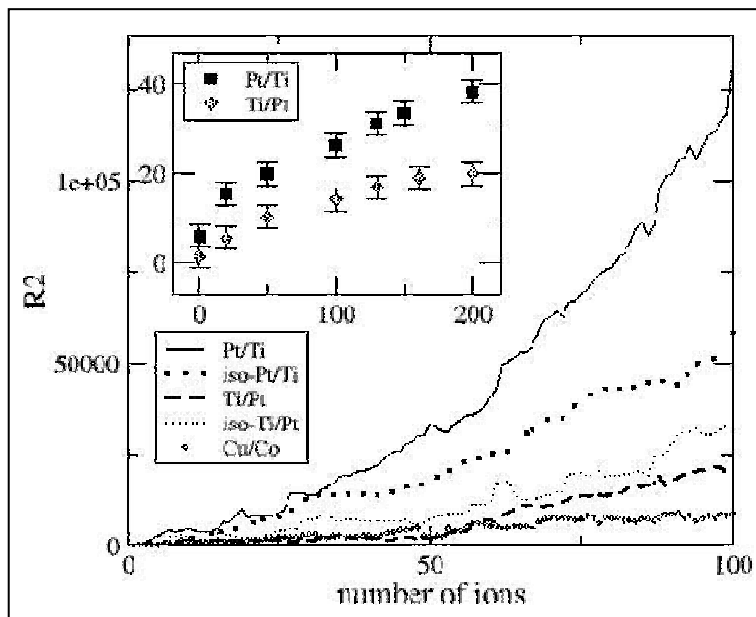
For the various application of the ion sputtering the knowledge of the sputtering yield is necessary. Still there are practically no data for sputtering

yield for grazing angle of incidence and low ion energy conditions. AES depth profiling can be applied for measuring relative sputtering yield if sample with well known structure is depth profiled. Ni/C multilayer was used for this purpose and we found that unexpectedly the C sputtering yield is higher than that of Ni at sputtering angles above  $80^\circ$  [21]. TRIM simulations agreed well with the experimental findings. This simulation also showed that the low scattering power of C is responsible for the strange behavior.



### ***Simulated ion-sputtering: anisotropy induced interdiffusion (OTKA F-037710)***

P. SÜLE, M. MENYHÁRD



Intermixing in metallic bilayers has been studied by atomistic simulations and the obtained results are compared with Auger electron spectroscopy depth profiling (AESDP) data. A new c-shell script code is written to simulate ion-sputtering. The experimentally observed asymmetry of intermixing in Pt/Ti has been reproduced and the mechanism of broadening at the interface is explained by

a new model. We find that a backscattering process occurs at the anisotropic interface. The scattered particles increase the energy density which leads to local lattice instability and to the enhancement of interdiffusion. In strongly anisotropic bilayers the enhancement of interdiffusion occurs leading to anomalously fast diffusion (superdiffusion) [165].

In the figure given above we show the evolution of the square of atomic displacements along the depth direction. We find that a strong asymmetry in mixing develops in agreement with the AESDP measurements carried out in our Laboratory. The saturation of broadening is also shown in the inset figure for Ti/Pt under the effect of 0.5 keV Ar ion bombardment. The saturation is not reached, however, for Pt/Ti, in which a wider broadening occurs.



## Thin Film Physics Laboratory

### **Quantitative Electron Microscopy (OTKA T043437)**

J. L. LÁBÁR, B. PÉCZ, G. RADNÓCZI, V. KOVÁCS-KIS, G. SÁFRÁN, B.P. BARNA, G. CZIGÁNY, L. PUSKÁS, A. JAKAB

Indexing of diffraction patterns from single-crystalline grains in the TEM is hindered by the limited accuracy of electron diffraction measurements. The new module in the ProcessDiffraction program overcomes this limitation by simultaneously indexing several diffraction patterns from the same grain, recorded under defined tilt-conditions. Accuracy is further enhanced by applying a new automatic procedure to fine-tune the identified location of the center of the pattern, a parameter, critical to the achieved accuracy. [97]

On the basis of previous years' results, the first steps were taken to establish quantitative phase analysis for nanocrystalline „powder” samples, examined in the TEM by high energy electron diffraction. The method established in the ProcessDiffraction program is similar to the Rietveld-method, which is well established in XRD. Optimization details are slightly different. The intensities of the individual diffraction lines are separated, extracted and compared to calculated ones to estimate the relative amount of crystalline phases present in the analyzed volume. Details of whole profile fitting are elaborated in last years Yearbook. Optimization of the model-parameters is done with the Downhill Simplex method. Theoretical diffracted intensities are calculated with the kinematical approximation, with possibility of minor correction for slight dynamic effects. The main limitation of the present version originates from this kinematical approximation, since very thin, nanocrystalline samples can only satisfy the validity condition for this approximation. Extension to thicker samples and / or larger grains is planned in coming years.

Two-phase test samples with characterized ratio of the phases were prepared by vacuum evaporation. Grain size <10 nm and layer thickness < 20 nm was applied in all cases. Phase ratio was measured by a quartz oscillator during deposition and further confirmed by EDS composition-analysis. Phase ratios, measured by our diffraction method agreed well with the true values for the small number of test samples, examined up-to-now. Accuracy is  $\approx 10\%$  and the detection limit is  $\approx 5\%$ . [99] Validation of the method on the basis of a larger number of samples is in progress.

Phase	Vol% [Quartz]	Vol% [SAED]
Al [fcc]	50	49
NiO [fcc]	50	51

Phase	Vol% [EDS]	Vol% [SAED]
Cr [cP8]	77	73
Ag [fcc]	23	27

Phase	Vol% [EDS]	Vol% [SAED]
Ni [fcc]	76	83
Ag [fcc]	24	17

Phase	Vol% [EDS]	Vol% [SAED]
Cr [cP8]	2	0
Ag [fcc]	98	100

Phase	Vol% [EDS]	Vol% [SAED]
Ni [fcc]	95	96
Ag [fcc]	5	4

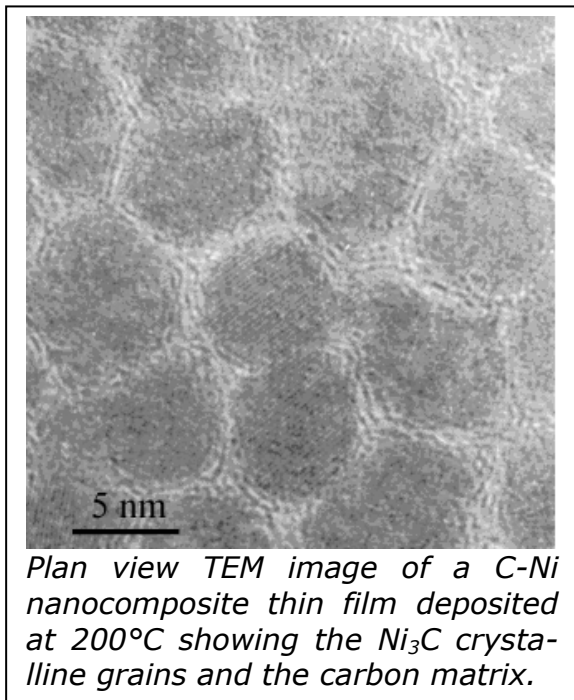
***New Fullerene-like Materials (FULLMAT)  
EU5, HPRN-CT-2002-00209 (202-2006)***

Our work, within the EU5 framework *New Fullerene-like Materials*, aims the understanding the formation and properties of magnetron-sputtered carbon-metal and carbon nitride-metal nanocomposite films. In industrial production pure carbon and carbon-nitride films have been already used as protective coatings. The metal addition should widen the spectrum of applications. These possible future applications are magnetic data storage, displays, tailored nano-containers for foreign materials, and protective coatings with enhanced tribological and bonding properties [30, 89, 94, 151, 161, 189, 190].

*Structural and mechanical properties of C-Ni nanocomposite films*

Gy. J. KOVÁCS, K. SEDLÁČKOVÁ, R. GRASIN, Zs. CZIGÁNY, G. SÁFRÁN, O. GESZTI, G. RADNÓCZI

C-Ni nanocomposite thin films were deposited by dc magnetron sputtering between 25°C and 800°C onto SiO<sub>2</sub> (300 nm thickness) covered Si substrates. Correlation was found between structure and mechanical properties of C-Ni films.

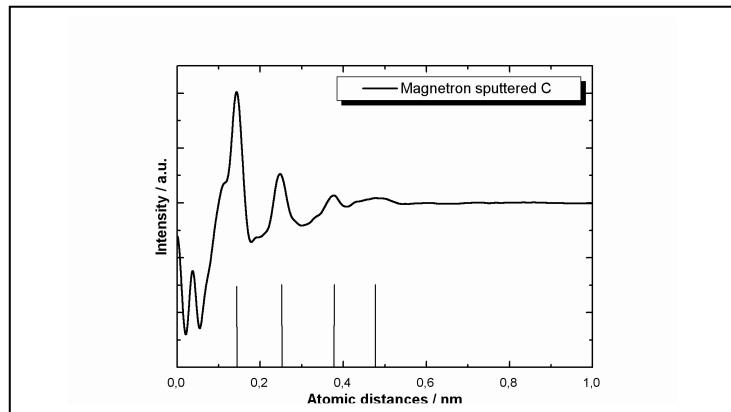


The columnar structure with Ni<sub>3</sub>C crystallites (~20 nm diameter) and 1–2 nm thick carbon matrix was characteristic for the films prepared below 400°C. HRTEM analysis of the films revealed that carbon was present in the matrix as disordered (amorphous) and graphite-like carbon. In films prepared at 600–800°C the columnar structure of Ni<sub>3</sub>C crystalline grains changed to globular Ni crystallites. The Ni grains (size ~10–100 nm) were separated by the 2–5 nm thick graphite-like carbon matrix.

The mechanical properties (hardness and elastic modulus) showed a distinct variation with the changing deposition temperature. The films prepared at 25–400°C were 9–14 GPa in hardness and had an elastic

modulus of 117–120 GPa. The observed variations can be interpreted on the basis of the structure of the films: The high values of hardness are related to the hard amorphous carbon matrix and to the columnar morphology and hardness of the Ni<sub>3</sub>C phase. The relatively low hardness of 2–4 GPa and low elastic modulus of 40–50 GPa measured on samples deposited at high temperature suggest that the soft graphite-like behaviour becomes dominant [161].

From the diffraction pattern of amorphous carbon samples using the Process Diffraction program we determined the pair correlation function ( $G(r)$ ) and the normalized pair correlation function ( $g(r)$ ) which gives the distribution of the atomic distances in the material.

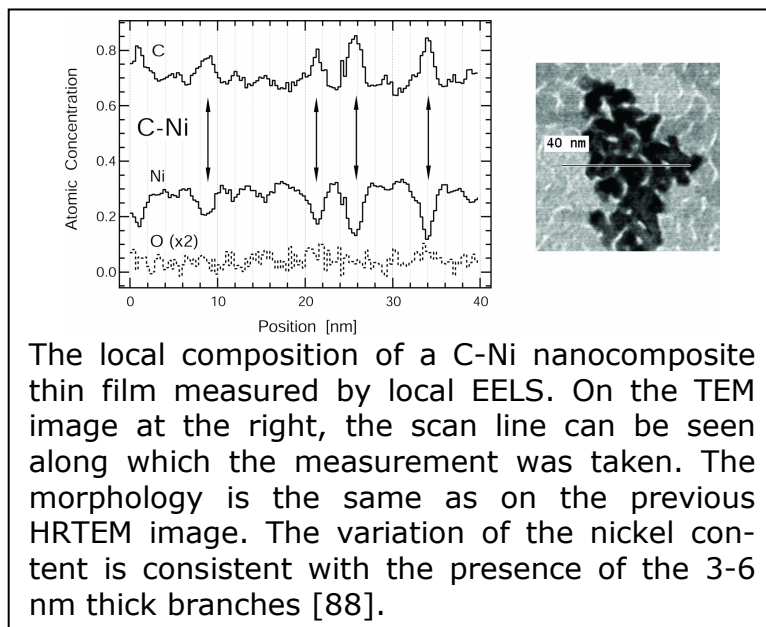


### *Spectroscopic properties of C-Ni and CN<sub>x</sub>-Ni nanocomposite thin films*

Gy. J. KOVÁCS, A. KOÓS, G. RADNÓCZI

(in cooperation with MTA SZFKI – M. Veres

– and with CEMES-CNRS, France – G. Bertoni, V. Serin, C. Colliex)



The local composition of a C-Ni nanocomposite thin film measured by local EELS. On the TEM image at the right, the scan line can be seen along which the measurement was taken. The morphology is the same as on the previous HRTEM image. The variation of the nickel content is consistent with the presence of the 3-6 nm thick branches [88].

Scanning tunneling microscopy / spectroscopy (STM/STS) investigations were taken to explore the electric properties of the surface. Despite the presence of nickel in the nanocomposite, metallic conductivity can be hardly found on the surface. Graphitic (zero band gap semiconductor type) and semiconductor type conductivity with 1-2 eV band gap are characteristic for the films.

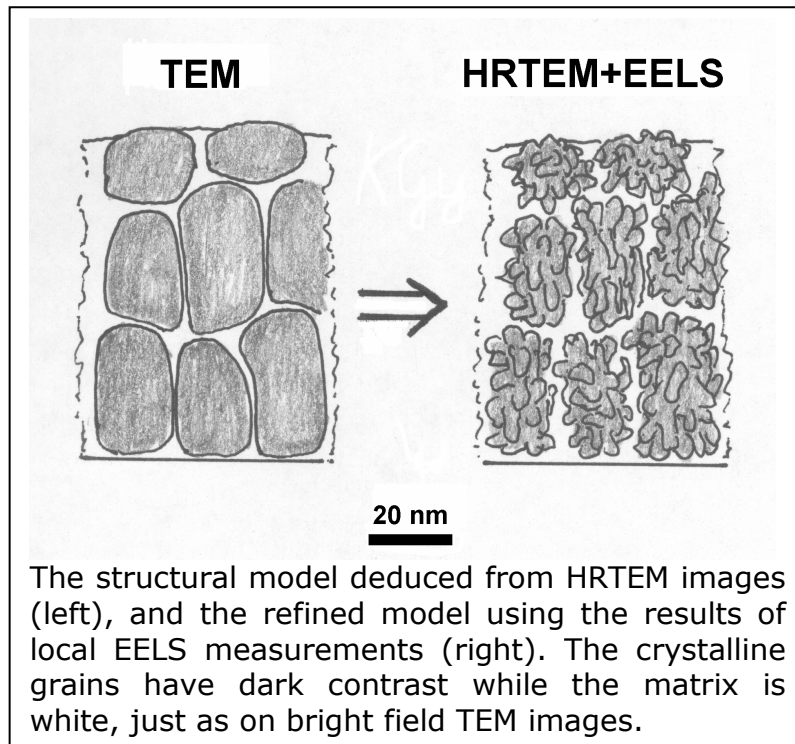
The comparison with

other, pure nickel, pure carbon and pure carbon-nitride films shows that the graphitic type conductivity arises from the amorphous C/CN<sub>x</sub> matrix, while the semiconductor type conductivity can arise from the fullerene-like shells of the matrix and from the uncovered top of oxidized Ni particles [89].

Local EELS measurements (on samples grown at low deposition temperatures up to 200°C) revealed the composition of the matrix and the crystalline dispersed phase. These measurements were extremely important to clarify the real structure of the nanocomposite films, completing our structural model based on the TEM investigations. Previously, from the TEM images we concluded that the films grown at low temperatures have a simple, regular columnar structure, where the columns are 20 nm in diameter, 50-100 nm in height, and are separated by 1-2 nm thin layers of the matrix. This model was in contradiction with both the global and local compositions measured by EDS and EELS. The contradiction was successfully eliminated by a refined model, where the columns have a finer spatial structure. The crystallites form elongated tree-like grains, with 3-6 nm wide branches. The

branches are separated by  $\sim 1$  nm thin layers of the matrix. Further EELS investigations are in progress on samples grown at higher temperatures [89].

Raman spectroscopy has proven to be effective in tracing the structural changes of the matrix with the changing deposition temperature. The  $1000 - 1700 \text{ cm}^{-1}$  range of the spectra can be interpreted just as in the case of graphite-like amorphous carbon films. This range consists of a D peak around  $1350 \text{ cm}^{-1}$  and a G peak around  $1580 \text{ cm}^{-1}$ . With the increasing deposition temperature both the significant shift of the D peak to lower wavelength and the increasing relative amplitude of the D peak show the increased ordering of the matrix. These changes in the spectra are due to the increasing number of carbon six-rings, and due to the increasing size of the coherent clusters composed from the six-rings. Another interesting part of the spectra is the band between  $2000$  and  $2300 \text{ cm}^{-1}$ . This band is related to the sp bonded nitrogen in the matrix. The band disappears with increasing deposition temperature despite that a measurable fraction of nitrogen remains in the film. We expect that local EELS will give the answer.



**Hybrid Substrates for Mass Production of  
High Frequency Electronics, HYPHEN  
(FP6 IST 027455)**

B. PÉCZ, L. TÓTH, L. DOBOS, F. RIESZ, Gy. Z. RADNÓCZI

This project started effectively in October 2005. The goal of the project is to prepare hybrid substrates like single crystalline Si, or SiC layers on polycrystalline SiC substrate. The substrates will be prepared by smart cut and wafer bonding technologies. High quality GaN layer will be grown onto the hybrid substrates and devices will be prepared. MFA does throughout characterisation of the substrates and epitaxial layers in the project.

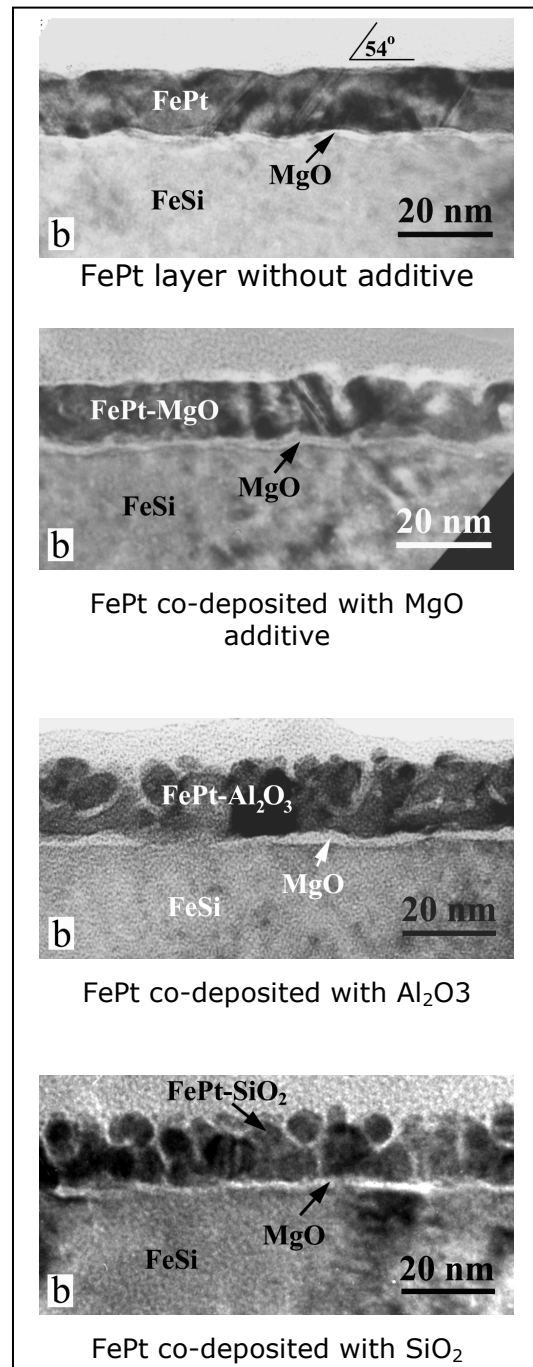
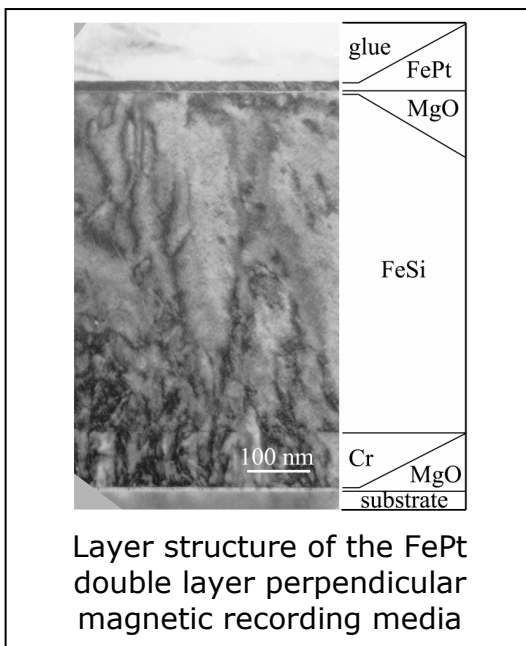
**Nano-structure formation in perpendicular magnetic recording media (MFA-AIT Consignment Agreement for Research)**

G. SÁFRÁN, T. SUZUKI\*, J. ARIAKE\*, N. HONDA\*, K. OUCHI\*, O. GESZTI, P. B. BARNA and G. RADNÓCZI

\*Akita Research Institute of Advanced Technology (AIT), 4-21 Sanuki, Araya, Akita 010-1623, Japan

Perpendicular magnetic recording (PMR) media promising Tbit/in<sup>2</sup> storage densities in computer hard disks appeared on the market right now (2005, Toshiba, Showa Denko). In a co-operation with AIT, we studied the formation of thin nanostructures of FePt PMR media prepared with MgO, Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> additives. Samples were deposited by magnetron sputtering on sapphire with a layer sequence of / MgO seed-layer/ Cr under-layer/ FeSi soft magnetic under-layer/ MgO intermediate layer/ FePt-oxide recording layer/. The effects of MgO, Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> additives on the morphology and orientation of the FePt layer were investigated by TEM. The samples exhibited (001) orientation of the L1<sub>0</sub> FePt phase with the mutual orientations of sapphire substrate// MgO (100) [001]//Cr (100)[1-10] // FeSi(100)[1-10]// MgO (100)[001]// FePt (001)[100]. The morphology of the FePt films varied due to the co-deposited oxides: The FePt layers were continuous and segmented by stacking faults aligned at 54° to the surface.

In the MgO-added samples, both components (FePt and MgO) were grown epitaxially on the MgO intermediate



layer, so that a nano-composite of intercalated (001) FePt and (001) MgO was formed.

Al<sub>2</sub>O<sub>3</sub> addition resulted in a layered structure, ie. an initial continuous epitaxial FePt layer covered by a secondary layer of FePt-Al<sub>2</sub>O<sub>3</sub> composite.

Films with SiO<sub>2</sub> addition, beside the oriented columnar FePt grains, exhibited a fraction of misoriented crystallites due to random secondary nucleation.

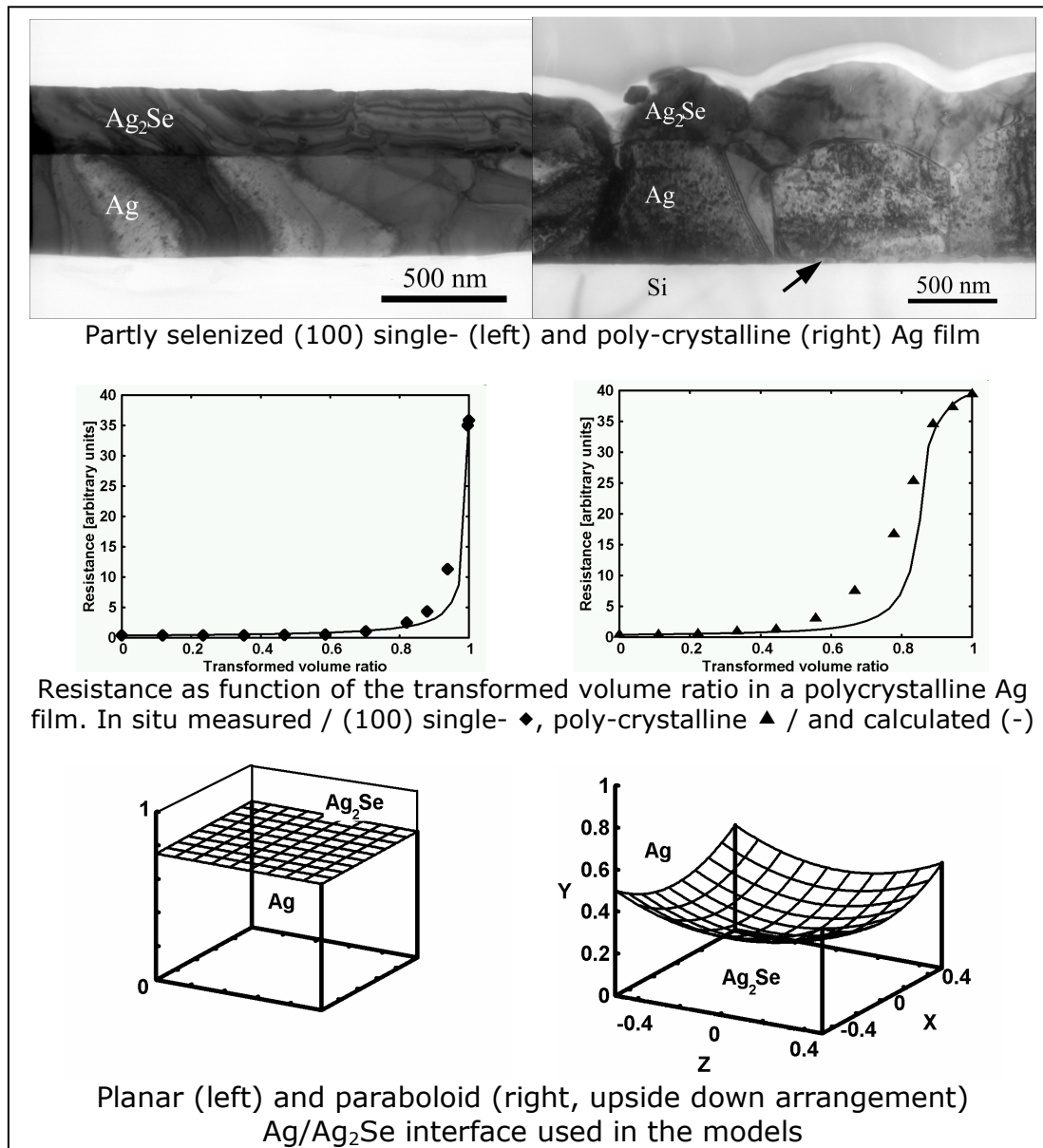
The revealed microstructures and formation mechanisms may facilitate the improvement of the structural and magnetic properties of the FePt-oxide composite perpendicular magnetic recording media.

**Formation of oriented ionic-conductors and  
semiconductors on non-oriented substrates  
(OTKA T035270)**

G. SÁFRÁN, P. PANINE\*, Gy. J. KOVÁCS, O. GESZTI

\*Laboratoire de Spectrométrie Physique Groupe RMN/P B.P. 87 F 38402 Saint Martin d'Hères CEDEX France

Superionic and semiconductor compound thin films were studied within the



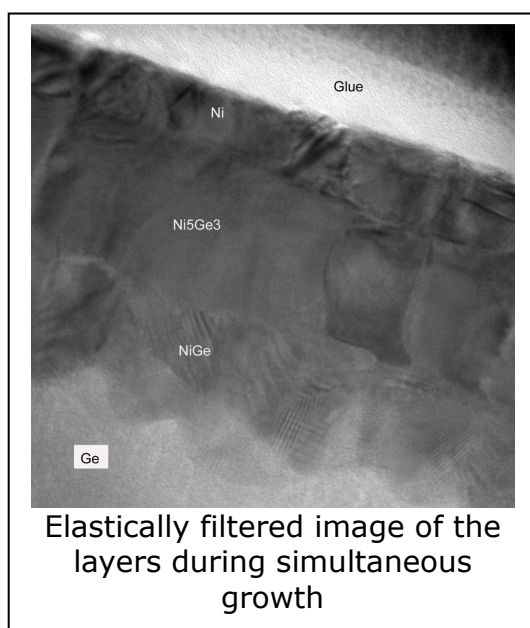
project. CdSe, CdTe and ZnSe can be applied for photovoltaic purposes, while  $\text{Ag}_2\text{Se}$ , due to its linear GMR properties, for magnetic field sensors. The structure forming mechanism was studied in subsequently vacuum deposited single crystalline (SC) and polycrystalline Ag film and Se by TEM, in situ electrical measurements and computer simulation. The influences of crystal defects were revealed during the reaction process.  $\text{Ag}_2\text{Se}$  phase starts to form at dislocations, and penetrates uniformly into (001) SC silver films. A planar interface between the metal and the compound is built up, which propagates across the film until complete selenization. In poly-Ag, however, the reaction occurs preferentially at the grain boundaries and an arch shaped interface is formed. Simultaneously, the Se diffuses along the GB-s to the substrate and reacts with the Ag there. From that stage the reaction occurs on both sides of the Ag layer until completing the selenization. The self-controlling process results in stoichiometric  $\text{Ag}_2\text{Se}$ . On cooling, (001) crystal orientation is forming due to polymorphic phase transition. The in situ electrical measurements revealed a delayed sudden increase and an early, moderate increase with an inflexion point of the electrical resistance vs. deposited Se thickness curves in single- and polycrystalline Ag, respectively. Substituting electrical circuits and numerical calculations were applied for modelling the evolution of the electrical resistance during selenization. The calculations reproduce well the electrical and TEM results. The revealed formation mechanisms contribute the tailoring of the properties of thin  $\text{Ag}_2\text{Se}$  layers and may be extensible for the description of the compound phase formation in numerous two-component systems.

**Early stages of reactions between Ni and Ge**  
**(bilateral research cooperation with the Paul Cézanne University,**  
**Marseille, France)**

JL LÁBÁR, F NEMOUCHI\*, D MANGELINCK\*, C BERGMAN\* and A JAKAB

\* L2MP, Paul Cézanne University, Marseille

Ni monosilicide has just been introduced in the mass production of Si devices in 2005 as connection and interconnection by IBM. Germanide thin films are also under current interest for their use in integrated microelec-

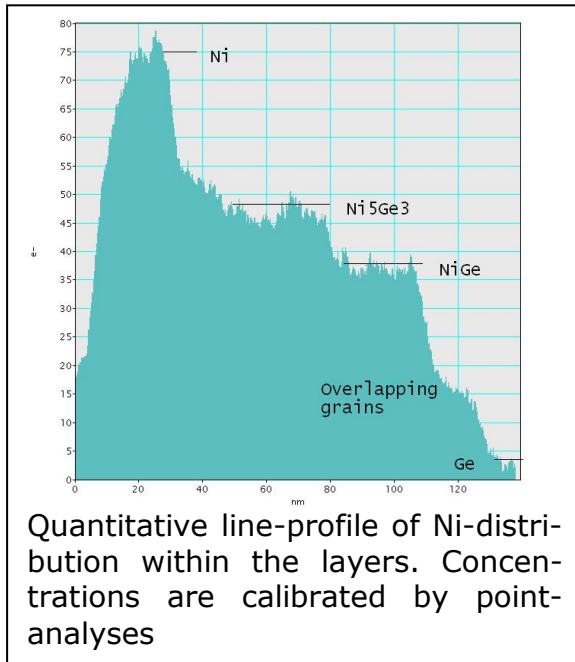


tronic devices. They are useful for low power consumption or high-speed devices as MOSFET transistors due to the high mobility of both holes and electrons in germanium. Thin film germanide reactions are often declared to be the same as silicide reactions that were far more studied. It is usually reported that the growth of thin film nickel germanides is sequential with two phases in the sequence: the first one is a Ni-rich phase, then the monogermanide NiGe grows. Although the available reports agree on the second and final phase (NiGe), they disagree on the first phase. Some authors report orthorhombic  $\text{Ni}_2\text{Ge}$ , while others monoclinic  $\text{Ni}_5\text{Ge}_3$  or hexagonal  $\text{Ni}_3\text{Ge}_2$ .

In order to solve the controversy and the open questions in the literature, samples, composed of a nanometric nickel film (10-50 nm) deposited on germanium substrates (both amorphous and crystalline), have been examined by both X-ray diffraction (XRD), energy filtered transmission electron microscopy (EFTEM) and electron energy loss spectrometry (EELS).

On the basis of detailed comparison of diffraction data we showed that the Ni-rich phase is  $\text{Ni}_5\text{Ge}_3$ . We also showed that all the contradictory literature data were based on practically the same experimental data, but they did not realize the problem of similar composition and diffraction patterns of several phases and attributed their measurements to only one of them.

Both an in-situ heat treatment in the TEM and ex-situ examination of separately heat treated samples proved that in contrast to the usual situation in thin films, we can observe a simultaneous formation of two phases,  $\text{Ni}_5\text{Ge}_3$  and NiGe. The phase competition continues until the (50 nm) Ni-film is to-



tally consumed. From that point NiGe is growing at the expense of  $\text{Ni}_5\text{Ge}_3$ . Simultaneous growth is rare in thin-film systems where sequential growth is generally obtained. The observed phase competition also disproves the similarity with the Ni-Si reactions.

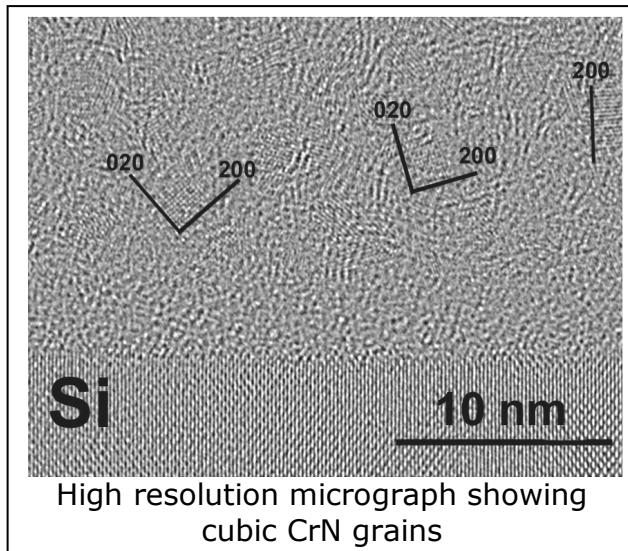
The switch from a sequential to simultaneous growth during thin film reaction might be quite important for industrial applications and especially for microelectronics. From a fundamental point of view, the difference between sequential and simultaneous growth may help to understand the phenomena that happen at the interface and that affect the kinetics.

### ***Nanocomposites for Piston/Liner Systems (EU-FP6 NMP3-CT-2003-505622)***

B. PÉCZ, L. TÓTH, É. HEGEDŰS, I. KOVÁCS

Nanocomposites coatings have been widely investigated in recent years due to their mechanical and tribological properties. Selflubricating Metal and Ceramic Matrix NanoComposites are materials consisting of a self lubricating matrix with dispersed metal or hartstoff nanoparticles. For Piston/Liner systems these particles may be a refractory metal like tungsten and chromium or a carbide or nitride of these metals. The solid lubricant would be graphite, molybdenum disulfide, h-BN. In this project Cr-B-N coatings were reactively sputtered from a  $\text{CrB}_2$  target onto Si (001) substrate at Leoben University. The main variable in this series of experiments was the nitrogen content of sputtering gas ( $\text{Ar-N}_2$ ). At low nitrogen content (3%  $\text{N}_2$ ) in the sputtering gas nanocrystalline structure was found. From the electron diffraction pattern the stable hexagonal phase of  $\text{CrB}_2$  (JCPDS 34-0369) was identified. By increasing the nitrogen (23%  $\text{N}_2$ ) according to the large magnification electron micrographs the mean crystallite size is less than 1 nm,





although an inhomogeneous, two-phase structure can be observed. High resolution electron micrographs of sample with the largest nitrogen content (68% N<sub>2</sub>) processed with high-pass filter, show several cubic CrN grains in (001) orientation. The amorphous matrix between the nanocrystals is most probably BN (see figure).

In the NAPILIS project MFA is responsible for the materials characterisation of the new coating layers. Mainly

transmission electron microscopy is applied, but also X-ray analysis is used. The task requires an intensive application of high resolution microscopy.

### ***Clay minerals in the environment***

#### ***(cooperation with the Institute for Geochemical Research)***

V KOVÁCS KIS, T NÉMETH<sup>1</sup>; P SIPOS<sup>1</sup>

<sup>1</sup>Hungarian Academy of Sciences, Institute for Geochemical Research

One of the hot topics in environmental sciences is the study of the behaviour of toxic and bioessential trace elements in soils. Adsorption capacity of the soil forming solid phases determines the distribution and migration properties of these trace elements. From this point of view, the most important inorganic soil components are clay minerals, mainly swelling clay minerals such as smectites and vermiculites. They are built up by two layers of (Si, Al)O<sub>4</sub> tetrahedra (T) with a layer of (Mg, Fe, Al)O<sub>6</sub> octahedra (O) between them. The size misfit between the T and O layers results extremely small grain/crystallite size, and the cation substitution both in the tetrahedral and octahedral layers requires charge compensation in the interlayer space to reach a chemically neutral state. These two special properties make smectites the crucial phases in adsorption processes.

In this cooperation we study the competitive adsorption of heavy metal ions (Pb<sup>2+</sup>, Cu<sup>2+</sup>, Zn<sup>2+</sup>, Ni<sup>2+</sup>) of sewage sludge on different soil clays by analytical TEM. Significant part of the sewage sludge is used in soil melioration because of its favorable mechanical properties and organic matter content, but during long term application heavy metal ions can be mobilized from the mud. The goal is to reveal how the different soils react to the increasing heavy metal ion content. The nano-mechanism of metal ion sorption and the change in site occupancy in the O layer will be studied by quantitative electron diffraction.

TEM study of soil from the maritime Antarctica also forms part of this cooperation. At this point we expect to find if there are recent weathering related to the global warming on the studied area (King George Island). TEM studies revealed such phases that are produced by chemical processes in the soil: smectites, vermiculite and halloysite, the latter one was previously unknown from antarctic soils.

### ***Growth mechanism, synthesis and microscopy of wide bandgap semiconductors (OTKA T047141)***

B. PÉCZ, Á. BARNA, J. LÁBÁR, L. TÓTH, L. DOBOS, B. VEISZ, Zs. MAKKAI, Gy. Z. RADNÓCZI, V. HEERA\*, H. WEISHART\*, W. SKORUPA\*

\*Forschungszentrum Rossendorf, Dresden, Germany

The present research subject covers the growth mechanism of wide band-gap semiconductors, silicon carbide (SiC), diamond and III-nitrides (GaN, InN and AlN), their contacts, solid phase reactions in them and the characterisation of the above structures by transmission electron microscopy.

Our goal is to synthesize new phases by ion implantation at high temperature in single crystals. As we earlier published, SiC grains can be prepared in single crystalline diamond lattice by high temperature Si ion implantation. The dose and the implantation temperature were studied by us in details. Raising the temperature from 900°C to 1000°C helps effectively the annealing out of defects and the formed SiC grains are larger. However, further increasing of the temperature is not advantageous, because that leads to the graphitization of diamond.

Nanograss like AlInN layers were characterized and a model was set up, which describes the bent crystals.

Al, Au, Ti/Al and Ti/Au contacts were deposited onto GaN and annealed up to 900°C. The annealed contacts were characterized both by electrical measurements and structural investigations by the help of X-ray diffractometry and transmission electron microscopy. We have experienced and explained that the electrical parameters of the as-deposited Ti/Al contacts are different from the parameters of the as-deposited Ti/Au contacts.

### ***Atomic arrangement in soot: carbon nanostructure of environmental interest (cooperation with the University of Veszprém)***

V KOVÁCS KIS, J LÁBÁR, M PÓSFAI<sup>1</sup>

<sup>1</sup>University of Veszprém, Department of Earth and Environmental Sciences

Soot, as the strongest absorbent of shortwave radiation in the atmosphere, has a strong influence on the radiation balance of the Earth. In order to be able to assess the optical properties of atmospheric soot, detailed information on its structure is required. The widely accepted structural model for soot assumes the presence of graphene sheets that consist of a net of hexagons formed by carbon atoms, as in graphite. The stacking of concentrically wrapped, curved graphene sheets results in a typical onion-like structure. However, it has long been known from bulk spectroscopic studies that soot formation involves the growth of layers from aromatic rings, and that soot contains other elements besides carbon.

In this cooperation we studied the structure of atmospheric soot using electron-diffraction-based pair distribution function (PDF) analysis, and compared it with other carbon structures. The atomic distances in soot differ from those in graphite in two notable aspects. First-neighbour atomic distances are as small as 0.134 nm, much shorter than in graphite or in amor-

phous carbon, and suggest the occurrence of a significant amount of small-sized aromatic clusters with a high molar ratio of hydrogen. Furthermore, the measurements provide evidence for the presence of five-membered rings as well. Aromatic components can strongly influence the optical properties of soot particles, whereas the presence of five-membered rings induces the curved nanostructure.

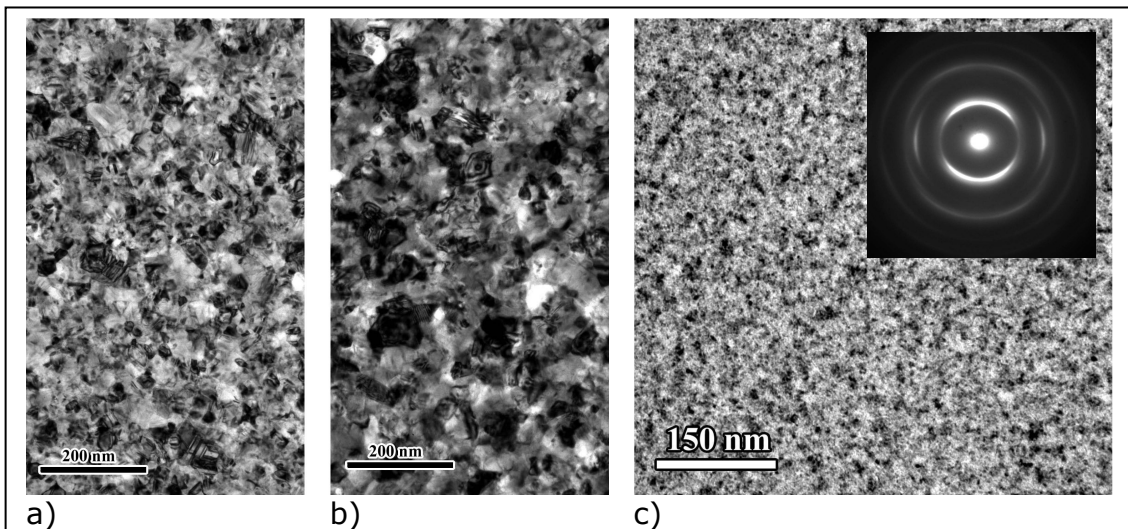
***Effect of additives on the structure formation of polycrystalline Copper films***

F. MISJÁK, P.B. BARNA, G. RADNÓCZI

Understanding the promoting or inhibiting effect of surfactant adatoms on thin film growth is important because it may provide a new route for controlling thin film deposition processes, contribute to the understanding of metal-metal nanocomposite layers and enable better engineering of the structure on atomic level. Recently we have investigated the influence of In or Ag as surfactant and oxygen as inhibitor on the structure evolution of vapour-deposited Cu films.

The films were prepared at pressures of  $10^{-5}$  and  $10^{-6}$  mbar oxygen partial pressure at 25 and 180°C substrate temperatures ( $T_s$ ) either on amorphous C films or on cleaved NaCl and Si substrates. Cu and the metallic additives were co-deposited by applying thermally heated tungsten evaporation sources.

In Cu films, grown with In addition, In and oxygen from the residual atmosphere play role in the morphological development of the layers. In acts as a promoter (surfactant), oxygen is an inhibitor. The interplay of the two additives in the development of the morphology and texture as a function of their quantities has been investigated.



a)

b)

c)

Fig. 1:

TEM images of 38 nm thick Cu films prepared on NaCl substrates in  $5 \times 10^{-6}$  mbar.

a) undoped Cu film deposited at 180 °C

b) In doped Cu film deposited at 180 °C. An increase in the grain size can be observed

c) shows a Ag-Cu nanocomposite film having a strong 111 texture

If the Cu films are grown in  $10^{-5}$ - $10^{-6}$  mbar and at  $T_s=25^\circ\text{C}$ , oxygen acts as an inhibitor and a small grain ( $20\pm 10$  nm grain size) film develops. Increasing  $T_s$  to  $180^\circ\text{C}$  leads to a larger grain size of about 40 nm in  $10^{-6}$  mbar. No texture formation is observed due to the inhibition of selection processes. The effect of In (5-10 vol%) can be detected only in  $10^{-6}$  mbar and at  $T_s=180^\circ\text{C}$  resulting in doubling of the grain size (Fig. 1.a and b). At higher In concentrations (20 vol%) a reaction between In and Cu occurs and a  $\text{Cu}_9\text{In}_4$  phase develops, with a definitely larger grain size ( $30\pm 10$  nm), compared to Cu or In doped Cu layers grown at the same ( $T_s=25^\circ\text{C}$ ) temperature. The obtained film is composed of Cu grains and a majority phase of  $\text{Cu}_9\text{In}_4$  which apparently shows smaller sensitivity to the retarding effect of oxygen than copper.

Addition of Ag to Cu instead of In leads to similar results. Ag concentrations close to the Ag-Cu eutectic composition (40at% of Ag), however, result in metal-metal nanocomposites of 5-10 nm grain size and strong 111 texture (Fig. 1c).

The Hungarian National Science Foundation (OTKA T-043437 and T048699, M-041689 and M 028154) is acknowledged for partly supporting this work.

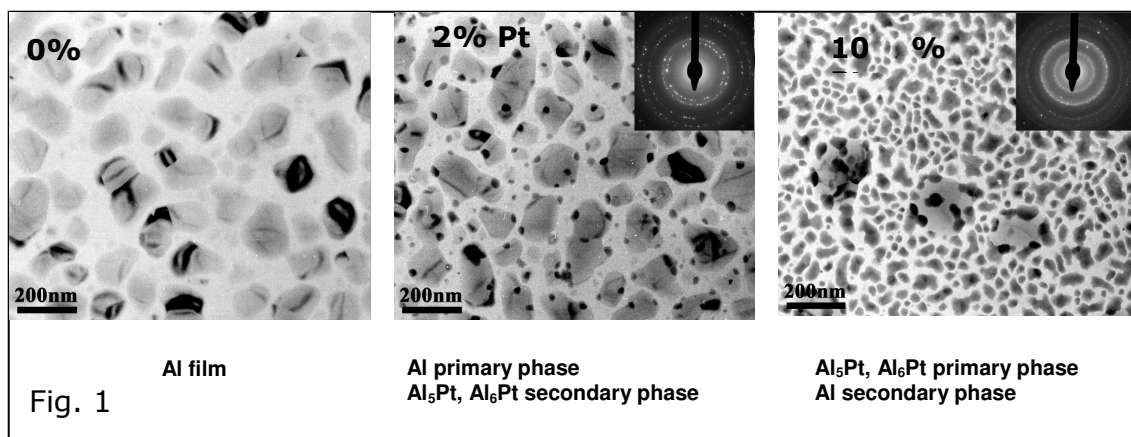
### ***Nucleation and growth of phases during co-deposition of multicomponent thin films***

A. KOVÁCS, P.B. BARNA, G. RADNÓCZI, L. SZÉKELY, A. DÉVÉNYI<sup>1</sup>, D. BIRÓ<sup>2</sup>.

<sup>1</sup>Center of Advanced Studies in Physics of Romanian Academy, Bucharest, Romania

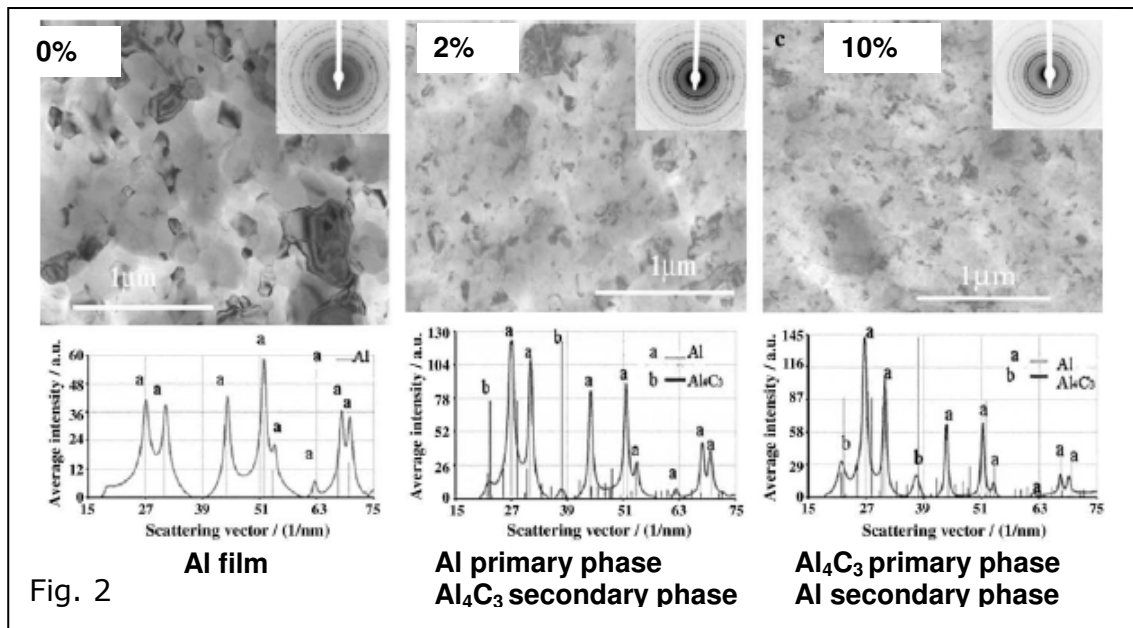
<sup>2</sup>Petru-Mayer University and Sapientia University, Tg-Mures, Romania (OTKA 048699)

Multicomponent multiphase thin films with their unique physical and chemical properties have received increasing interest during the last decades. The phases constituting these structures are determined primarily by the type and concentration of material constituents and by the methods of preparation and process parameters. By changing the concentration of material constituents one can control the nucleation sequence of phase.



Experiments revealed that both the nucleation of primary and secondary phases and the growth mode (2D or 3D) as well as the competitive growth of these phases control the pathway of structure evolution. These phenomena were investigated in the frame of that project in Al-Pt and Al-C systems. Surface chemical reactions are the means by which the condensing

species integrate themselves into the growing structure. The atomic growth processes of the phase nucleating on the substrate at the very beginning of the condensation (primary phase, primary nucleation) segregate the species which are not consumed by the building of that phase (excessive species).



This segregation results in an increased surface concentration of the excessive species leading to the formation of new phase(s) (secondary phases) on the growth surface by „delayed” nucleation. That is the stage at which the competitive growth of the primary and secondary phases starts and will control the structure evolution. These processes were investigated in co-deposited Al-Pt (Fig. 1) (Kovács A., PhD Thesis) and Al-C (Fig. 2) (Biro D., Kovács A., Székely L., Dévényi A., Barana PB., Surface and Coatings Technol., in print) systems.

***The initial states of wetting and spreading of Sn on Al surfaces: the fundamental process of the Stranski-Krastanov growth mode (OTKA 048699, Hungarian-Austrian TeT Project)***

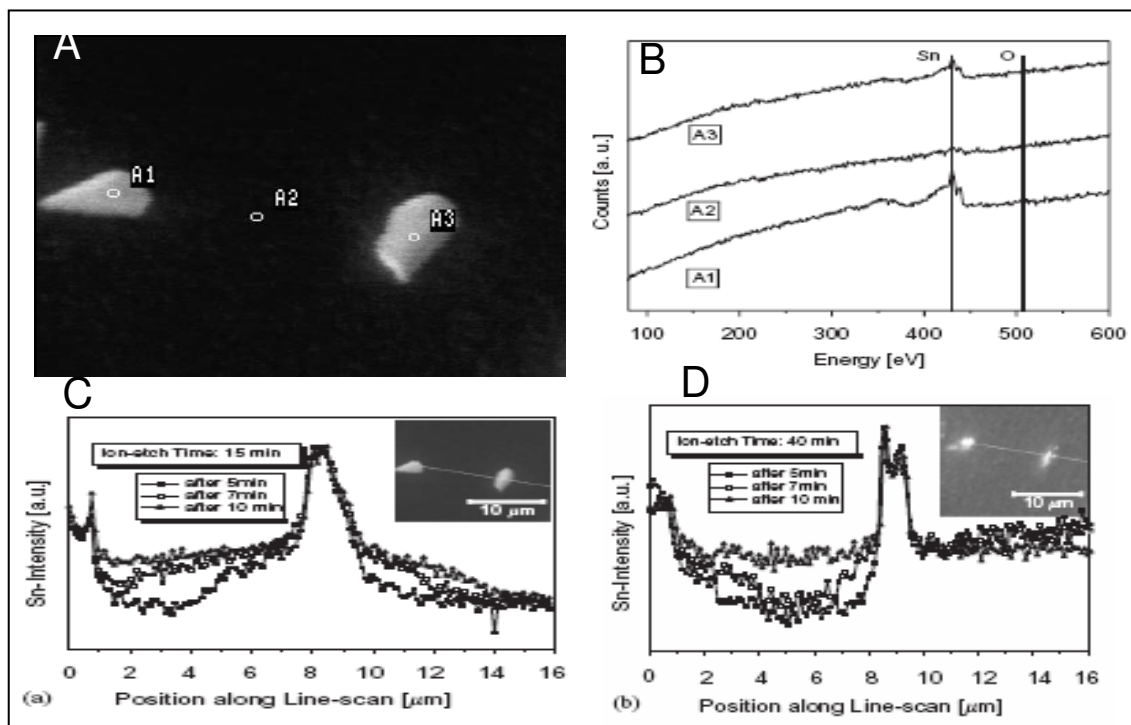
P. B. BARNA, A. KOVÁCS, E. KLEIN<sup>1</sup>, B. SCHWARZ<sup>1</sup>, C. EISENMENGER-SITTNER<sup>1</sup>, C. TOMASTIK<sup>2</sup>

<sup>1</sup>Institute für Festkörperphysik, E-138, TU, Wien, Wiedener Hauptstrasse 8-10, A-1040 Wien, Austria

<sup>2</sup>Institute für Allgemeine Physik, E-134, TU, Wien, Wiedener Hauptstrasse 8-10, A-1040 Wien, Austria

Tin (Sn) deposited on polycrystalline aluminium (Al) surfaces shows a Stranski-Krastanov growth mode which means that before Sn islands nucleate a thin Sn wetting layer is formed and could be detected between the 3D grown Sn islands. In the present work the evolution of the Sn wetting layer on the polycrystalline Al film surface has been investigated at room temperature in model experiments by scanning AES [79]. If the wetting layer developed already during the formation of an Sn film is removed from the Al surface by sputter cleaning in UHV (Figs A and B, AES point analysis) it reforms by a solid state wetting process (Figs. C and D). The sources of

the Sn atoms forming the wetting layer are in that case the Sn islands, which are not removed during sputtering from the Al surface due to their size. Nonetheless, it was observed that not every island acts as an Sn emitter (Fig. C). It is shown that this selective Sn emission is a consequence of the chemical composition and the crystallographic structure of the Sn islands. Regarding the chemical composition of the Sn islands each residual trace of oxygen has to be removed to facilitate the emission of Sn atoms from the island boundaries. In addition wetting is only initiated if the sputter cleaning process results in a visible damage of the islands, thus increasing the roughness of their surface (Fig. D). From this rough interface Sn atoms can emerge more easily than from a crystallographically smooth surface due to their lower coordination. By monitoring line scans obtained from scanning auger electron spectroscopy the diffusion coefficient of the Sn atoms could be estimated from the progress of the rim of the wetting layer around the islands.



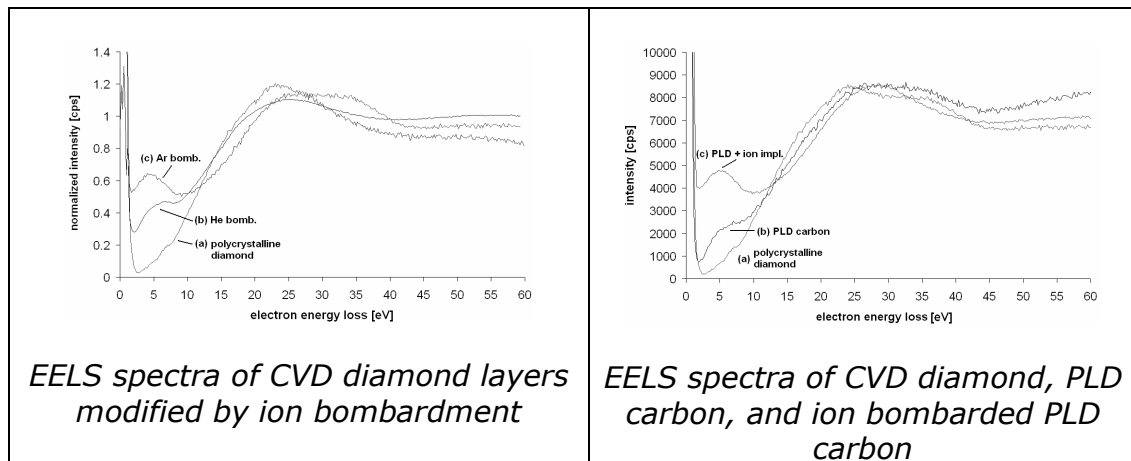
## Thin Film Nanostructures Laboratory

### **Nanostructured coatings developed by surface modification techniques (NKFP OM 00287/2002)**

G. PETŐ, A. KARACS, G. KOVÁCH

*Physical measurements on high-density nanocrystalline, protective carbon layers: an electron energy loss spectroscopy (EELS) study.*

Characterizing the amorphous carbon structures the most important parameter is the rate of graphite like ( $sp^2$ ) and diamond like ( $sp^3$ ) chemical bonds. With the help of EELS method, the  $\pi - \pi^*$  transition could be detected, which is characteristic to graphite. After ion bombardment, the intensity of the  $\pi - \pi^*$  peak increased as it can be seen in the figures. Parallel with the enhancement of the  $\pi - \pi^*$  peak, the colour of the samples changed and their resistivity decreased indicating a more graphitic like character. The ion bombardment, following deposition, is advantageous for layer adhesion and for stress decreasing inside the carbon layer. The optimal features of carbon protective film could be achieved in case of 170°C substrate temperature and low self implantation during laser ablation [34, 88].



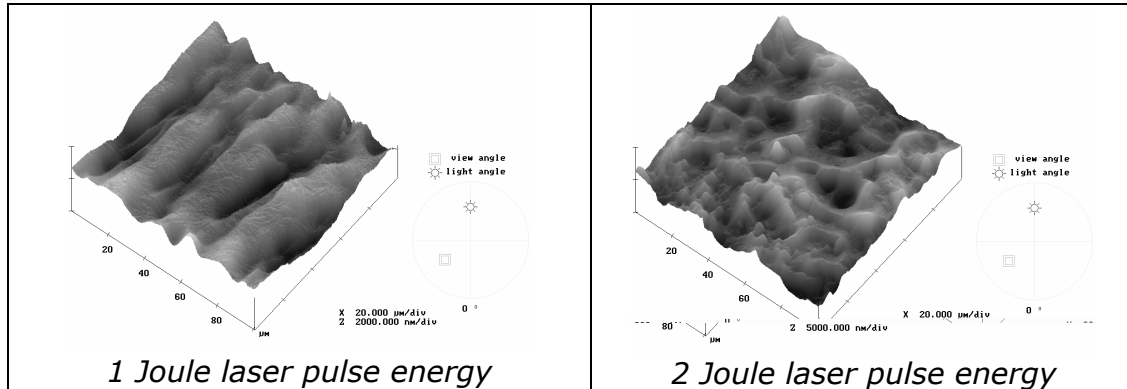
### **Development and application of functionalized interfaces in specified biochemical and chemical systems (NKFP 3/A 058-04/200)**

G. PETŐ, A. KARACS, T. HORÁNYI, G. MOLNÁR

*Surface morphology modification of Ti model materials by pulsed laser shots.*

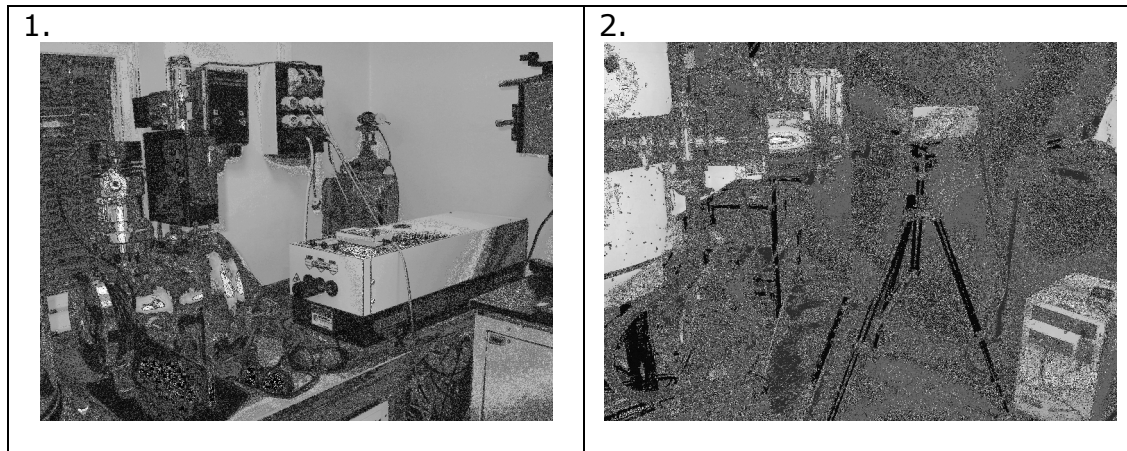
A new method was elaborated for surface treatment of titanium implant materials, which resulted more homogenous and engineered morphology. This new procedure essentially means grazing incidence pulsed laser shots, where the focused laser beam hits the Ti surface between 15-25° angles. The plasma cloud, which appeared as a consequence of the laser-matter interactions, is blown away by the light from the site of the beam incidence. In contrast to the conventional perpendicular incidence to the surface,

where the laser photons and the particles of the developing plasma were moved opposite to each other, causing uncontrollable situations. In case of 1 Joule pulse energy, by grazing incidence laser light hits, the morphology of Ti substrate became similar to a rippling water surface, or laminar flow, according to our experimental observations. While, the Ti surface morphology was similar to turbulent flow or rough hills at 2 Joule laser pulse energy (see AFM images.)



**Installation of new movable laser systems  
(GVOP-3.2.1.-2004-04-0320/3.0)**

G. PETŐ, A. KARACS, G. KOVÁCH, G. MOLNÁR



Two Nd/YAG lasers were installed in 2005 in our laboratory. The bigger one has 1600mJ/pulse energy at 1064 nm, with second harmonic (532 nm) and third harmonic (355 nm) generators. The smaller one has 800 mJ/pulse at 1064 nm, and it can be moved easily between the vacuum chambers.

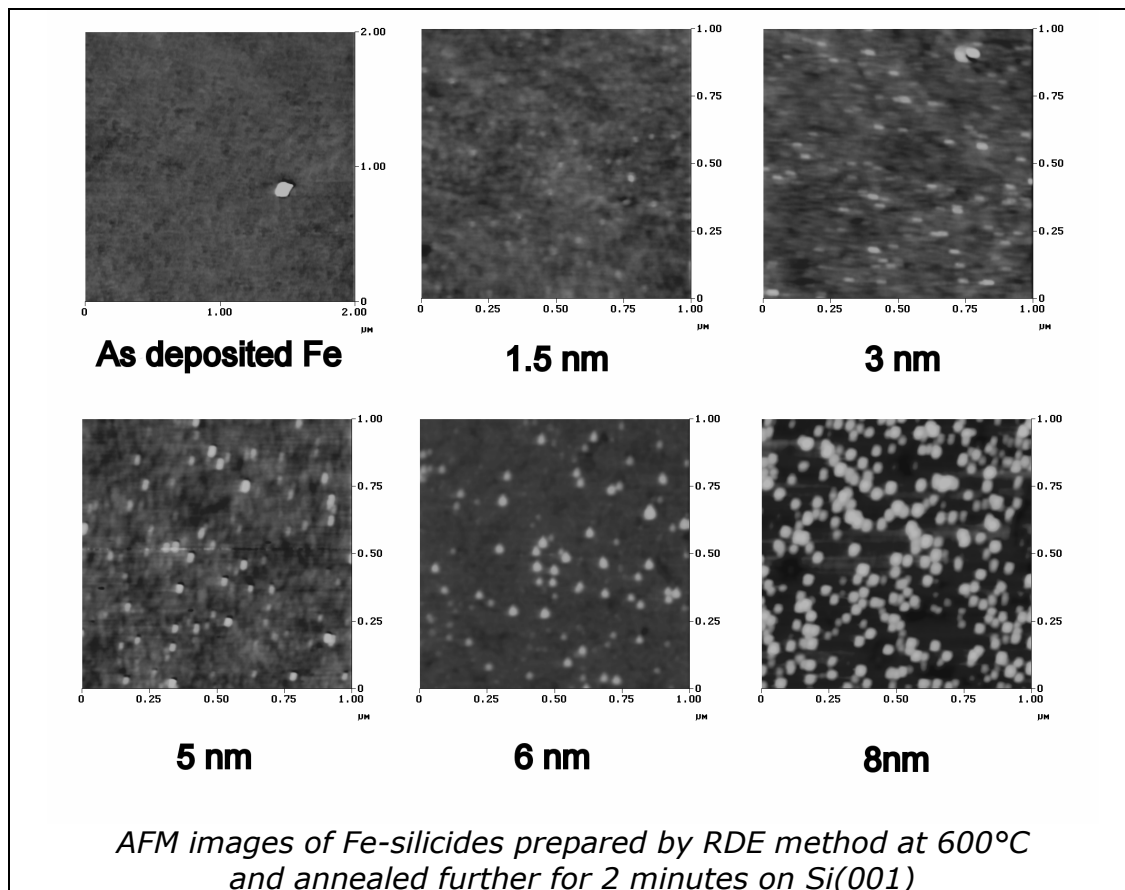
**Investigation of noise and electric parameters of  
quantum structures  
(Hungarian-Greek Intergovernmental  
S&T Cooperation program for 2005-2006)**

L. DÓZSA, G. MOLNÁR, Zs.J. HORVÁTH

Iron-silicides were grown on Si by reactive deposition epitaxy (RDE) method on Si(001). Silicides were investigated by electron microscopy, atomic force microscopy, and by infrared reflectance measurement. Self-assembled, is-



land like, oriented  $\beta$ -FeSi<sub>2</sub>,  $\alpha$ -FeSi<sub>2</sub> and  $\gamma$ -FeSi<sub>2</sub> were found to grow on Si(001) substrates. The properties of the reacted films were investigated first as a function of the thickness at the same short time annealing. After the RDE deposition of iron films onto Si(001) kept at 600°C and annealed further for 2 minutes dots are seen in the AFM images.



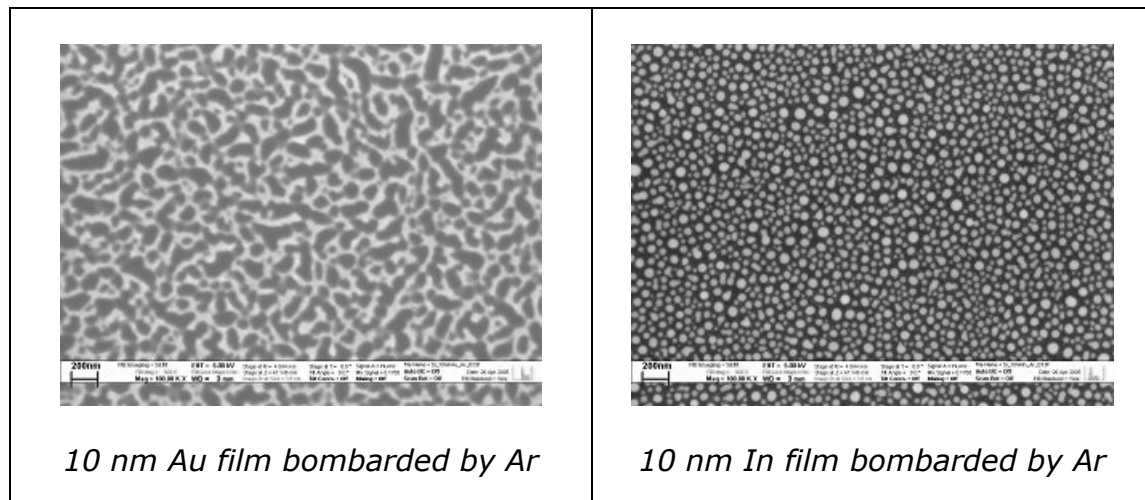
The density of islands increased with the growing thickness, but it was not a linear function of the available amount of Fe. Around 6 nm evaporated Fe thickness, should have been a critical thickness, above, the number of islands suddenly enhanced. These islands are randomly distributed on the surface of the Si(001) substrate. The typical size of an island was in the 20-50 nm range [113, 200, 201].

***Formation of metal nanoparticles and investigation of their electronic structure and catalytic features (Cooperation with the Chemical Research Center, Budapest)***

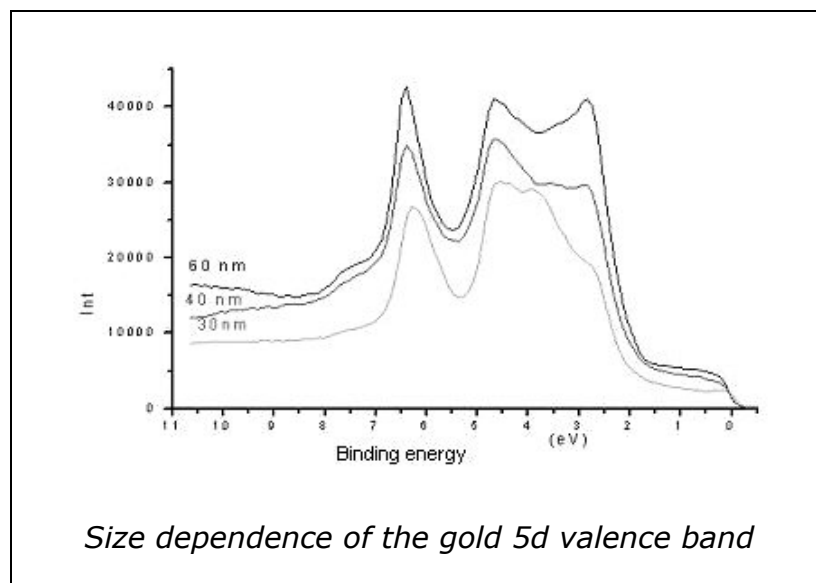
G. PETŐ, A. SZANYÓ, Zs. BAJI

Gold and indium layers were deposited onto native oxide covered Si(001) substrates. The samples were bombarded by Ne, Ar, Kr, and P ions at the same energy and dose, to investigate the effect of ion mass on the surface morphology of the metal films. The motivation of these experiments was to understand the effect of energetic ions on the formation of metal nanoparticles, which objects are useful in catalytic processes.

The samples were measured by SEM and UPS/XPS. As can be seen in SEM images, gold films suffered structural modifications from ion bombardment. While, indium layers melted into nanosized spheres as a consequence of their low melting point, during ion implantation.



The size dependent properties of the valence band of gold were investigated by UPS, since its resolution is quite good in this energy interval. The size dependence of Au 5d valence bands can be seen in the next figure. The line indicated "60 nm" can be regarded as a bulk state. The shape of 5d peak changed with decreasing Au thickness, and a new peak at 4 eV appeared.



## Microtechnology Department

<b>MEMS Laboratory</b>	<b>Laboratory of Optoelectronic Devices</b>	<b>Semiconductor Characterization Laboratory</b>
<p><b>Head:</b> Csaba DÜCSŐ, Ph.D.</p> <p><b>Staff:</b> György ALTMANN, technician Mária ÁDÁM István BÁRSONY, D.Sc. Ferenc BELEZNAY, D.Sc. Ábel DEBRECZENY Magdolna ERŐS, technician Csilla FARAGÓ, technician János FERENCZ, M.Sc., engineer Péter FÜRJES, Ph.D. Tamás, JÁSZI Alajos GONDOS, technician Ákos MAJOROS, engineer Attila NAGY, technician Margit PAJER, technician Edit Andrea PAP, Ph.D. dr. Imre SZABÓ, engineer Éva VÁZSONYI, research fellow János VOLK, Ph.D.</p>	<p><b>Head:</b> Béla SZENTPÁLI, Ph.D.</p> <p><b>Staff:</b> Olga KRAFCSIK Homokiné Ph.D., part time Zoltán LÁBADI, Ph.D. Ákos NEMCSICS, Ph.D., part time István PINTÉR, Ph.D. Bálint PÖDÖR, Ph.D., part time dr. Sándor PÜSPÖKI engineer Vilmos RAKOVICS, Ph.D. István RÉTI engineer Ms. Ferenc VARGA technician Ms. Katalin VÖRÖS Veresné engineer</p> <p><b>PhD Students (Advisor):</b> Edvárd Bálint KUTHI (Béla Szentpáli) Ágoston NÉMETH (Zoltán Lábadi)</p> <p><b>Engineering trainee (Advisor):</b> Géza LACZKOVICH (Béla Szentpáli)</p>	<p><b>Head:</b> Gábor BATTISTIG, Ph.D.</p> <p><b>Staff:</b> Edvard BADALJAN engineer László DÓZSA, Ph.D. Tibor EPPICH Konrád, engineer Zoltán HAJNAL, Ph.D. Zsolt J. HORVÁTH, Ph.D. Nguyen Q. KHÁNH, Ph.D. Zsuzsa PÜSPÖKI engineer András STER Vo Van TUYEN, Ph.D. (on leave) József WAIZINGER engineer Zsolt ZOLNAI, Ph.D.</p> <p><b>PhD Students:</b> Péter BASA Anita PONGRÁCZ Péter SZÖLLŐSI</p>

## MEMS Laboratory

### **Development of force sensor structures**

*Robust force sensor chip for industrial application (OM support, "FORCESEN" project)*

Mária ÁDÁM, Csaba DÜCSŐ, Péter FÜRJES

The 18 month project started in April 2004, aims at the development of discrete force sensors for automotive and precision instrument industry. On the basis of the preliminary technology tests and model calculations, Si chips of the specified functionality were designed and processed in 2005.

Due to the required high operational temperature (160°C), conventional p+ diffused resistors isolated by *pn* junctions can not be considered for the formation of the piezoresistor bridges. Therefore, MESA-like poly-crystalline silicon resistors isolated by thermally grown SiO<sub>2</sub> layers were fabricated on the top of the alkaline etched membranes. Beside the appropriate geometric design of the single crystalline Si membranes going to be exposed to a point-like load in the final device, the main effort was put into the selection of the optimum material properties of the poly-crystalline Si resistors. The doping level and crystallite size not only determines the sensitivity of the sensor, but their effects on temperature dependence of the resistivity and the sensitivity had to be considered as well. The final version of the sensor chips were fabricated by the end of the project.

*Micro-force sensor with increased shear sensitivity (follow-up research of the Széchenyi-NKFP "TELESENSE" project)*

Mária ÁDÁM, Csaba DÜCSŐ, Éva VÁZSONYI

Silicon based three-dimensional (3D) force sensor was designed and fabricated for detection of normal and shear forces. The mono-block sensor chip contains a rectangular Si rod emerging out of the centre of the membrane. The technology involves ion-implanted piezoresistor formation on the back

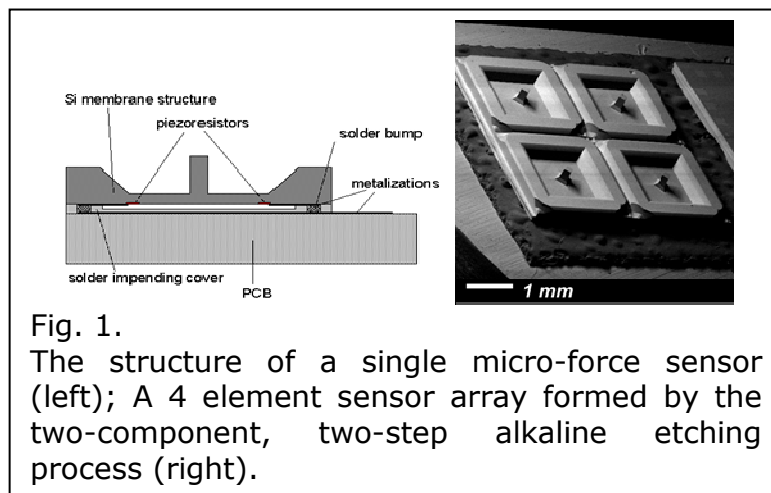


Fig. 1.

The structure of a single micro-force sensor (left); A 4 element sensor array formed by the two-component, two-step alkaline etching process (right).

side and a novel anisotropic etching on the front side of an n-type wafer. The novel two-component, two-step anisotropic etching process forms the rectangular side wall rod and the membrane simultaneously, using a double layer silicon oxide and nitride mask. A mask-less alkaline etching in the second step results in the central rod protruding over the chip surface while leaving a frame of reduced thickness around the membrane in order to pro-

vide mechanical stability (Fig. 1.). The cavity underneath the membrane is formed by bonding, facilitating also the signal read-out from the ion-implanted strain gauge resistors at the bottom (backside) of the membrane. The results of the mechanical test of the realised 3D Si force sensors show good fit to the theoretical predictions.

*Integrated micro-force sensor array (follow-up research of the Széchenyi-NKFP "TELESENSE" project)*

Mária ÁDÁM, István BÁRSONY, Csaba DÜCSŐ, Péter JÓNÁS (SZTAKI), Tibor MOHÁCSY, Éva VÁZSONYI

The major goal of the project is the integration of porous Si micromachining technique into conventional CMOS processing technology. Elaboration of a reliable method may open new routes in design and manufacturing of monolithically integrated smart sensors with embedded 3D elements. According to our best knowledge, no proposals for combination of porous Si micromachining and CMOS process have been presented so far.

In our demonstration device an integrated CMOS decoder provides the sequential read-out of the 8x8 element 3D micro-force sensor (see MFA yearbook, 2004), each consists of 4 resistors and their reference transistor pairs. All the 8 lines are powered by dedicated current generators also integrated on the chip.

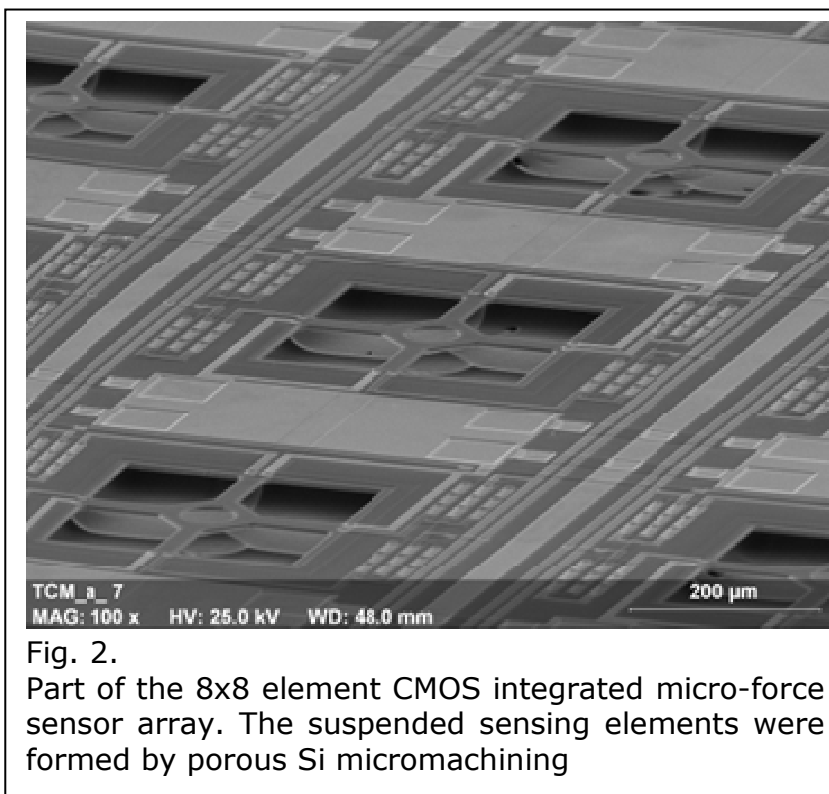


Fig. 2.

Part of the 8x8 element CMOS integrated micro-force sensor array. The suspended sensing elements were formed by porous Si micromachining

The main processing steps were developed and alternative processing sequences were investigated in 2005. Although the applied 11 mask, 2 metal, 5 $\mu$ m, n-well CMOS process represents an old generation of IC manufacturing, it clearly demonstrates the feasibility of the combined technology. As the main technical barriers against the integration of the 3D porous Si processing

do not depend on the feature size of the CMOS circuit, a proven method can directly be introduced into a more complex, multilevel, submicron CMOS process.

The final electrical and functional tests of the fabricated array-chip will be accomplished by the appearance of the present yearbook. Part of the manufactured 8x8 taxel element chip is shown in Fig. 2.

## **Development of novel methods in Si micromachining (OTKA TO47002)**

### *Micro-membranes from porous Si multilayers*

Csaba DÜCSŐ, István TAKÁCS (BME)

Porous Si double layers of high difference in their porosity, i.e. low porosity top-layer and high porosity layer underneath can be transformed into a closed membrane by appropriate vacuum and heat treatment in combination with a followed up epitaxial Si layer deposition.

Taking the existing technology of MFA into consideration, we have started the elaboration of a modified process what enables us to form closed membrane and micro-fluidic channels. The final target is the fabrication of an integrated miniature pressure sensor for in vivo medical application. In order to define the appropriate process parameters required for the structural rearrangement we have investigated various combinations of vacuum treatments, annealing processes in reductive atmosphere and poly-crystalline Si or Si<sub>3</sub>N<sub>4</sub> depositions (Fig. 3.)

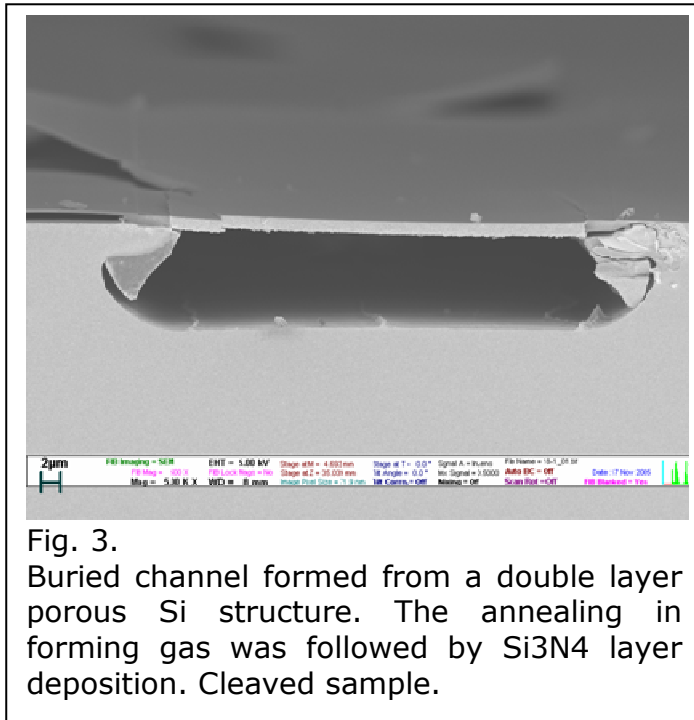


Fig. 3.

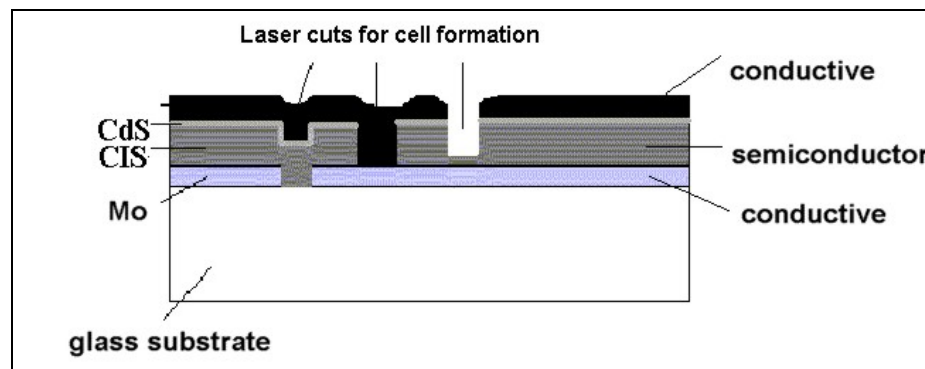
Buried channel formed from a double layer porous Si structure. The annealing in forming gas was followed by Si<sub>3</sub>N<sub>4</sub> layer deposition. Cleaved sample.

## Laboratory of Optoelectronic Devices

### **Solar Cell Innovation Center (NKFP 3/025/2001)**

Zoltán LÁBADI, Ágoston NÉMETH, Sándor PÜSPÖKI, Vilmos RAKOVICS, Ákos NEMCSICS, István RÉTI, Béla SZENTPÁLI, Ferencné VARGA, Katalin VÖRÖS VERESNÉ

The overall aim of the project is to develop a thin film preparation system for R&D on solar cells with CuInGaSe active layer. The consortium went through a restructuring; the MTA MFA took over the leadership. The planned solar cell structure is shown in the figure below.



In 2005 the deposition of contact layers for CIGS solar cells was researched. The purpose of the work is to develop an optimal technology for the deposition of transparent front contact layer for a CIGS solar cell. The structure consists of an undoped ZnO buffer layer and an Al doped conductive ZnO (ZAO) layer. The magnetron sputtering of the ZAO layer takes place from a Zn:Al (2% m/m) metallic target in Ar:O<sub>2</sub> atmosphere.

The technological parameters of the deposition of the ZAO layer have been studied, and the region where the suitable layer forms was established. In this technology the conductive and transparent ZnO film is deposited successfully at room temperature.

The layers are qualified by spectral transparency, sheet resistance. The specific resistance values are in the mOhmcm range.

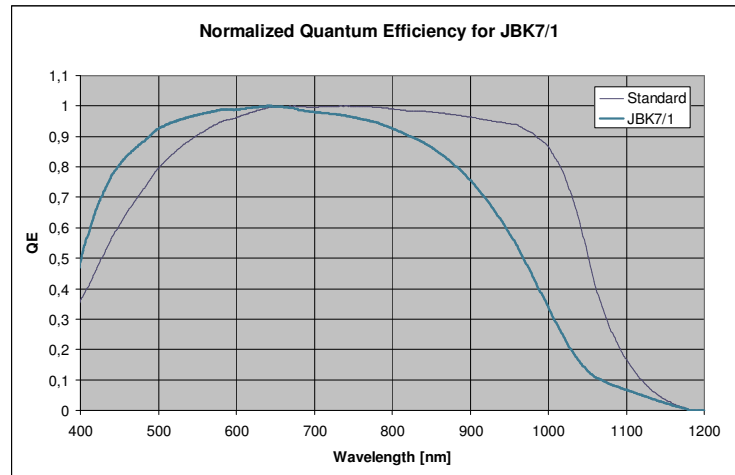
### **Indoor light cell**

Béla SZENTPÁLI, István PINTÉR, Edvard KUTHI, Csaba DÜCSŐ, Mária ÁDÁM Antalné, Zoltán LÁBADI, Ágoston NÉMETH, Vilmos RAKOVICS, Tibor MOHÁCSY

The aim of the project is to develop „solar cells” optimised for indoor lighting, i.e. fluorescent light at about 700 lux intensity. The devices are planned to supply wireless indoor sensors. The project is cooperative; the partner is the Tsukuba Research Laboratory of Tateyama Kagaku Co. Ltd. (Tsukuba, Japan.)

The Plasma Immersion Ion Implantation (PIII) technology was applied for this task. This technology was developed in earlier years during the ADVOCATE (EU-FP6: ENK6-CT-2001-00562, 2001-2004) project. The PIII technique is a very low energy (100-1000eV) implantation. It is used for Phosphorous doping of the emitter of silicon solar cells. Due to the low energy

implantation and the rapid thermal annealing the emitters are very shallow (0.2...0.3  $\mu\text{m}$ ). The shallow emitter and the properly designed antireflection coating result in an enhanced efficiency at the bluish-white fluorescent light. The figure below shows comparison of the normalised efficiency of the indoor light cell structure (JBK7/1) and the usual Si solar cell.



### ***The origin of electronic noise in semiconductor sensors (OTKA T 037706)***

Béla SZENTPÁLI, Vilmos RAKOVICS, Tibor MOHÁCSY, István BÁRSONY, István RÉTI, Mária ÁDÁM Antalné

The lower limit of the sensitivity of any sensor is limited by the noise, fluctuation generated in them. The magnitude of this noise determines the dynamic range of the sensor too. Namely the maximum of the perceptible signal, which results in a proportional output signal is also limited. In 2005 the noise properties of ion-implanted resistors were investigated. These are the piezo-resistive elements in pressure sensors. This investigations are important in respect to the development of the tactile sensor in which many (in the present version 256) piezo-sensors are integrated. The Hooge-type  $1/f$  noise was found in these resistors, the value of  $\alpha$  is about  $1.5...3 \times 10^{-4}$ , which can be interpreted well with the mobility reduction due to the Coulomb scattering of dopants. The quality of the p-n junction between the B doped resistor and the n-type substrate can influence the total noise. The soft reverse characteristics occurs extra noise.

A further achievement in this project is the building up the low-frequency noise laboratory. In 2005 a new spectrum analyser and numerous preamplifiers were installed.

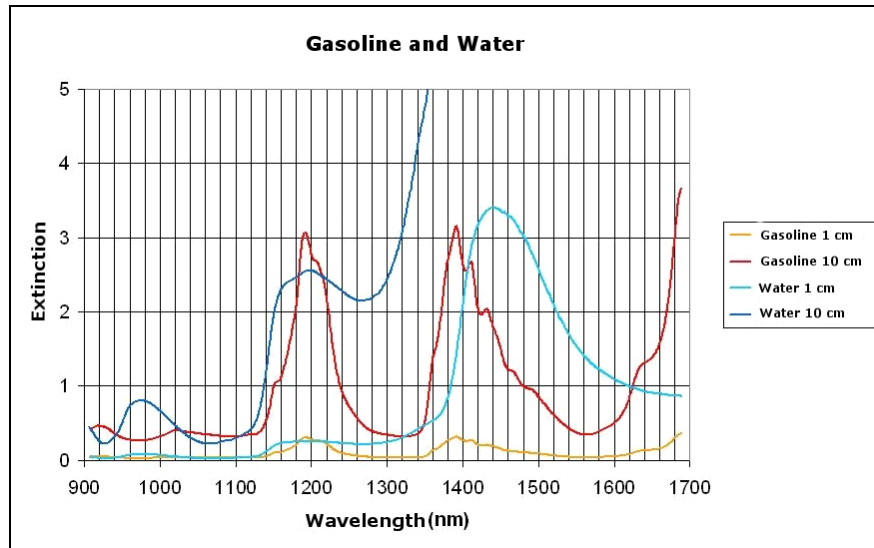
### ***Research and development of custom wavelength IR sources and detectors***

Vilmos RAKOVICS, János BALÁZS, Sándor PÜSPÖKI, István RÉTI, VARGA Ferencné (Magdi), Kati VÖRÖS Veresné

The general aim of the project is the fabrication and development of IR LEDs emitting in the 1000-1700 nm wavelength range. The devices are used mainly in portable IR spectrometers. In 2005 two projects utilized this technique.

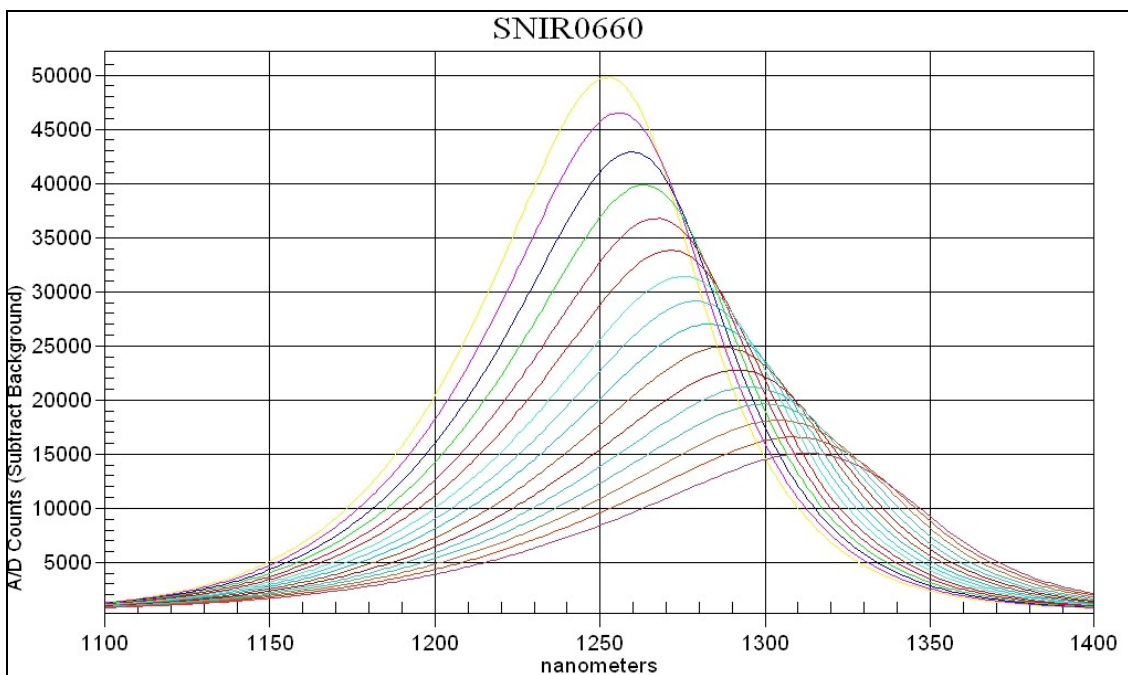


1. The AQUANAL (NKFP) project, which aims the analysis of the phreatic water in Hungary. The related task is the detection of hydrocarbons in the water by IR absorption. The figure below shows the absorption spectra of the water and the petrol as it was measured in our laboratory.



We can conclude from the absorption spectra that the detection of petrol in as received water samples is hopeless, the extraction of petrol is necessary.

2. The co-operative project with Ricola Ltd., Finland. Here the necessity of IR absorption measurement under high temperatures (oil industry) arised. The figure below shows the shift of the emitted spectra of our IR LED in the temperature range between 25 °C and 170 °C. The measurement also shows the decrease of the emitted light power. Other experiments ensured that the reliability of the LEDs remain unchanged, so - taking into account the temperature dependences shown in the figure - the devices can be used at elevated temperatures too.



**Closed Space EMC**  
**(GVOP-3.1.1.-2004-05-0354/3.0)**

Béla SZENTPÁLI, Géza LACZKOVICH

The general aim of the project is the realization of electromagnetic compatibility (EMC) test in closed space. The standard EMC investigations in the radiated frequency range (usually above 1 MHz) are performed in open air avoiding the reflections. In Hungary, there is no such measuring platform. The measurement can be fulfilled also in an anechoic chamber and/or in TEM cells. Naturally in these spaces more or less reflections are always present. Therefore the direct measurement of the radiating field is strongly recommended in the course of the EMC test.

The project is co-operative; the partner is the Bonn-Hungary Ltd. The task of the institute is the development of a field meter, which has only minimal disturbance on the field. The EMC measuring standard demands field uniformity below 6 dB. On the basis of an earlier project (AKP 96/2-604 2,3; 1997-98) a high frequency E-field probe was constructed from a resistive transmission line. In the frequency range from 300 MHz to 1 GHz this structure has a maximum reflection of about 0.4 dB. For comparison the reflection of the thinnest available coaxial cable (1.8 mm outer diameter) of the same length is 20 dB.

## Semiconductor Characterization Laboratory

### ***Physics and Technology of Elemental, Alloy and Compound Semiconductor Nanocrystals***

*(Supported by the Hungarian Scientific Research Fund under Grant No. T048696, and by the European Commission in the frame of FP6 project SEMINANO No. 505285 )*

Zsolt J. HORVÁTH, M. ÁDÁM, János BALÁZS, Péter BASA, László DOBOS, László DÓZSA, Tivadar LOHNER, György MOLNÁR, Péter PETRIK, Péter SZÖLLŐSI

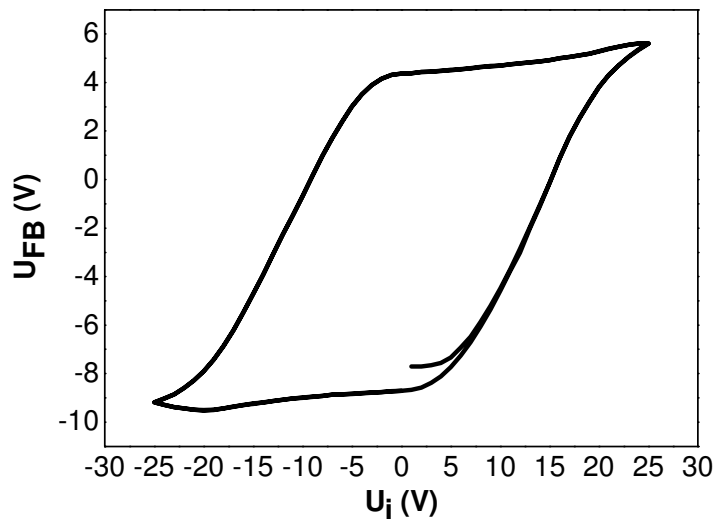
Dielectric layers with embedded semiconductor nanocrystals are studied in order to overcome difficulties of non-volatile memory devices connected with technology scale down, and to develop Si-based LEDs. One of the methods used for creating these structures is the deposition of a  $\text{SiO}_2/\text{Si}/\text{SiO}_2$  or  $\text{SiN}_x/\text{Si}/\text{SiN}_x$  thin film structure, where the nanocrystal formation takes place in the middle layer.

In this work the formation of Si nanocrystals (ncs) in sandwiched  $\text{Si}_3\text{N}_4/\text{nc-Si}/\text{Si}_3\text{N}_4$  structures, and the formation of Ge ncs in sandwiched  $\text{SiO}_2/\text{nc-Ge}/\text{SiO}_2$  layers were investigated using spectroscopic ellipsometry, cross-sectional transmission microscopy (XTEM), electron energy loss spectroscopy (EELS), atomic force microscopy (AFM), and scanning electron microscopy (SEM).

The  $\text{Si}_3\text{N}_4/\text{nc-Si}/\text{Si}_3\text{N}_4$  structures were prepared by Low Pressure Chemical Vapour Deposition (LPCVD) at 830°C on top of both 'n' and 'p' type Si substrates. The top and bottom stoichiometric silicon nitride layers were grown by at a gas flow rate of  $\text{SiH}_2\text{Cl}_2$  and  $\text{NH}_3$  of 21 and 90 sccm, while the middle nc-Si layer with a gas flow rate of  $\text{SiH}_2\text{Cl}_2$  of 100 sccm. The thickness of the bottom layer is 14-16 nm in these structures, while that of the upper layer is 30-32 nm. The duration of the deposition of the middle layer was varied which resulted in a varying thickness of the middle layer from 9 to 23 nm, as obtained by ellipsometry. A comparison of the duration of deposition with these values indicates that the growth rate was much higher during the nucleation of Si grains. The Si content of the middle layer for 1 min was 45% only, while for 3 and 5 min a nearly continuous nc-Si layer was obtained. It was found by XTEM and EELS that the deposition time of 1 min results in a discontinuous middle nc-Si layer, where Si nanocrystallites are separated from each other by the silicon nitride. This is in good agreement with spectroscopic ellipsometry measurements, which yielded 45% Si and 55%  $\text{Si}_3\text{N}_4$  content for the middle layer of this sample. In this sample, well defined Si ncs have been obtained with grain size in the range of 5-10 nm. The effect of annealing on the nanostructure of  $\text{Si}_3\text{N}_4/\text{Si}/\text{Si}_3\text{N}_4$  structures is under investigation. The electrical behavior of these structures was also examined. The best memory hysteresis curve obtained on the thinnest sample is shown in Fig. 1.

For the formation of Ge nanocrystals (nc) (001) oriented Si wafer covered by thermally grown 100 nm  $\text{SiO}_2$  layer prepared at 1100°C in dry  $\text{O}_2$ , were used as substrates. The wafers were loaded into an oil free evaporation chamber (Varian VT-460), and the system was evacuated down to  $1 \times 10^{-8}$  Torr. Ge ingot of 99.999% purity was supported on a molybdenum plate,

and it was evaporated using an electron gun, at an evaporation rate of 0.01-0.03 nm/s, at a pressure of  $1 \times 10^{-7}$  Torr. During evaporation the substrate temperature was kept at 350°C. Samples with four different nominal Ge layer thicknesses were prepared, namely: 0.6, 1.2, 1.8, and 2.4 nm. After germanium evaporation and cooling down, the wafers were cut in two parts, and the first halves of the wafers were covered by CVD SiO<sub>2</sub> with a thickness of 100 nm, grown at 430°C from SiH<sub>4</sub> and O<sub>2</sub> using N<sub>2</sub> gas carrier. The size and partial distribution of Ge nanocrystals were studied on the other halves of the wafers by atomic force microscopy (AFM) and scanning electron microscopy (SEM). The same data – and so the effect of the deposition of the covering CVD SiO<sub>2</sub> layer on Ge ncs – are under study on the first part of the wafers after the deposition of the CVD SiO<sub>2</sub> layer, by XTEM. The obtained AFM and SEM images indicate that Ge ncs have been formed on all samples during the evaporation with size of 10-30 nm.



*Fig. 1.*  
Memory hysteresis curve (the change of the flat-band voltage as a function of writing/erasing pulses with increasing/decreasing amplitude) for the thinnest Si<sub>3</sub>N<sub>4</sub>/nc-Si/Si<sub>3</sub>N<sub>4</sub> sample

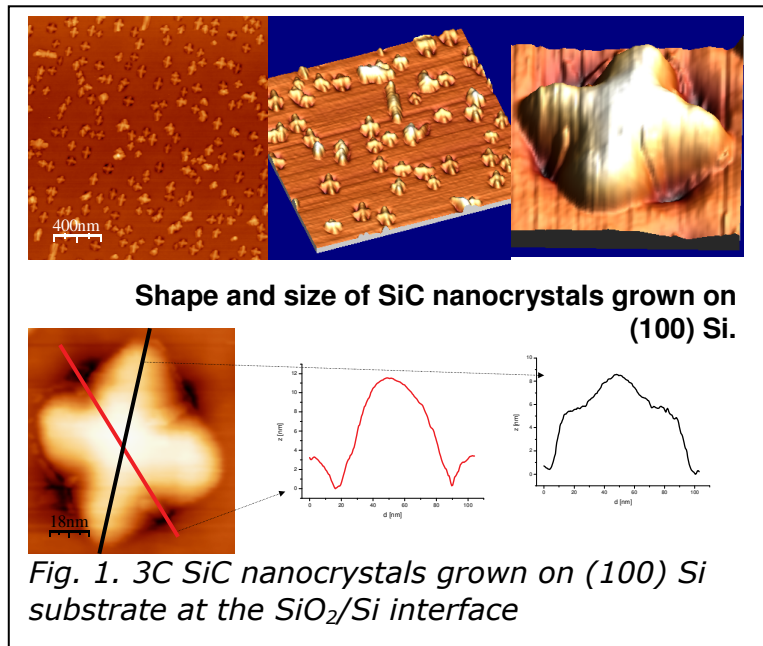
**Nanograins and nanolayers in semiconductor structures – electrical and photoelectrical properties (OTKA T048696)**

Zsolt J. HORVÁTH, Péter BASA, László DÓZSA, Péter PETRIK, Bálint PÓDÖR, Zsolt ZOLNAI

In this project the electrical behaviour of different semiconductor structures are studied, which contain either nanocrystals or thin layers with a thickness of a few nanometer. main goal is to establish the relation between the electrical behaviour and the device structure.

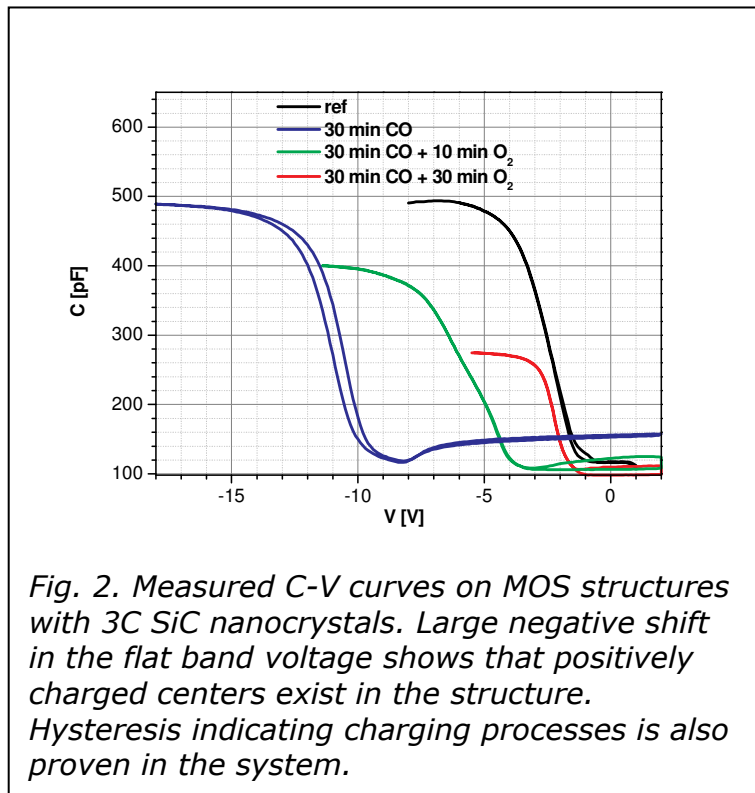
**SiC nanocrystals at the SiO<sub>2</sub>/Si interface: electrical behaviors**  
 Gábor BATTISTIG, Anita PONGRÁCZ, Zoltán HAJNAL, Zsolt MAKKAI, Attila TÓTH

Conventional non-volatile memory transistors use stacked floating gate for charge storage. These structures are not able to keep up with the downscaling of Si technology. A valuable solution to overcome scaling limitations to replace the floating gate by many discrete trapping centers. A non-continuous semiconductor nanocrystal region in the gate-oxide is a good candidate to realize such a structure.



*Fig. 1. 3C SiC nanocrystals grown on (100) Si substrate at the SiO<sub>2</sub>/Si interface*

Our group has already shown that a simple reactive annealing of SiO<sub>2</sub>/Si structure in CO containing ambient produces 3C-SiC nanocrystals epitaxially and void-free grown at the SiO<sub>2</sub>/Si interface. With a further oxidation step these nanocrystals can be isolated from Si into SiO<sub>2</sub> matrix creating a potential structure for charge storage.



Structures with nanocrystalline SiC were investigated in order to determine their structural and electrical properties depending on the various technological parameters applied. Electron microscopy was used to obtain information about the size distribution, nucleation density and volume fraction of the nanocrystals (Fig. 1). MOS structures with 3C-SiC nanocrystals were produced for current-voltage and capacitance – voltage measurements (Fig. 2). The results indicate that the high-tem-

perature annealing did not damage our structure and a reversible carrier injection was observed in the system.

***Research of SiC and other wide band gap semiconductors  
(OTKA grant No T035273)***

László DÓZSA, György MOLNÁR, Károly SOMOGYI, Béla SZENTPÁLI, Attila L. TÓTH, Edvard BADALJAN, Ákos MAJOROS, János FERENCZ, István FICZERE

SiC technology was developed to prepare ohmic, rectifying contacts and MOS structures prepared by dry oxidation. The ohmic contact was produced by evaporating Ni and annealing for 30 min at 950 °C. I-V, C-V, and DLTS measurements were applied for investigation electrical properties. A high temperature measuring chamber (500-600 °C) was manufactured. Most of the research work in the project was carried out in MBE grown InAs/GaAs quantum dot structures prepared in Parma, MOVPE quantum well samples prepared in Prague, and  $\beta$ -FeSi<sub>2</sub> quantum structures prepared in MFA.

***$\beta$ -FeSi<sub>2</sub> nanocrystals on silicon  
(Hungarian-Greek Bilateral Project GR-35/03)***

László DÓZSA, György MOLNÁR, Béla SZENTPÁLI, Attila L. TÓTH, Zsolt J HORVÁTH, Anita PONGRÁCZ, Péter BASA

Fe on Si-based quantum structures were investigated by current-voltage, capacitance-voltage, deep level transient spectroscopy (DLTS), noise measurements, by atomic force microscopy (AFM), scanning capacitance microscopy (SCM), scanning and transmission electron microscopy (TEM, SEI), by infrared reflection and transmission (FIR), secondary ion mass spectroscopy (SIMS), and by photoluminescence (PL) measurements. The  $\beta$ -FeSi<sub>2</sub> quantum structures were grown by depositing Fe and annealing at 400 - 600°C temperature. FIR results have shown the RT deposited Fe results in polycrystalline  $\beta$ -FeSi<sub>2</sub>, but in samples prepared by RDE the ratio of the beta phase is small. SIMS measurements show the deposited Fe remains near the surface, there is no significant diffusion of Fe into silicon at the RDE deposition temperatures. TEM has identified  $\alpha$  and  $\gamma$  phases in the grown  $\beta$ -FeSi<sub>2</sub> quantum structures. DLTS shows the point defects generated by the growth process compensate the dopants in the silicon, and PL shows the generated point defect drastically reduce minority carrier lifetime in the silicon near the surface.

***Temperature controlled sample holder for the  
DLS-83E spectrometer  
(GVOP-3.2.1-2004-2004-04-0322/3.0)***

László DÓZSA, Vilmos RAKOVICS, Sándor PÜSPÖKI, Anita PONGRÁCZ, Péter BASA

In the frame of the project a Deep Level Spectroscopy setup for measuring point defects in semiconductors was realized. The measuring setup fits to the material science and semiconductor device activity of the Institute. The measurements can be carried out in the 12-320 K range using the Lake-shore 330 temperature controller, and in the 80 K- 550 K temperature range using the sample holder financed by the project. In the project new options were installed in the DLS spectrometer: optical excitation mode and

FET measurement mode. The project integrates the deep level spectroscopy into the material research activity of the Institute.

***Preparation and investigation of silicon-based nanostructures  
(Academic exchange program)***

László DÓZSA, N.A. GALKIN (Vladivostok)

Investigations of the optical, electrical and structural behaviour of silicon-based nanostructures with buried semiconductor silicide precipitates ( $\beta$ -FeSi<sub>2</sub>, CrSi<sub>2</sub> and Mg<sub>2</sub>Si). DLTS on the  $\beta$ -FeSi<sub>2</sub> samples received from Russia show the iron silicide growth process created defects which compensate the shallow dopant in p-type silicon. It is in agreement with the results achieved in Budapest on n-type silicon.

***Transport and defects in Quantum structures  
(Academic exchange program)***

László DÓZSA, P. HUBIK (Prague)

In the project InGaAs/InAs quantum layer structures were investigated by photoluminescence, AFM, TEM, SEM and by DLTS. The quantum layers were grown in Prague. TEM, PL and DLTS show defect free structures. AFM and SEM show rough morphology in some of the samples, which correlates with the broadening of the PL peak.

## Photonics Department

<b>Laboratory for Nondestructive Analysis</b>	<b>Semiconductor Photonics Laboratory</b>	<b>Bioengineering Laboratory</b>
<p><b>Head:</b> Tivadar LOHNER, Ph.D.</p> <p><b>Staff:</b> Csaba DARÓCZI Imre EÖRDÖGH Miklós FRIED, D.Sc. György JUHÁSZ Péter PETRIK, Ph.D. Olivér POLGÁR Ferenc RIESZ, Ph.D. Károly SZÁSZ Gábor VÉRTESY, D.Sc.</p> <p><b>PhD Student (Advisor):</b> Csaba MAJOR (dr. Miklós Fried) Antal GASPARICS (dr. Gábor Vértesy) István E. LUKÁCS (dr. Ferenc Riesz)</p>	<p><b>Head:</b> Miklós SERÉNYI, Ph.D.</p> <p><b>Staff:</b> János BALÁZS dr. András HÁMORI György KÁDÁR, D.Sc. Sándor KURUNCZI Ph.D. Zsolt LACZIK, Ph.D. (on leave) János MAKAI, Ph.D. (part time) dr. Miklós RÁCZ (part time) Péter TÖRÖK, D.Sc. (on leave) Péter VARGA, Prof. Emeritus, D.Sc. Ferenc VONDERVISZT, Prof., D.Sc. (part time)</p> <p><b>Technical Staff:</b> Mrs. M. RÚZSA JANKÓNÉ Mrs. L. MÉSZÁROS</p> <p><b>PhD Student:</b> Norbert NAGY</p>	<p><b>Head:</b> György KOZMANN, D.Sc.</p> <p><b>Staff:</b> Krisztina SZAKOLCZAI Kristóf HARASZTI Andrea CSALÓTZKY BOLGÁR</p>



## Laboratory for Nondestructive Analysis

### ***Ion beams in physical nanotechnology (OTKA T043704, Head: Prof. József Gyulai)***

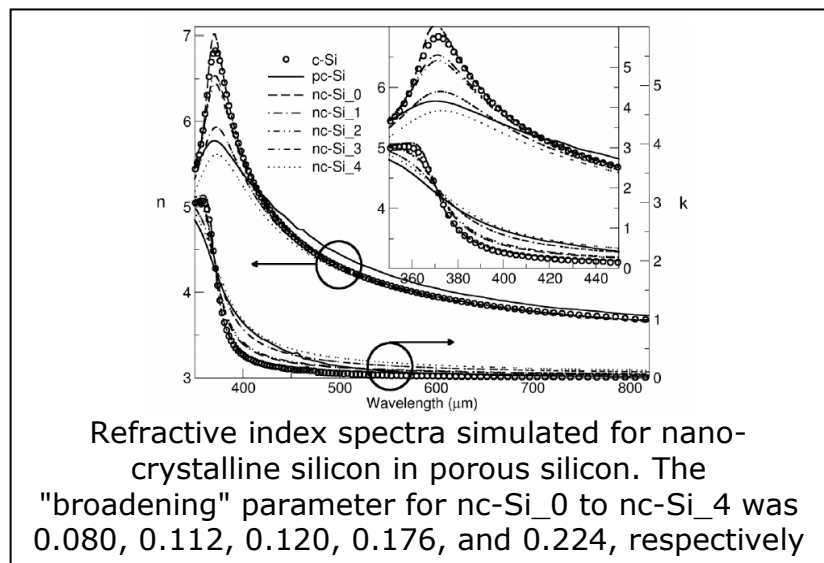
Tivadar LOHNER, Péter PETRIK

Realistic optical models were elaborated on basis of studies performed by spectroellipsometry and cross-sectional transmission electron microscopy for cavities and damaged zones created by He ion implantation in silicon [141].

### ***Development of optical models for ellipsometric study of multicomponent materials (OTKA T04701)***

Miklós FRIED,  
Tivadar LOHNER,  
Péter PETRIK

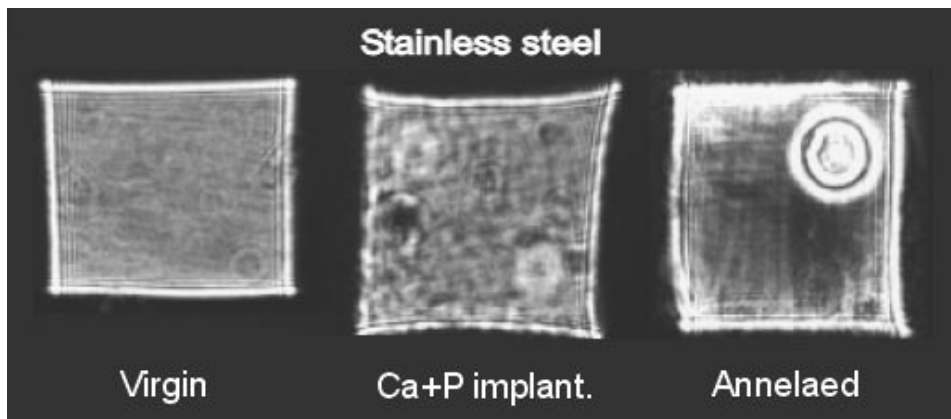
We developed optical models for the ellipsometric characterisation of porous silicon structures [142]. We would like to establish correlation between the parameters of the dispersion relation and the microscopical structural properties of the materials studied.



### ***Quantitative Makyoh topography (OTKA T037711)***

Ferenc RIESZ, István E. LUKÁCS

Systematic investigations were carried out on the morphology of various substrates for hydroxi-apatite layer growth modified by ion implantation and annealing for biomedical application using Makyoh-topography [154].



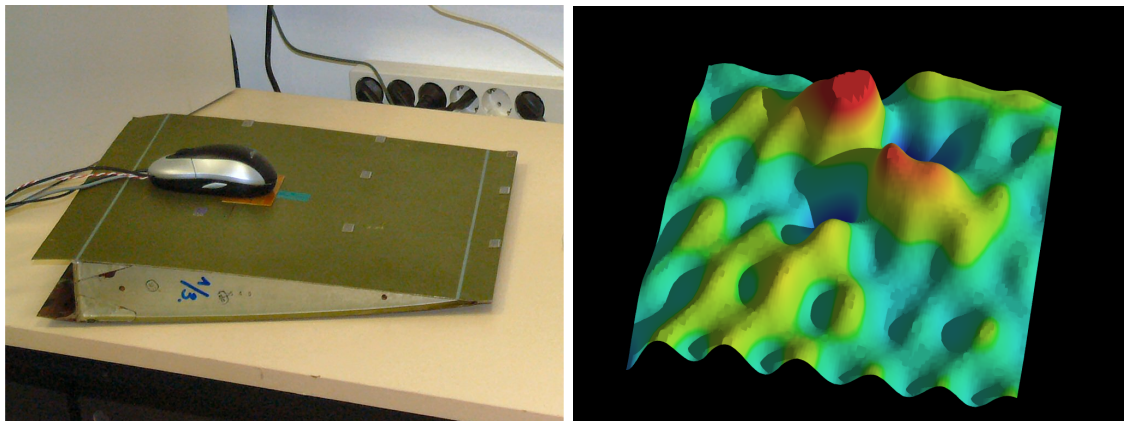
***Detection of the degradation of structural materials by  
electromagnetic nondestructive methods  
(OTKA T035264)***

Gábor VÉRTESY, Antal GASPARICS, Csaba DARÓCZI

Novel methods have been developed for nondestructive electromagnetic material evaluation.

One of them is based on systematic measurement of magnetic minor hysteresis loops. It is possible to follow the structural degradation of ferromagnetic materials by this method. The effectivity of this method has been proved by measurements. The plastic deformation of cold-rolled stainless steel has been characterized by this method [192]. As a theoretical background for the hysteresis modeling, the hysteresis properties of a two dimensional array of small magnetic particles were studied as a test bed for the Preisach model [193].

The other method is the application of a high sensitivity magnetic field sensor (Fluxset sensor) for eddy current investigations [191]. Mapping procedure has been developed for safety checking methods of different parts of airplanes and helicopters (see the figures below).



***Application of novel electromagnetic nondestructive techniques  
(EURATOM-EFDA Fusion Underlying Technology Workprogramme)***

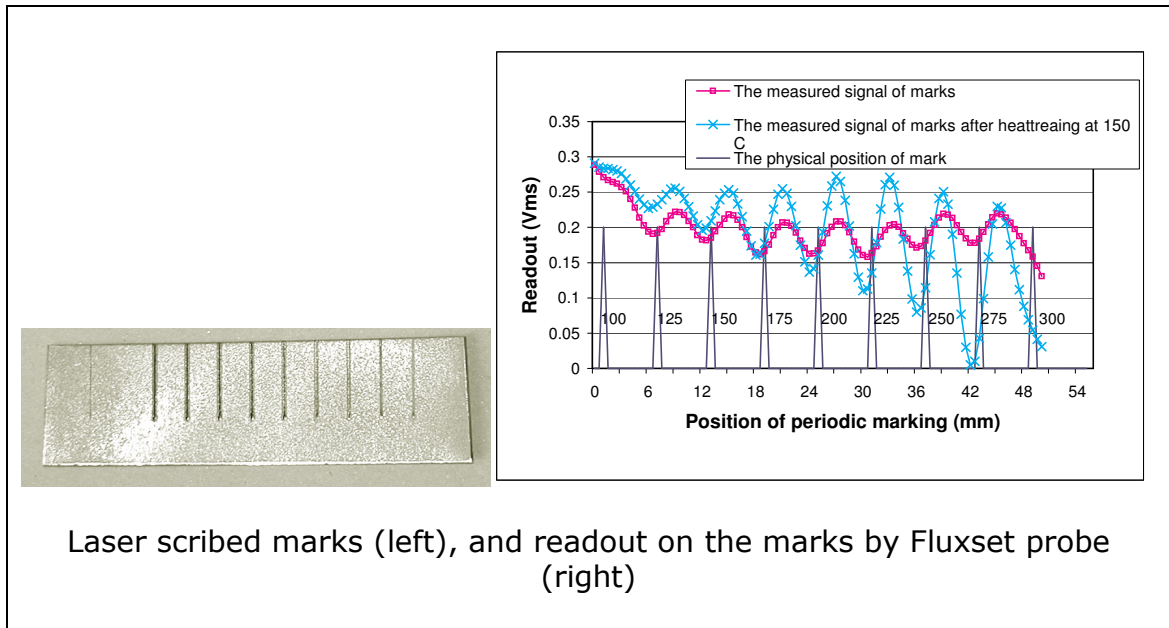
Gábor VÉRTESY, Antal GASPARICS

The objective of the work has been to develop a complex way of characterization of degradation of austenitic stainless steel, which is a frequently used structural material in nuclear reactors. The relationship between the magnetic hysteresis parameters and the structural changes occurring during mechanical loading of materials have been determined. The basic experimental tool was the measurement of the series of hysteresis loops by the special device, developed by us. The basic theoretical tool was the special analytical method based on an appropriate original modification of Preisach model of the magnetisation process. The whole process is called as Magnetic Adaptive Testing.

***Electromagnetic reading system of laser marked logistic bar codes  
(GVOP-3.1.1- 2004 – 05 -0452/3.0, Head: Gábor Vértesy)***

Gábor VÉRTESY, Antal GASPARICS

Stable marker stripes have been created by CO<sub>2</sub> laser irradiation in the surface layer of steel aiming identification of parts of industrial machineries during production steps. The markers have been investigated by the Fluxset magnetic sensor [193] and very good signal/noise ratio has been detected (see Fig. below).



***Development and application of special image processing methods  
(Head: Imre Eördögh)***

Imre EÖRDÖGH, Károly SZÁSZ

Special image processing methods were developed and applied for solving medical, dosimetric and fabrication-related technological tasks [133, 157].

## Semiconductor Photonics Laboratory

### **AQUANAL (NKFP 3A/079/2004, Head: István Bársony)**

András HÁMORI, Miklós SERÉNYI, Sándor KURUNCZI, Norbert NAGY

The aim of the project is the analysis of the natural water basis using micro- and nanosensors. Interferometric and fluorescence methods were developed for the monitoring of the oil film on the surface of the water. Characterization of Salmonella FliS flagellar chaperone binding to flagellin was performed for optical detection of the heavy ionic pollution.

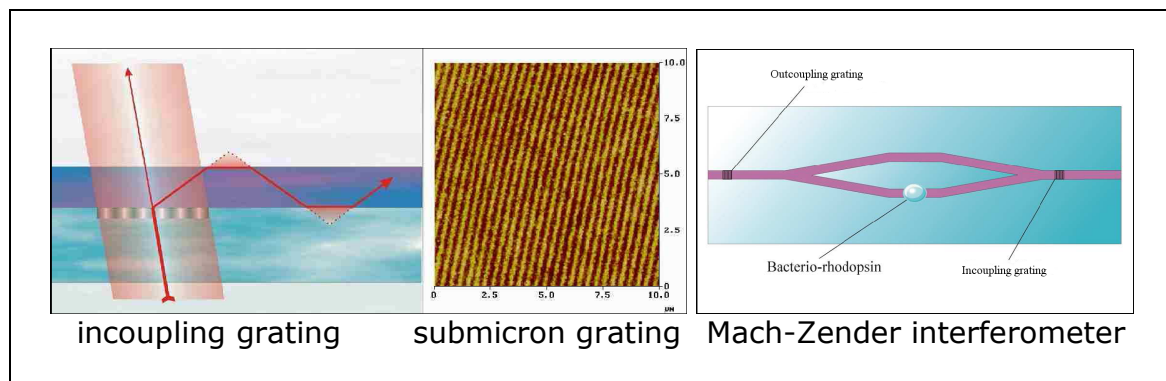
### **Optical setup for Makyoh topography (OTKA No. T037711)**

J. MAKAI

### **Opto-electronic devices based on the protein Bacteriorhodopsin (NATO Project Number: Sfp974262)**

M. SERÉNYI, A. HÁMORI, N. NAGY

Monomode waveguiding sensor, different waveguides including in-, and out-coupling grating, and Mach-Zender interferometer was prepared on Suprasil substrate by Ta<sub>2</sub>O<sub>5</sub> thin film.



### **Solar cell made of CIGS (NKFP 3/025/2001)**

J. MAKAI; J. BALÁZS

We developed methods for in-situ control during the deposition of CIS/CIGS layers by measurement of transmission and reflection.

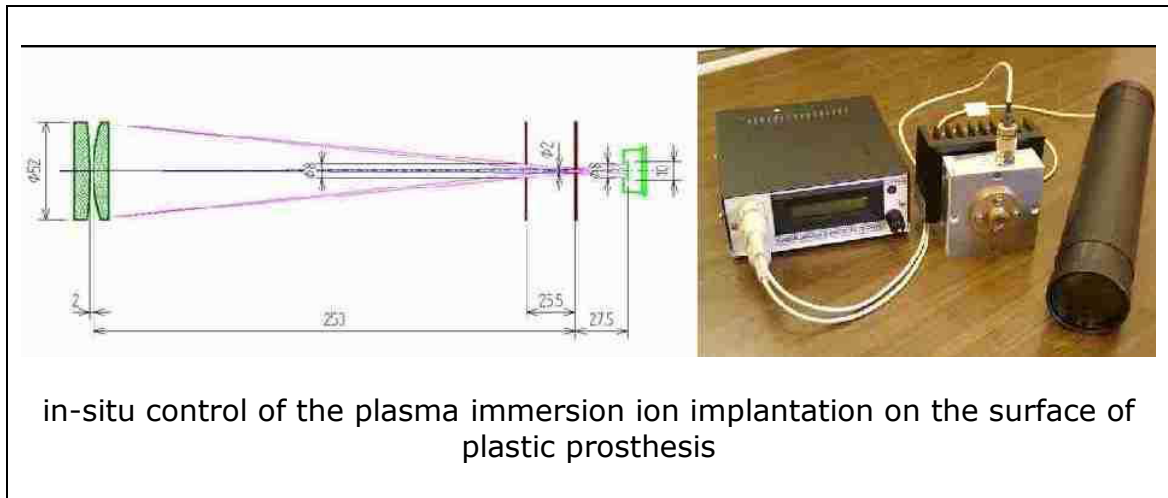
### **Development of long life-cycle human-body hip-prosthesis (NKFP 1/013/2001)**

M. SERÉNYI, M. RÁCZ

The aim of the project to enhance the life-time of human articular prosthesis by ion implantation.

We developed an optical method for the in-situ control of the plasma immersion ion implantation caused hardness change on the surface of plastic

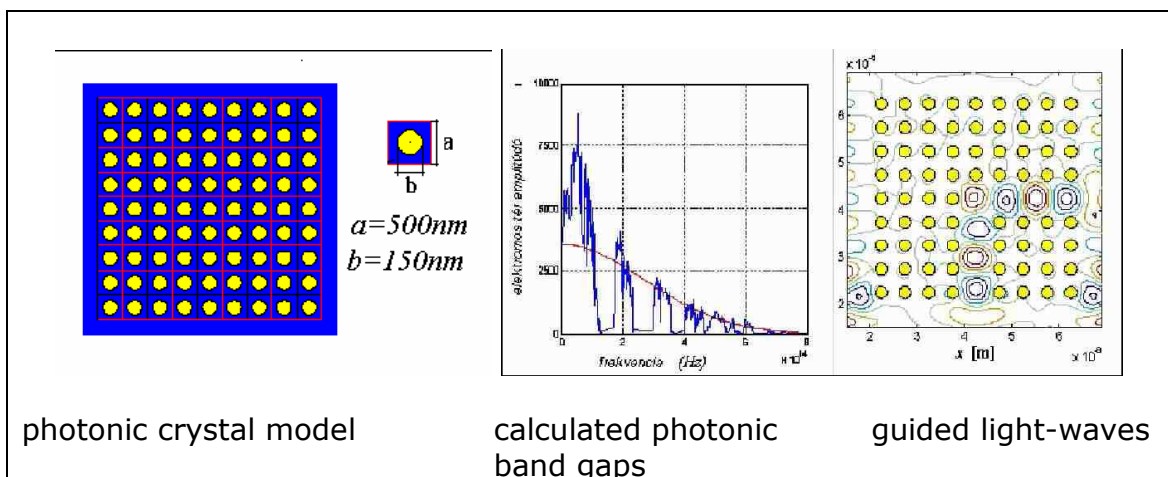
prosthesis. The method is based on the spectral reflection of the surface depending on the implanted ion dose. The device (containing semiconductor diode-laser) is capable of in-situ, real-time control during plasma immersion ion implantation (PIII) of surfaces.



### ***Electromagnetic waves in artificial periodical structures (OTKA T 046696)***

G. KÁDÁR, J. GYULAI, I. BÁRSONY, B. SZENTPÁLI, G. BATTISTIG, P. VARGA, A. HÁMORI, A. TÓTH, J. BALÁZS, J. VOLK, N. NAGY, Zs. SZABÓ

A research project for the modelling, fabrication and characterisation of photonic crystals (periodic structures of light wavelength scale) has been launched this year by a group of persons belonging to various departments of the Institute. Experimental results were obtained in porous silicon based one-dimensional periodic structures. In the first year the main effort was the development of a computer model for the simulation of the propagation of electromagnetic waves in one- and two-dimensional photonic crystals by using the finite difference time domain (FDTD) method. The model was tested and applied in rectangular two dimensional lattices for the calculation of the energy band structure and band-gaps as well as for the simulation of the propagation of a "forbidden energy" wave along a defect line of a photonic crystal model as seen in the figures.

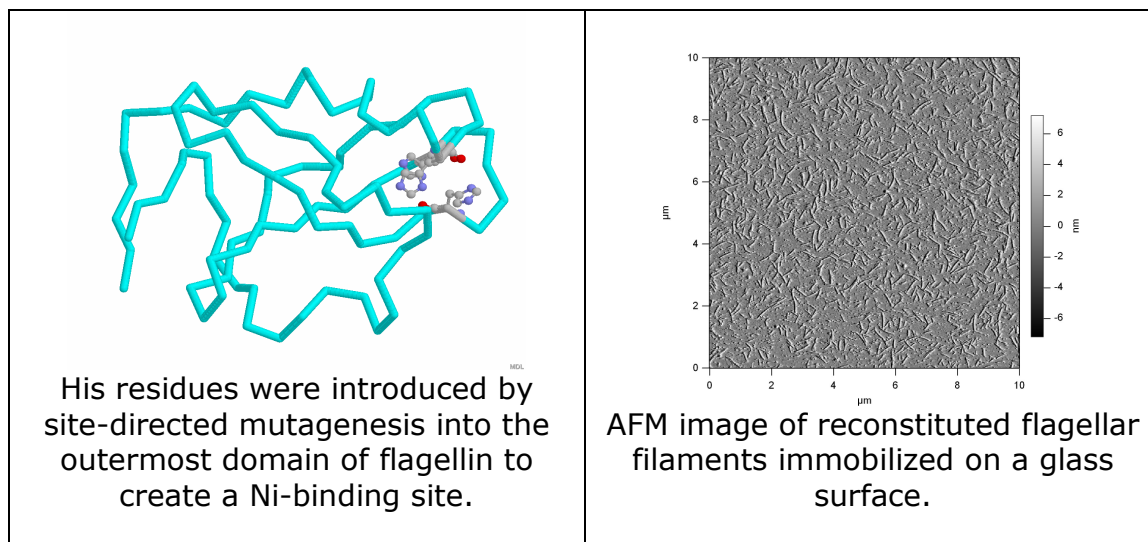


### **Laboratory of Nanosensorics**

Living organisms have been using molecular nanotechnology over the past 4 billion years with great success. Molecular machines of living cells are mainly made of proteins, have the capability for self-assembly and can fulfill complex functions in a highly controlled fashion. Given their key role in natural molecular machines, proteins are obvious candidates for work in self-assembling nanosystems.



The Laboratory of Nanosensorics - as a joint unit with the Department of Nanotechnology, University of Veszprém - was established in 2005. Major research interest is focused on the development of integrated optical waveguide biosensors which apply self-assembling protein-based sensing elements. These biosensors are intended for use in various medical and environmental applications.



Flagellin is the subunit protein of bacterial flagellar filaments. Flagellin-based artificial receptors capable of efficient recognition and binding of target molecules are under development using directed evolution and rational protein design. Flagellin receptors, due to their polymerization ability, can be used to build various filamentous structures which are stable, resistant to proteases, and can be preserved for a long period of time.

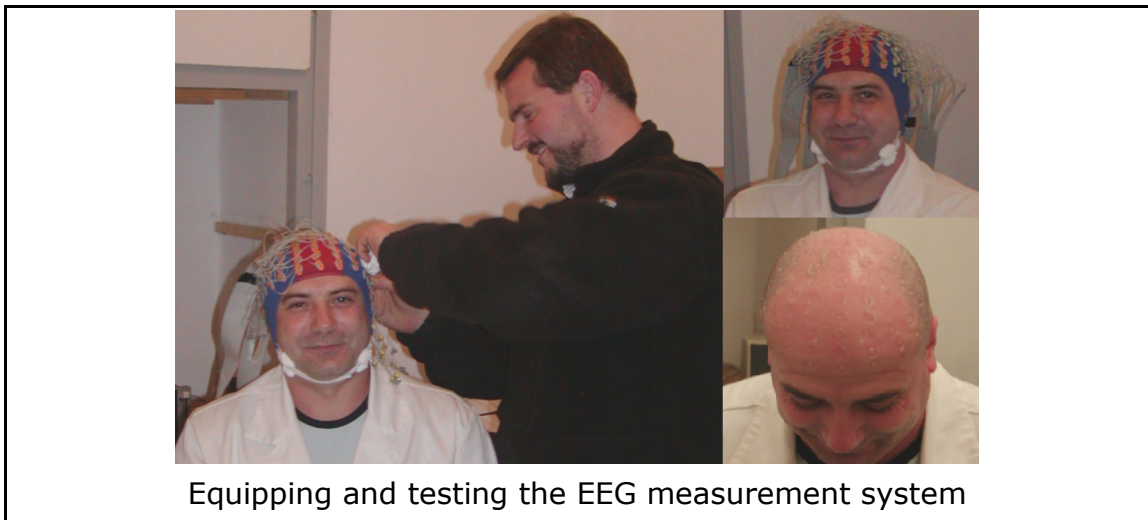
Starting from a certain type of flagellin receptors, filaments of desired length can be prepared with a very high binding site density on their surface. Additionally, filamentous receptor structures can be polymerized from differently modified flagellins. These block copolymers can recognize and bind different target molecules in different regions, or they can be immobilized through a certain region containing specifically modified subunits, while their other parts are involved in molecular recognition. These supramolecular objects may serve as basic recognition units for biological sensors and diagnostic kits.

## Bioengineering Laboratory

### ***Developing high-resolution brain electro-mapping (BEM) (NKFP 2/004/2004)***

GY. KOZMANN, K. SZAKOLCZAI, K. HARASZTI

The most recent research area of the Department is Brain Electro Mapping (BEM). The essential feature of BEM is to grasp surface (scalp level) manifestation of brain bioelectrical phenomena associated to physiological or pathological activity. Based on 128 channel low noise EEG records and head anatomy assessment by MRI, the final goal is to provide source level representation by different approaches of inverse computations (e.g. Laplacian maps, cortical potential and/or current density estimates, concentrated equivalent current dipole sources, etc.) In the frame of the very same project, in cooperation with the National Institute of Psychiatry and Neurology, high spatio-temporal resolution brain plasticity research is contemplated. According to the preliminary expectations the new imaging modality integrated into the imaging laboratory, may provide useful contribution to cost effective follow-up studies, and optimized rehabilitation procedures.



Equipping and testing the EEG measurement system

In 2005 we have upgraded our previous 64 channel mapping system up to a 128 channel. A new data acquisition software system has been developed and tested in laboratory. In order to reduce magnetic and electronic interference, currently a Faraday cage is to be implemented.

### ***Intelligent physiological telemonitoring system (GVOP AKF 0196/2004)***

GY. KOZMANN, K. SZAKOLCZAI, K. HARASZTI, A. CSALÓTZKY BOLGÁR

The aim of the project is to develop an intelligent measuring and supervising system for monitoring and transmitting of physical, circulatory and emotional status, work load and environmental load. The major components of the system comprise robust wearable sensors (EKG, O<sub>2</sub> saturation, pulse temperature, physical activity, etc.) and signal conditioners with bluetooth or cable connection to the local portable data acquisition module. Data processing will be carried out in two steps, locally and in a centralized surveillance system.



In 2005 we have installed a local test laboratory capable of physical exercise measurements, a set of sensors has been developed and tested with the contribution of an industrial subcontractor. Based on our previous research we have started to create a mathematical model to explore relations of ECG, blood pressure, pulse and respiration.

***Control of multi-joint movements: electro-mechanical model  
(OTKA T 34548)***

J. LACZKÓ

A concept of a general mathematical model and a computer simulation for neural control of limb movements has been developed based on a common work with the New York University. The model generates muscle forces and joint rotations as a function of activation patterns of motoneuron pools while biomechanical parameters of the neuro-musculo-skeletal system were considered.

First we worked on a direct problem: joint rotations and limb movement patterns has been computed from given frequencies of neural impulses originated from motoneuron pools. On the other hand an inverse model has been developed to provide discharge rates of motoneuron pools that lead to the given joint rotations and limb movements. This inverse problem has infinity of solutions and we approached it assuming that each joint were controlled by one flexor-extensor muscle pair and only one member of the muscle pair was active in a given moment. Possible motoneuron firing rates were computed from joint rotations measured in rats during swimming and walking. Experimental data were received during the common work with the researchers of the New York University. The effect of gravity on movement patterns and the sensitivity of the model to the change of muscle force-muscle length relations and to the change in posture were analyzed.

Additionally we participated in developing neuroprostheses by electrical stimulation of leg muscles of spinal cord injured patients.

***Search for repolarisation disparity parameters  
(OTKA F035268)***

GY. SÁNDOR, K. SZAKOLCZAI, A. PINTÉR

Diagnosing patients with non-ST elevation acute coronary syndrome (ACS) is difficult, because the electrical abnormalities of the heart do not evoke measurable departures on standard 12 lead ECG. ACS develop due to myocardial ischemia and as a result of ACS three main types of cardiac diseases may occur: non-Q myocardial infarction (NQMI), unstable angina (UA) and Q wave myocardial infarction (QMI). NQMI and UA are more frequently associated with malignant arrhythmias and sudden cardiac death than QMI. By complex nonparametric statistical methods we have found significant relations between combination of major vessel lesions and potential losses on BSPM in patients with non ST elevation ACS, which cannot be detected by ECG just only by invasive methods. Furthermore, a stable connection was revealed between the steady-state spatial dispersity of depolarization activation sequence (represented by QRS integral map) and ventricular repolarization (represented by QRST integral map). Consequently, chronic pathologic state changes of depolarization phase infer changes of repolarization properties characterized by QRST integral map.

## Nanotechnology Department

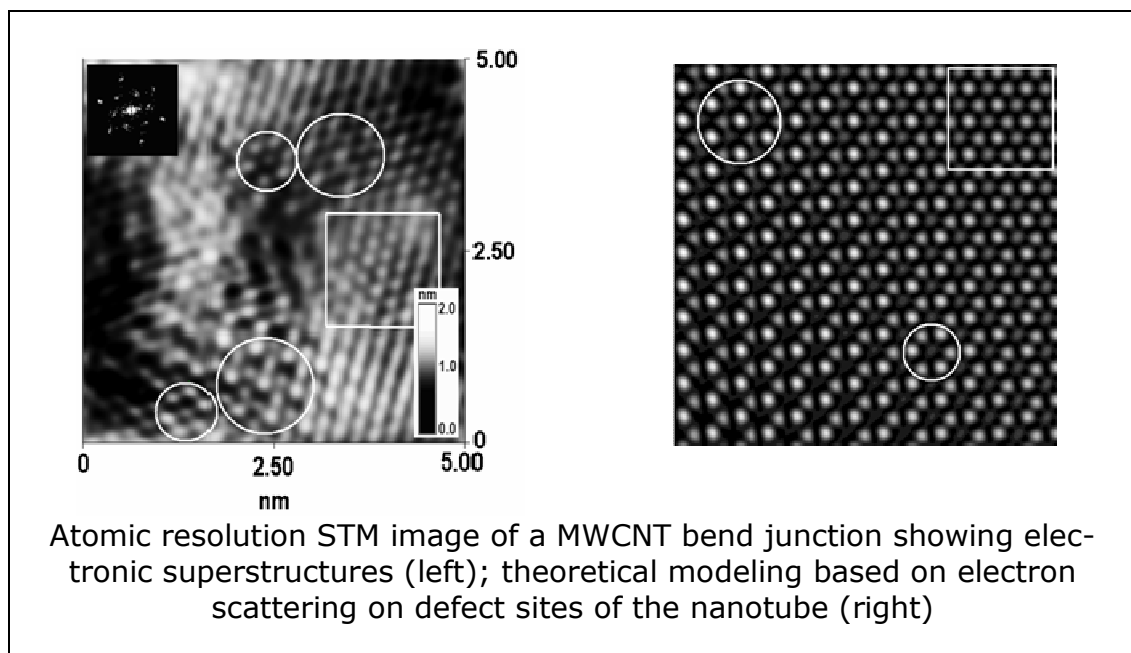
<b>Nanostructures Laboratory</b>	<b>Ceramics and Composites Laboratory</b>	<b>Complex Systems Group</b>
<p><b>Head:</b> Zsolt E. HORVÁTH, Ph.D.</p> <p><b>Staff:</b> József GYULAI, Prof. Emeritus, member of the HAS László P. BIRÓ, D.Sc. Attila Lajos TÓTH, Ph.D. Zofia VÉRTESY, Ph.D. Géza I. MÁRK, Ph.D. Antal A. KOÓS, Ph.D.</p> <p><b>PhD Students (Advisor):</b> Enikő HORVÁTH (A. L. Tóth) Krisztián KERTÉSZ (László P. Biró) Zoltán OSVÁTH (László P. Biró) Levente TAPASZTÓ (László P. Biró &amp; G. I. Márk)</p> <p><b>Technician:</b> Margit SÁRKÁNY</p>	<p><b>Head:</b> Péter ARATÓ, D.Sc.</p> <p><b>Staff:</b> Csaba BALÁZSI, Ph.D. Zsuzsanna Ilona KÖVÉR Judit PFEIFER, Ph.D. Ferenc WÉBER</p> <p><b>PhD Students (Advisor):</b> Judit BABCSAN KISS (Péter Arató) Nikoletta KAULICS (Péter Arató) Balázs FÉNYI (Csaba Balázsi)</p>	<p><b>Head:</b> György SZABÓ, Ph.D.</p> <p><b>Staff:</b> István BORSOS Zoltán JUHÁSZ, Ph.D. Géza ÓDOR, D.Sc. Attila SZOLNOKI, Ph.D.</p> <p><b>PhD Student:</b> Jeromos VUKOV</p>

## Nanostructures Laboratory

### ***Production, modification and characterization of carbon nanotube-like nanostructures based on physical, chemical and simulation methods (OTKA T043685)***

L. P. BIRÓ, Z. E. HORVÁTH, Z. VÉRTESY, G. I. MÁRK, A. A. KOÓS, K. KERTÉSZ, Z. OSVÁTH, L. TAPASZTÓ

Bend-junctions of multiwall carbon nanotubes grown by the injection CVD method were investigated by STM. Atomic resolution images revealed position dependent modulation of the electronic density of states, attributed to the scattering of electrons on defect sites present in the junction region. We developed a theoretical model based on the interference of the scattered electrons, suitable to interpret the experimentally observed long-range interference patterns by considering coherent scattering processes allowed at finite bias voltages in carbon nanotubes. The model predicts that complex charge density oscillations present near defects are tunable by varying the position of the Fermi level.



### ***Nanotube-based gas sensor (MEH-MTA strategic research grant NANOGAS)***

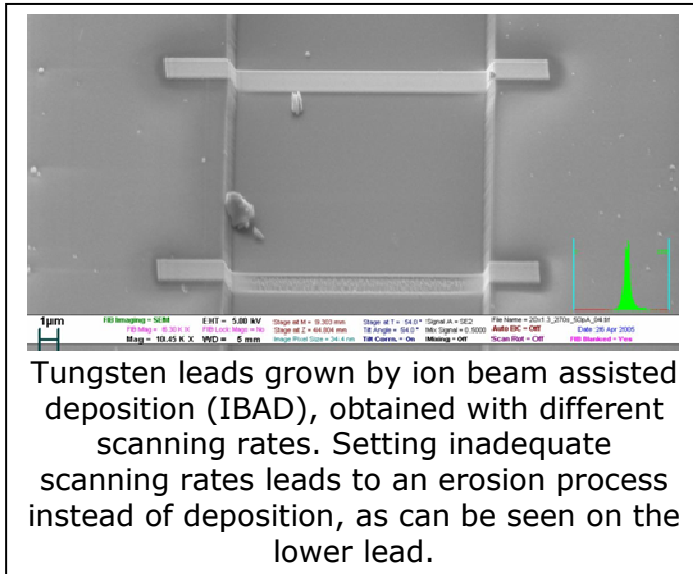
J. GYULAI, L. P. BIRÓ, Z. E. HORVÁTH, Z. VÉRTESY, A. A. KOÓS, K. KERTÉSZ

Resistance measurements on random networks of multiwalled carbon nanotubes, produced by a special deposition process, were carried out in the presence of different gas/vapor atmospheres. We showed that the nanotubes functionalized by various physical and chemical methods, can be made selectively sensitive on different gases/vapors. From arrays of such nanotube-based sensors we were able to build an operable vapor-recognizing system.

### **Nanopatterning of thin layers by focused ion beam (OTKA T049131)**

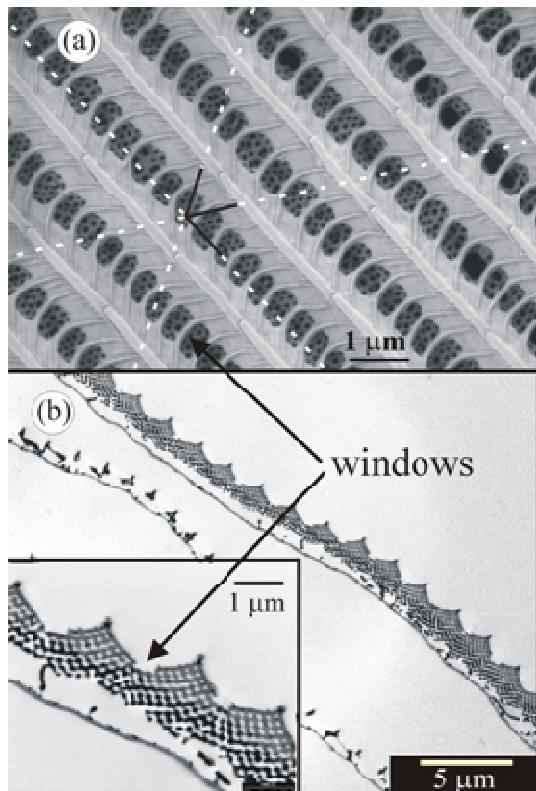
A. L. TÓTH, Z. VÉRTESY, E. HORVÁTH

We have carried out several deposition rate measurements on ion beam deposited (IBAD) tungsten layers. We studied the thickness of the tungsten layer deposited on regions of different areas, by scanning an ion beam of 50 pA. We found that the scanning rate is a critical factor in determining the equilibrium between the competitive processes of deposition / erosion. In situ resistance measurements were started on tungsten nano-wires deposited on a micro-heater. After some failed trials, resistance measurements were successfully carried out using a home made low current measuring device.



### **Photonic crystal type materials of natural origin (INCO-12915/2005 EU6 NEST-Pathfinder „BIOPHOT” and OTKA T042972)**

L. P. BIRÓ, Z. VÉRTESY, K. KERTÉSZ



The structure of the photonic crystal responsible for the color of the wings of *Cyanophrys remus* butterfly was found to be a completely regular hexagonal inverse opal structure, which gives the blue color in a complicated, angle dependent way, as it was demonstrated using spectro-goniometer measurements.

SEM (a) and XTEM (b) images of the wing scales of *Cyanophrys remus* butterfly responsible for its blue color. From SEM & TEM measurements one can observe the long range order (periodicity) of the structure in two transversal planes.

## Ceramics and Composites Laboratory

### ***Silicon Nitride-Based Ceramics and Composites (OTKA T043704)***

P. ARATÓ, Cs. BALÁZSI, F. WÉBER, Zs. I. KÖVÉR

The intensive study of ceramic composites started in this laboratory three years ago. The long-range aim is to develop new materials with a high level of synergism. Composites with silicon nitride matrix and carbon nanotube (CNT) reinforcement have been in the focus of our interest.

It is known that CNTs are characterised by exceptional mechanical and physical properties, however their incorporation into ceramic matrices gave only modest improvements. This discrepancy is caused by two facts, firstly, it is difficult to produce a homogenous distribution of CNTs in the ceramic matrix and secondly, their degradation at the temperature of sintering had to be prevented. First our team succeeded to find processing parameters providing the maintenance of carbon nanotubes in a silicon nitride based matrix.

In 2005 we continued the investigation of CNT/silicon nitride composites. Samples were prepared with different compositions, sintering techniques and processing parameters. Their micro and nanostructure were examined by scanning electron microscopy (SEM), X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR), mechanical and electrical properties were measured. We attempted to reach a better understanding the relationships between processing parameters, structure and properties.

Spark plasma sintering (SPS) is one of the advanced sintering methods, its main benefit is the high heating and cooling rate (100 K/min and 400 K/min, respectively). Samples made from our materials were sintered in Arrhenius Laboratory. 3 - 5 min holding at 1500 °C was sufficient to reach 95-99% of density. Density, hardness and modulus of elasticity of samples with 1% CNT was only slightly less than that of reference sample, no difference between the values of toughness was observed. The grain size in both cases was about 200 nm, comparing to 400-500 nm of ceramics after usual sintering. SPS equipment is too expensive for mass production, it is able, however, to provide particular information on the nanostructure of ceramics and composites.

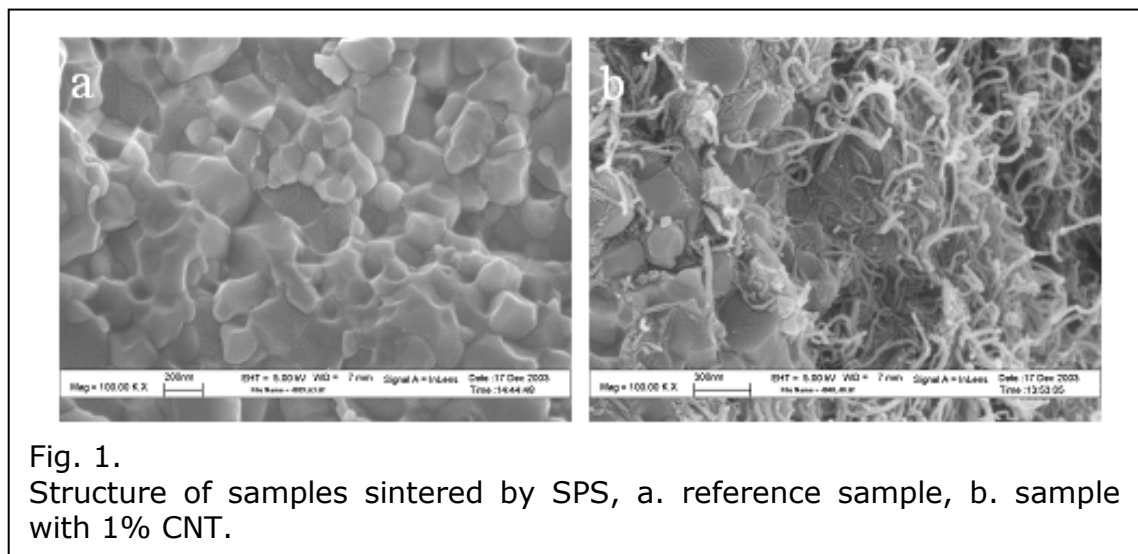
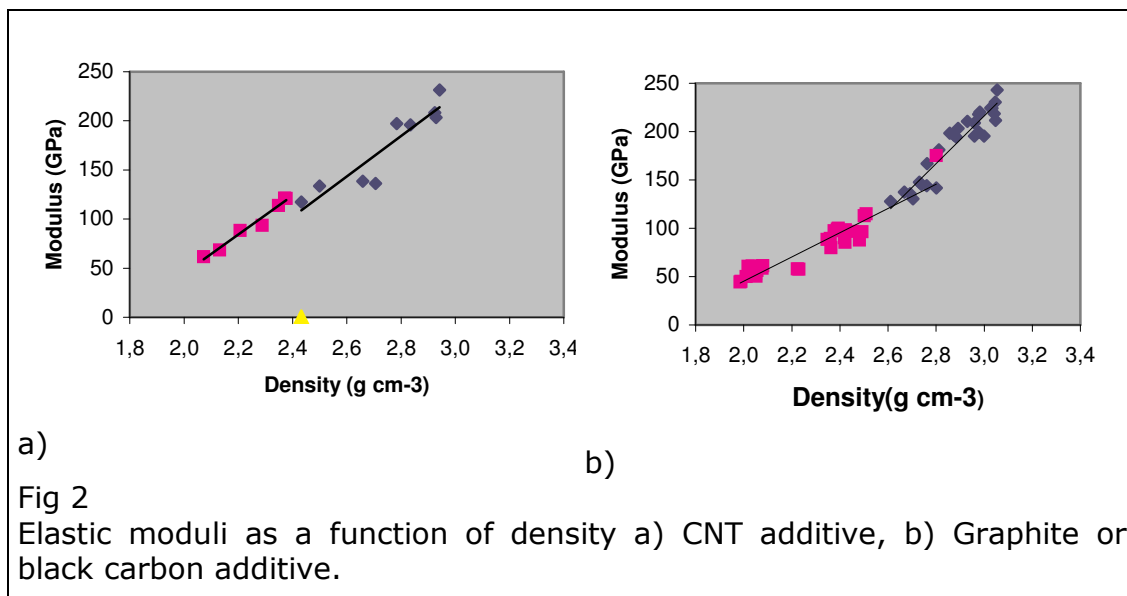


Image obtained by direct examination of structure can be supplemented by the information gained from results of measurements. The modulus of elasticity reflect well mechanism of deformation in the initial stage of sintering. Fig. 2b shows the modulus as a function of apparent density for samples made using carbon black or graphite addition. The data split into two groups. Density of samples with high carbon content (5% BC, 10% graphite, 10% BC) was less than  $2.6 \text{ g cm}^{-3}$ , the slope of density-modulus curve was  $125 \text{ GPa cm}^3 \text{ g}^{-1}$ . In the case of low carbon content (1% graphite, 1% BC, 5% graphite) the value of slope ( $247 \text{ GPa cm}^3 \text{ g}^{-1}$ ) was twice as much as in the low density range, nevertheless it agreed with the slope obtained for a series of samples non-containing carbon addition ( $234 \text{ GPa cm}^3 \text{ g}^{-1}$ ). It is thought that in the range of low density the redistribution of carbon is responsible for the densification and for the change of modulus of elasticity. When the density reached the critical value  $2.6 \text{ g cm}^{-3}$  the generation and growth of necks between particles became the controlling factor. When CNT was added the two groups can be recognised (Fig. 2a), their slopes, 197 and  $206 \text{ GPa cm}^3 \text{ g}^{-1}$ , were close. These results suggest that the strong interaction between CNT and matrix provides that in the initial stage the deformation is the same, the load is distributed.



In addition to the mechanical properties physical characteristics were also measured. The DC specific conductivity was determined co-operating with the Miskolc University. It was found that 3 wt. % CNT is sufficient to alter the transport properties of the HIPed composites. The order of magnitude of electrical conductivity of silicon nitride ceramics is  $10^{-11} - 10^{-12} \text{ S m}^{-1}$  while its value in the composite was as high as  $18 \text{ S m}^{-1}$  [46], at the same time the difference between mechanical properties of ceramic and composite was less than 50%. These data mean that the CNTs percolate providing the conductivity while the ceramics are bonded each to the neighbouring particles providing the mechanical strength. It is sure that a composite which is wear resistant, refractory and conductive will be used in a wide region.

### **Tungsten Oxide Functional Ceramics (MTA-OTKA-NSF)**

Csaba BALÁZSI, Judit PFEIFER

Tungsten oxide compounds, promising at sensing dangerous gases in the ambient have been prepared in order to use them as thin layers of functional ceramics. The synthesis was based on soft chemical methods: acidic precipitation and hydrothermal dehydration of potassium and sodium tungstate derivatives. The potassium tungstate precursor resulted in tungsten bronze structures with nanosize morphology. The same preparation method using sodium tungstate precursor resulted in metastable open structure derivatives,  $\text{WO}_3 \cdot 1/3\text{H}_2\text{O}$  and  $\text{h-WO}_3$  with nanosize morphology as well. Powders of  $\text{h-WO}_3$ ,  $\text{c-WO}_3$  and  $\text{m-WO}_3$  were used to deposit sensing layers at the Department of Materials Science & Engineering SUNY, Stony Brook. Responses of the sensors to  $\text{NH}_3$  and  $\text{NO}_2$  gases are shown in Fig 3.

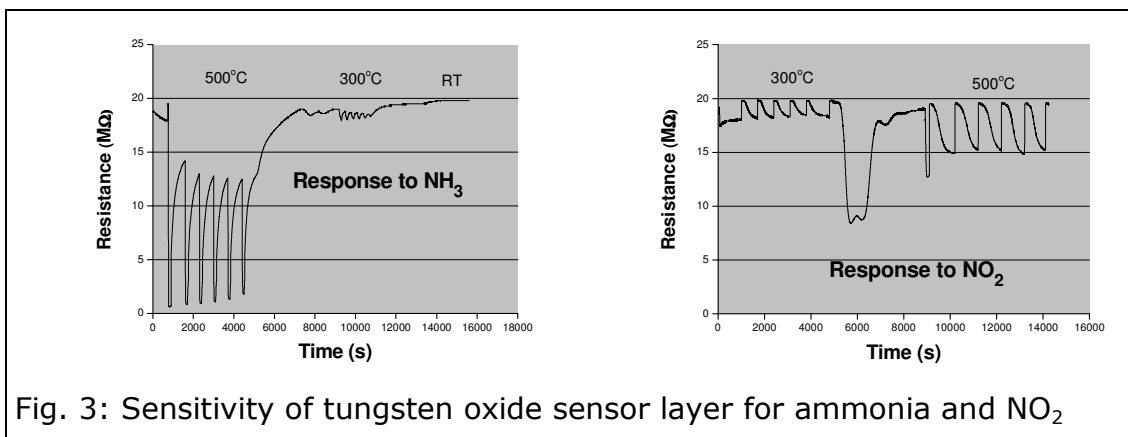


Fig. 3: Sensitivity of tungsten oxide sensor layer for ammonia and  $\text{NO}_2$

Another method for preparing tungsten oxide thin films was elaborated co-operating with Istanbul Technical University, Physics Department. The layer presented in Fig. 4 shows reversible electrochromic properties. The development of sensors indicating the concentration level of  $\text{NH}_3$  and  $\text{NO}_2$  gases by both resistivity and colour changes at the same time seems to be a real target.

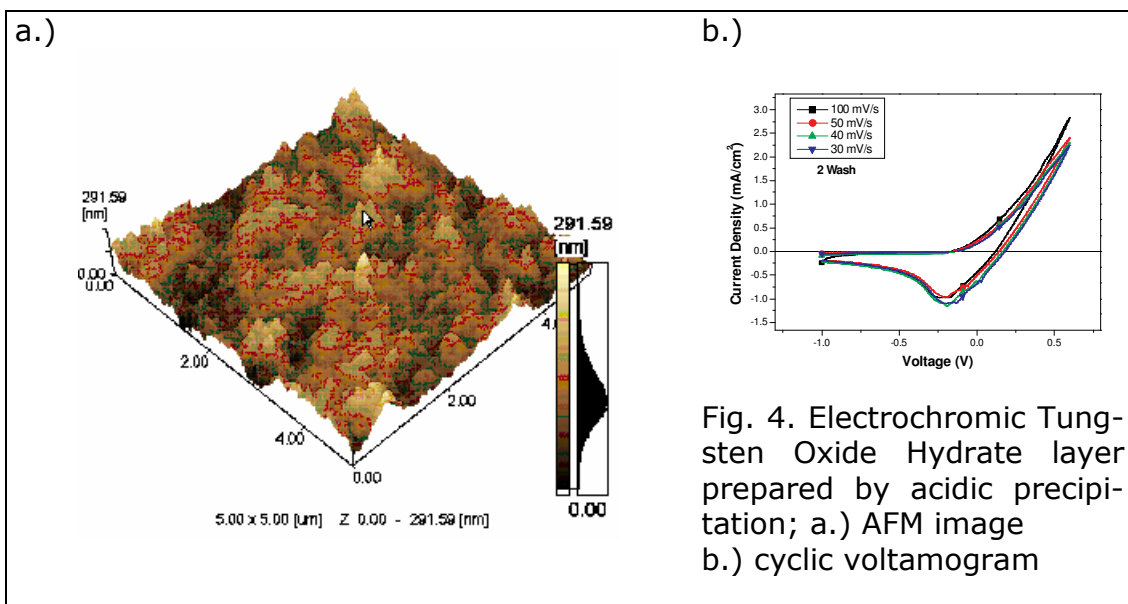


Fig. 4. Electrochromic Tungsten Oxide Hydrate layer prepared by acidic precipitation; a.) AFM image b.) cyclic voltammogram

## Hydroxyapatite and Polymer Based Bio-Compatible Composites

Csaba BALÁZSI, Ferenc WÉBER

The significant increase of the number of old people results in new aims for the materials of human implants. One of possible answers is to develop a material which does not damage the tissue at the surface of the implant and keeps an appropriate strength throughout decades of years. Another material imagined bears the mechanical load at the beginning, then promotes the formation of bone tissue and dissolves when its work becomes unnecessary. Experiments to work out processing technology for production materials with the mentioned characteristics are in progress in several research centres of the world.

Hydroxyapatite (HAP) is one of the ceramic materials often used in implants. Its bio-compatibility is fine, its strength, however, is not high. We developed a processing technology starting from natural raw materials for preparing bio-compatible hydroxyapatite based composites. The procedure is advantageous from the point of view of protection of environments and energy saving, too. Processing steps include techniques of soft chemistry and high temperature sintering, the size of particles is in the  $\mu\text{m}$  and  $\text{nm}$  ranges.

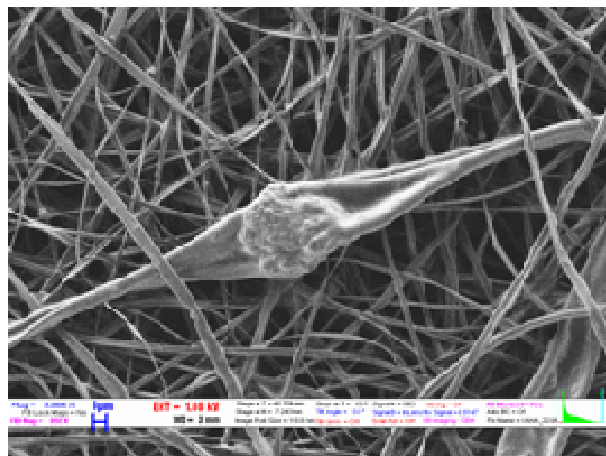


Fig. 6  
Fibrous structure of hydroxyapatite-polymer composite

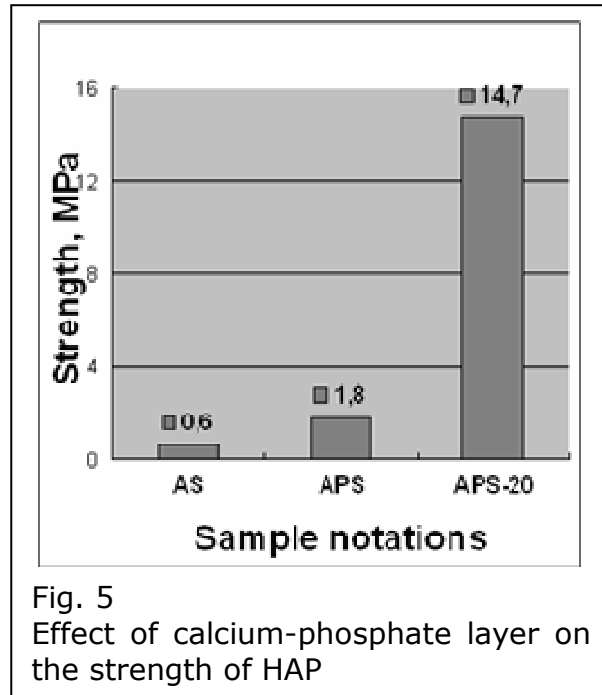


Fig. 5  
Effect of calcium-phosphate layer on the strength of HAP

Chemical vapour deposition was applied successfully to cover hydroxyapatite substrate by calcium phosphate nano and micro layers or fibres. The developed multilayers initiated a large increase of strength.

We began to study various kind of ceramic-polymer composites this year in co-operation with SUNY at Stony Brook. Electrospinning gave a 3D arrangement of polymer micro- and nano-fibres. This structure has high porosity and large specific surface, consequently provides good conditions for biodegradation.

In composites prepared in our laboratories hydroxyapatite nanoparticles were dispersed in a polymer matrix. It is thought that the nanograins may be particular places for the regeneration of bone tissue. Our experiments on the interaction between composite and tissues are continued.



## Complex Systems Group

### Evolutionary games (OTKA T-047003)

György SZABÓ; Attila SZOLNOKI; István BORSOS; Jeromos VUKOV

The frequency of cooperators is investigated in an evolutionary Prisoner's Dilemma game with two strategies (cooperator and defector) when the players are located on different two-dimensional lattices or regular random graphs (see Fig. 1).

We have studied the effect of payoff (i.e., the temptation  $b$  to choose defection), noise (temperature  $K$ ), and connectivity structures on the frequency of cooperators [60,124]. Cooperators become extinct if  $b$  is larger than  $b_{cr}$  depending on  $K$

and on the topological structure of connectivity. Two qualitatively different behaviors [function  $b_{cr}(K)$ ] can be distinguished as plotted in Fig. 2.

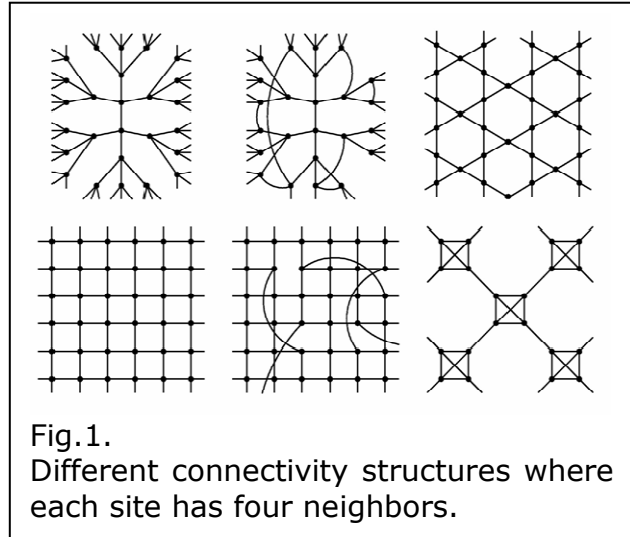


Fig.1. Different connectivity structures where each site has four neighbors.

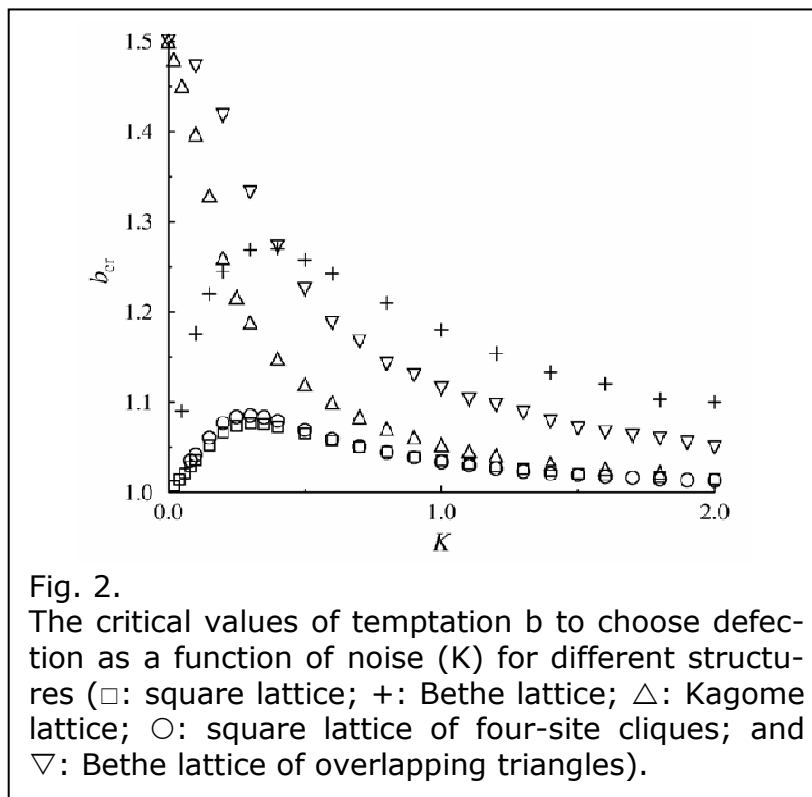


Fig. 2. The critical values of temptation  $b$  to choose defection as a function of noise ( $K$ ) for different structures ( $\square$ : square lattice;  $+$ : Bethe lattice;  $\triangle$ : Kagome lattice;  $\circ$ : square lattice of four-site cliques; and  $\nabla$ : Bethe lattice of overlapping triangles).

If the connectivity structure cannot be spanned by overlapping triangles (e.g., square- and Bethe lattices) than the system exhibits an optimal noise level ( $K$ ) where  $b_{cr}$  has a local maximum (resembling stochastic resonance). In the opposite case, the cooperation is maintained in the zero noise limit and  $b_{cr}$  decreases when increasing  $K$ . The highest  $b_{cr}$  values are found for the non-spatial connectivity structures.

## **Nonequilibrium phase transitions (OTKA T-046129)**

Géza ÓDOR; Attila SZOLNOKI

The nonequilibrium systems can also undergo phase transitions (e.g., extinctions) that can be classified by considering the universal features of the critical transitions. Our research is focused on some exceptions exhibiting unusual behaviors. The models are studied by Monte Carlo simulations and the extended versions of the mean-field methods [125].

### **Analysis of folk music**

Zoltán JUHÁSZ

Each melody can be represented by a point in the multi-dimensional melody space.

This method is applied to study the relations between the Hungarian and Eurasian folk music.

Adaptively weighted version of self-organizing mapping is developed to explore the basic roots of the Hungarian folk songs.

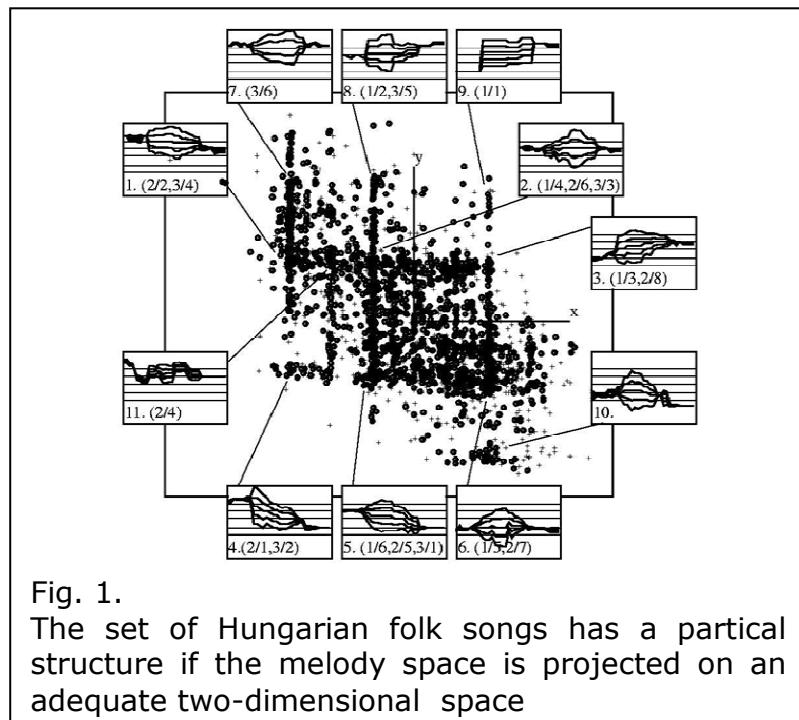


Fig. 1.  
The set of Hungarian folk songs has a partial structure if the melody space is projected on an adequate two-dimensional space

Several aspects of these techniques are used for the analysis of blood pressure pulses to diagnose some illnesses.

## *Activities*

## Scientific Promotions

### **László Péter BIRÓ**

*Synthesis and characterization of nanotube like carbon nanostructures*

D.Sc. – Hungarian Academy of Sciences

### **Miklós FRIED**

*Optical properties of ion implanted and annealed semiconductors,*

D.Sc. – Hungarian Academy of Sciences

### **János L. LÁBÁR**

*New methods in analytical electron microscopy and their applications*

D.Sc. – Hungarian Academy of Sciences

### **Ákos NEMCSICS**

Habilitation – University of West-Hungary, Veszprém

### **Antal Adolf Koós**

*Investigation of Carbon Nanotubes with Scanning Probe Microscopy and Transmission Electron Microscopy*

Ph.D. – Eötvös Loránd University, Budapest

### **Viktória Kovács-Kis**

*Examination of the SiO<sub>2</sub>-3D network in micro- and nano-crystalline, as well as amorphous samples*

Ph.D. – Eötvös Loránd University, Budapest

### **András Kovács**

*Development and transformation of phases in thin films as examined with the combinatorial method*

Ph.D. – Eötvös Loránd University, Budapest

### **Zsolt MAKKAI**

*Transmission electron microscopic study of III-nitrid and SiC nanograins*

Ph.D. – Budapest University of Technology and Economics, Budapest

### **Edit Andrea PAP**

Ph.D. – University of Oulu, Finland

### **Katalin SEDLACEK**

*Structural characterization of nanocomposite thin films*

Ph.D. – Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava

### **János VOLK**

*Porous Silicon Optical Elements*

Ph.D. – Budapest University of Technology and Economics, Budapest

### **Zsolt ZOLNAI**

*Irradiation-induced Crystal defects in Silicon Carbide*

Ph.D. – Budapest University of Technology and Economics, Budapest

### **Gyula MASA**

M.Sc. – Budapest University of Technology and Economics, Budapest

### **Tamás JÁSZI**

B.Sc. – Budapest Tech, Budapest

## Conferences and Symposia

Hungarian Nanotechnology Symposium  
(Network for Nanostructured Materials of ACC)  
21-22 March 2005, Budapest, Hungary

3rd Meeting of the International Union of Microbeam Analysis Societies,  
22-26 May 2005, Florence (Italy)

5th International Symposium on Hysteresis and Micromagnetic Modeling  
30 May – 1 June 2005, Budapest, Hungary

Summer School:  
Advanced Nanotechnologies, testing, production and application of  
nanoscale materials  
1-7 June 2005, Primorsko, Bulgaria

30th FEBS Congress - 9th IUBMB Conference  
2-7 July 2005, Budapest, Hungary

“Optical Amplifiers” (Optical Society of America)  
7-10 Aug 2005, Budapest, Hungary

SEMINANO 2005  
First International Workshop on Semiconductor Nanocrystals  
10-12 September 2005, Budapest, Hungary

24th Neumann Colloquium  
16-17 December 2005, Veszprém, Hungary

## MFA Seminar Talks

- 7 February 2005 Andreas REMSCHEID (RAITH AG, Dortmund)  
Electron beam lithography
- 9 February 2005 Dr. Sven LUBECK (Duisburg)  
Universal scaling functions of non-equilibrium phase transitions
- 16 February 2005 Dr. Alíz SIMON (ATOMKI, Debrecen)  
Investigation of novel materials by ion beam induced charge-microscopy
- 23 February 2005 Zoltán HAJNAL (MFA)  
Modelling of point defects and reactions at SiO<sub>2</sub>-SiC-Si interfaces
- 2 March 2005 Norbert KISS & Tamás SOMFAI (BME, Budapest)  
Studies of the geometric and electronic properties of carbon nanotubes
- 9 March 2005 Csaba BALÁZSI (MFA)  
Micro- and Nanocarbon additions to Silicon Nitride Ceramics
- 17 March 2005 Guy LELAY (Marseille)  
Self-assembled Ge nanodots and Si nanostructures and nanowires formed on silver surfaces
- 23 March 2005 János VOLK (MFA)  
Porous Silicon Optical Multilayers
- 30 March 2005 Mária HODOS (Szeged University)  
Rolling up the mystery of titanium-oxide nanotubes
- 22 April 2005 Zsolt MAKKAI (MFA)  
Electron-microscopic Investigations of Thin Film Group III – Nitrides and SiC Nanoparticles
- 2 May 2005 Zsolt ZOLNAI (MFA)  
Irradiation-induced crystal defects in silicon carbide
- 11 May 2005 A. A. Koós (MFA)  
Investigation of carbon nanotubes with Scanning Probe Microscopy and Transmission Electron Microscopy
- 12 May 2005 Zoltán BERÉNYI (Atomki, Debrecen)  
First experiences and result with the new SNMS instrument of the ATOMKI

- 18 May 2005 Gergely KOVÁCH (MFA)  
Variable bonding in carbon thin films
- 25 May 2005 Zoltán OSVÁTH (MFA)  
Investigation and modification of carbon nanotubes by ion beam and scanning probe techniques  
György Zoltán RADNÓCZI (MFA)  
Electron-microscopy of wide bandgap semiconductor films
- 9 June 2005 Csaba JÓZSA (Eindhoven UT)  
Precessional magnetization dynamics in microstructures
- 29 June 2005 Prof. Kazuaki SAKODA  
(Nat. Inst. Materials Science, Tsukuba)  
Selection rules for Light Scattering by Localized Eigenmodes of the Menger Sponge Fractal
- 24 August 2005 Prof. Kenneth HOLMBERG (VTT, Finland)  
Friction and wear of thin surface coatings - a modelling and simulation approach
- 7 Sept 2005 Jan KNAUP (Universität Paderborn)  
Theoretical investigation of reactions at solid state interfaces and their products
- 21 Sept 2005 Adam SOMLAI-FISCHER (architect, Budapest)  
About human-space interactions and novel technologies
- 28 Sept 2005 György Kádár (MFA)  
Precession rewriting of magnetic information bits
- 2 Nov 2005 Jerzy MORGIEL and Lukasz MAJOR  
(Institute of Metallurgy and Materials Sciences, Krakow)  
Examination of TiN/CrN hard coatings
- 9 Nov 2005 György KOVÁCS (MFA)  
Structural, mechanical and spectroscopic properties of C-Ni and CN<sub>x</sub>-Ni nano-composites
- 16 Nov 2005 Tadeusz WOSINSKI  
(Institute of Physics of the Polish Academy of Sciences)  
Anisotropic strain relaxation in lattice-mismatched III-V epitaxial layers
- 23 Nov 2005 Leonid A. CHERNOZATONSKII  
(Materials Research Group, Institute of Biochemical Physics, Russian Academy of Sciences)  
Electronic and Mechanical Properties of Carbon Nanotube Junctions

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- Roman BENES,  
Anton Paar, Graz, Austria
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- Dr. Lee JUNGIL,



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