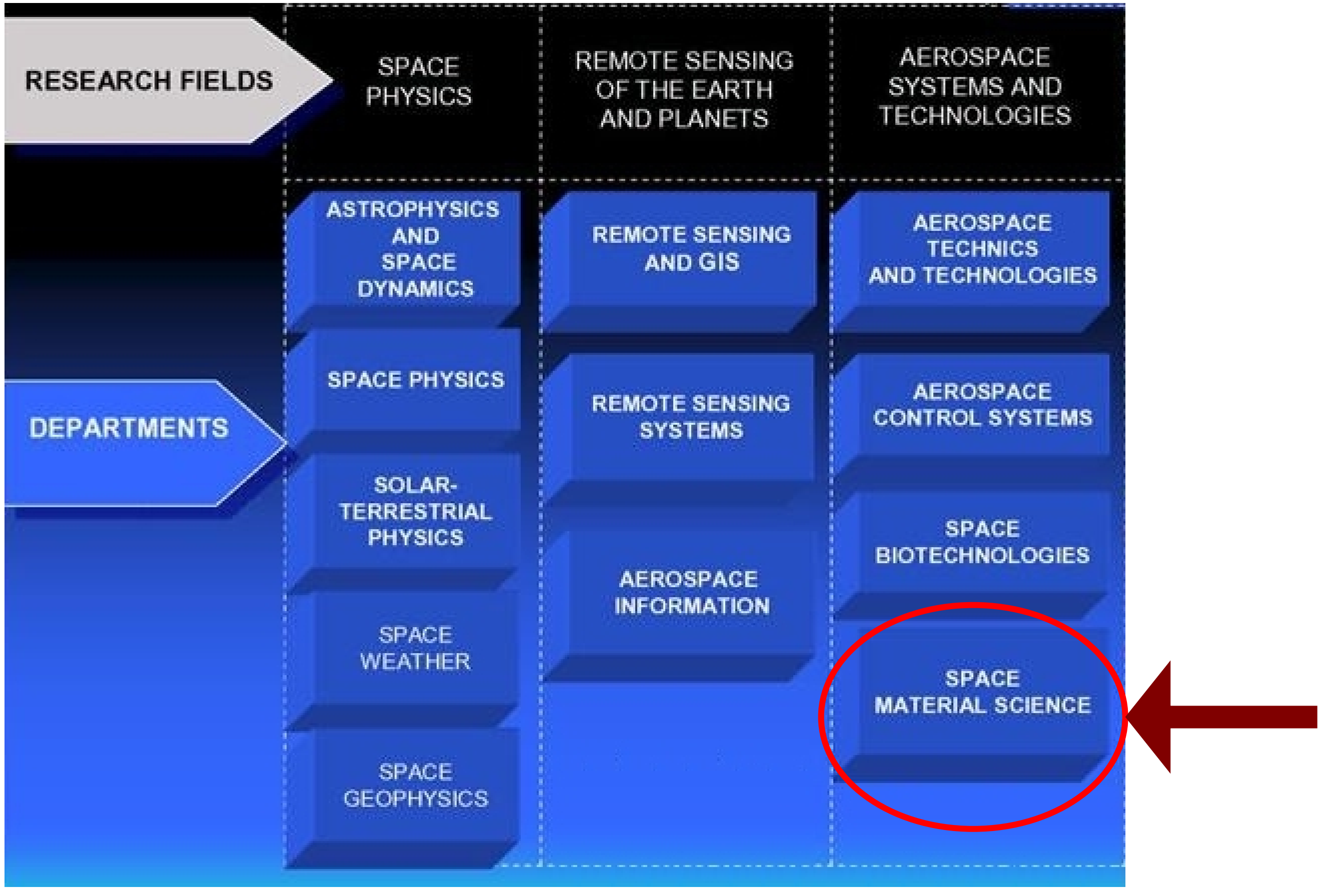
SPACE MATERIAL SCIENCE DEPARTMENT

SRTI - BAS



Overview - Research Scope

- Shock-wave synthesis of nano-diamonds
  - From mechanical engineering to biomedical science
- Response of solids and disperse media to shock-wave loading
- Multi-scale modeling of novel materials
  - Atomistic to Continuum Scale
- Vitreous carbon coatings technology
- Laboratory “Vacuum Investigations”
  - Testing and Calibration of scientific instruments for space experiments

Current Projects

"New Biodegradable Nanostructured Materials Enhancing Osteogenesis"
P.I. Julian Karadjov, PhD
Email: doktorka@abv.bg

"Multi-scale modeling of materials with enhanced performance subjected to extreme conditions - improving existing materials and predicting properties of new materials: metal alloys, composites, nanocomposites"
P.I. Roussislava Zaharieva, PhD
Email: rsz@space.bas.bg

Electroless Nickel Coatings with Reinforcing Nano- and Microsized Particles:
„New methods and tools for renovation shaft film extrusion”
„Nanostructured composite coatings based on nickel”
„Research on nano-modified metal alloys and their application in casting”
P.I. Zdravka Karagyozova, MSc
Email: karazuzi@yahoo.com

"Theoretical Investigation of the response of solids, powders and power mixtures to shock-wave loading. Applications to the synthesis of new materials."
P.I. Valentin Gospodinov, MSc
Email: vgospodinov@space.bas.bg

"Quantum Confined Stark Effect in some Nanostructures (QWs-Quantum Wells)"
P.I. Adelina Miteva, MSc
Email: admiteva@phys.bas.bg

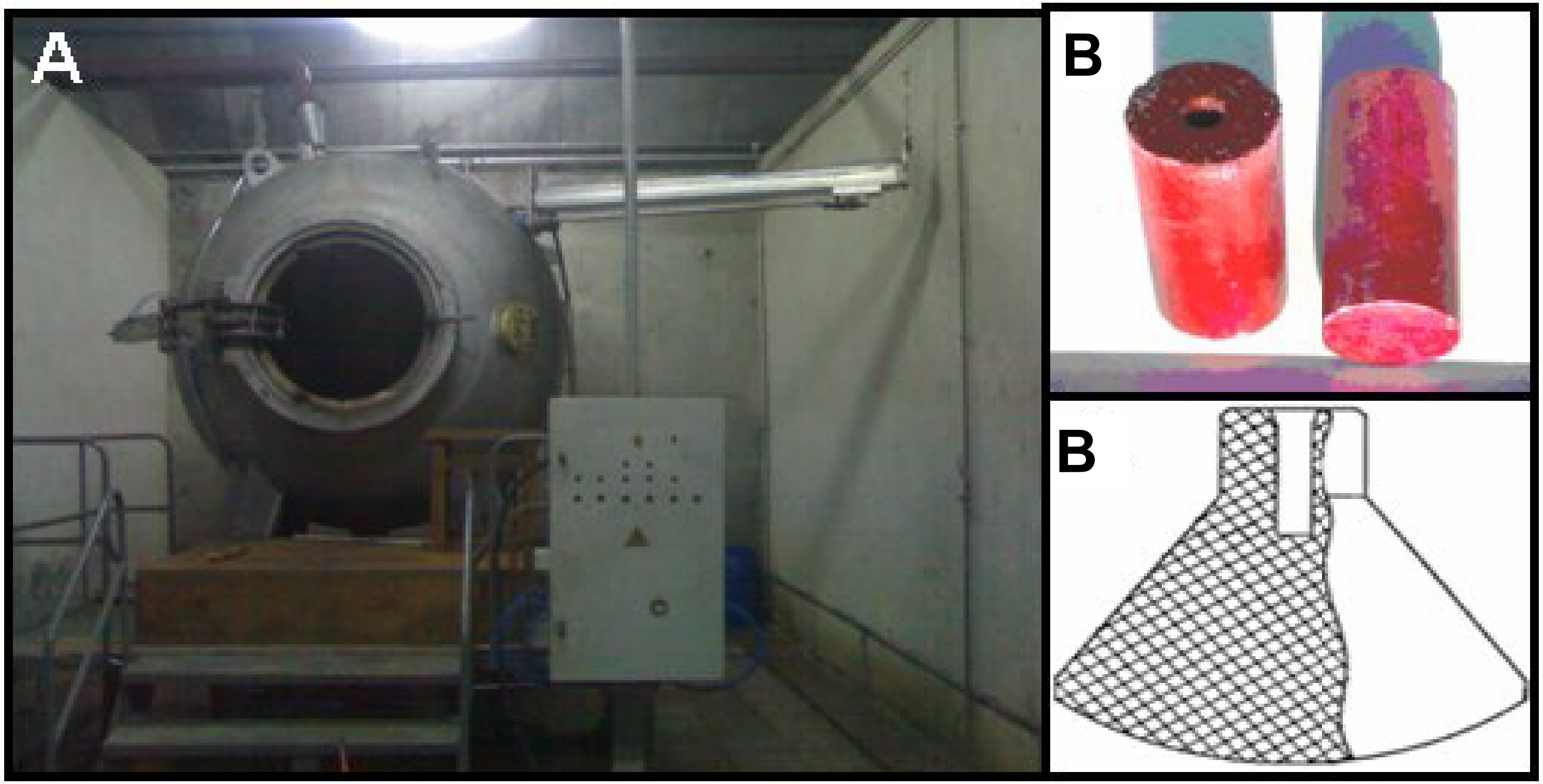
"Study of the tribological characteristics of a biocompatible ceramic material (Al_2O_3-$CaTiO_3$) coated with vitreous carbon for endoprosthesis orthopedic implants"
P.I. Dimitar Teodosiev, PhD
Email: dteod@space.bas.bg

Shock-wave / Detonation Synthesis of Nano-Diamonds

Ludmil Markov, SRTI-BAS
email: lmarkov@space.bas.bg

Synthesis and Properties of Nanodiamonds:

1. Mean size of ND nanoparticles → 4 ÷ 12 nm
2. Maximal size of ND aggregates → 60 nm
3. High surface to volume ratio → ~400 m^2/g
4. Stability of ND water suspension → up to 30 days
5. Extremely high purity with respect to heavy metal contamination (especially important for biomedical applications)



Detonation camera for ND synthesis

Different shapes of explosive charges

- tested to obtain ND with desired properties

Results: X-ray diffraction shows that the so obtained ND are reasonably pure (97-99% diamond, the rest are other carbon nanostructures)

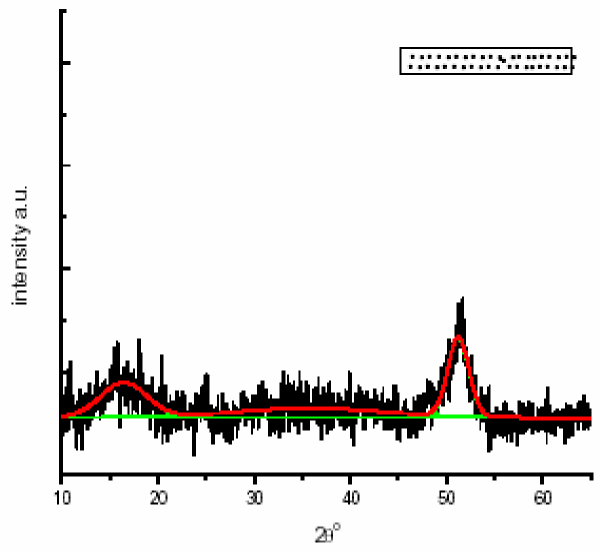


Figure 1. Powder X-Ray Diffraction Analysis of Cylindrical ND

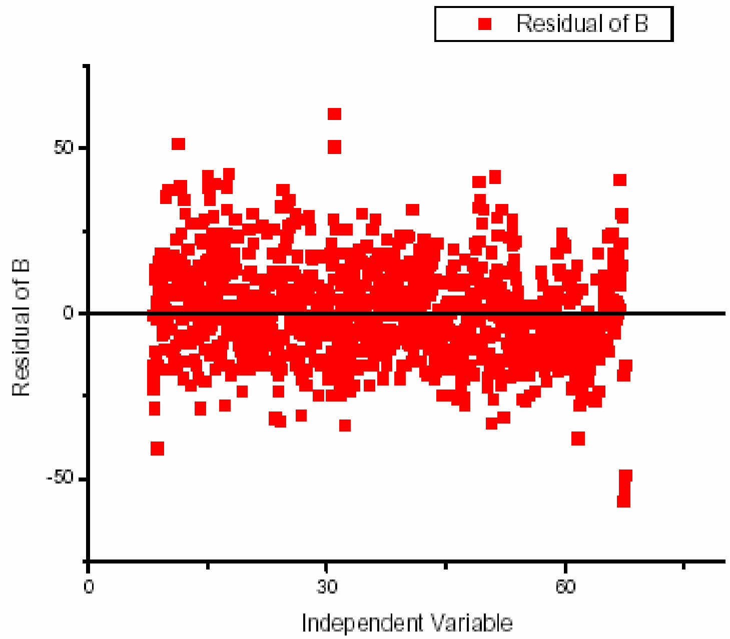


Figure 2. Residual difference plot of experimental and modeled diffractogram of cylindrical ND

MECHANICAL ENGINEERING APPLICATIONS OF NANODIAMONDS:

Electroless Nickel Coatings with Reinforcing Nano- and Microsized Particles

Zdravka Karagyozova, SRTI-BAS
email: karazuzi@yahoo.com

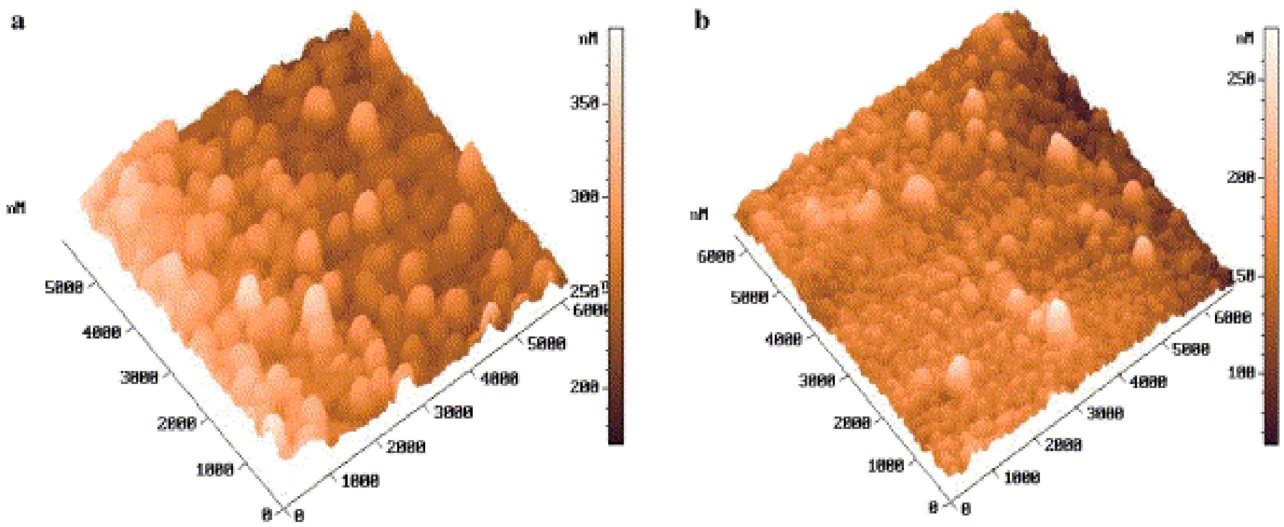


Figure 1. AFM images of Ni–P (a) and Ni–P–ND (b) electroless composite coating 6

Wear Test of Nickel Coatings

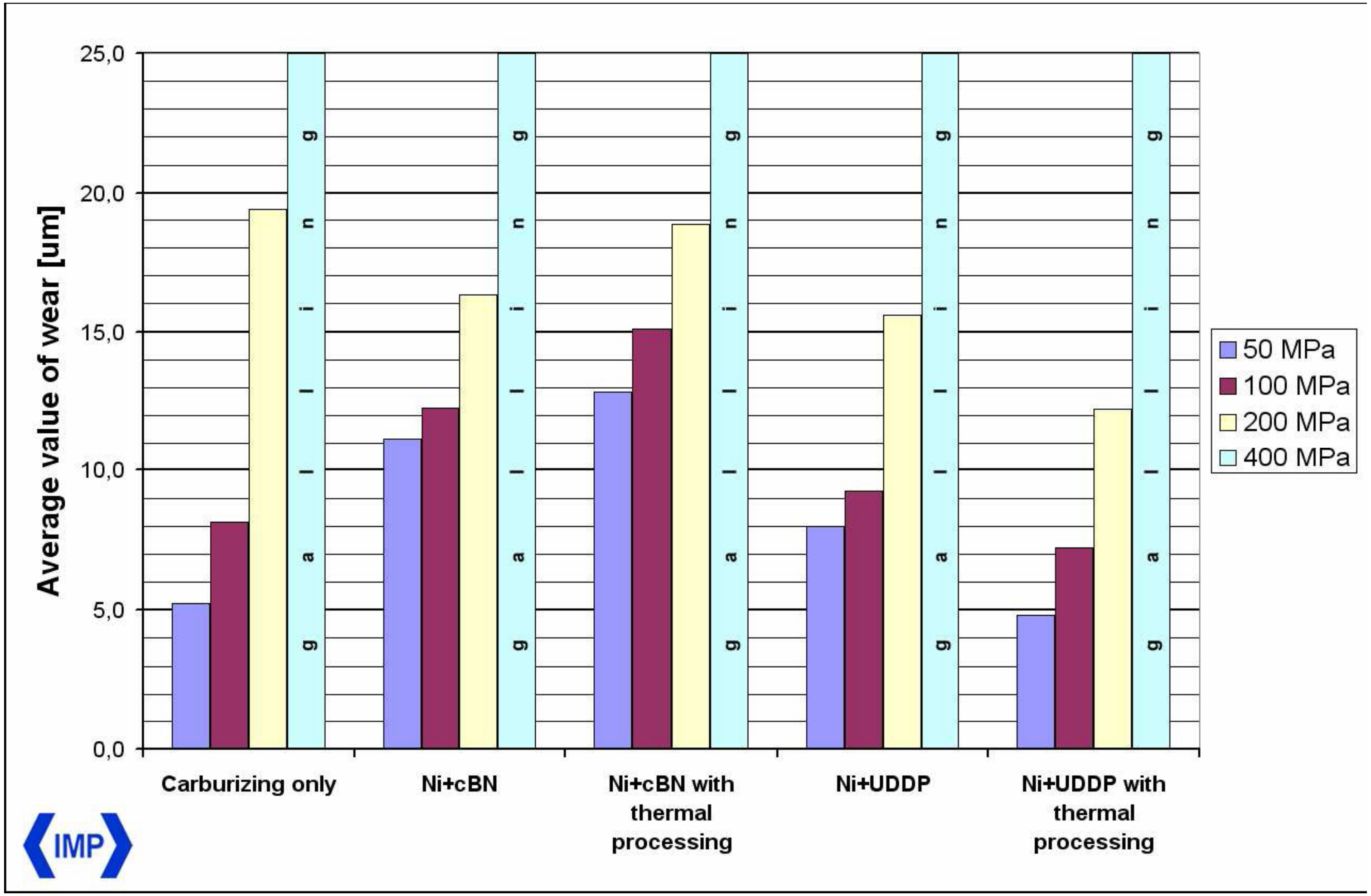
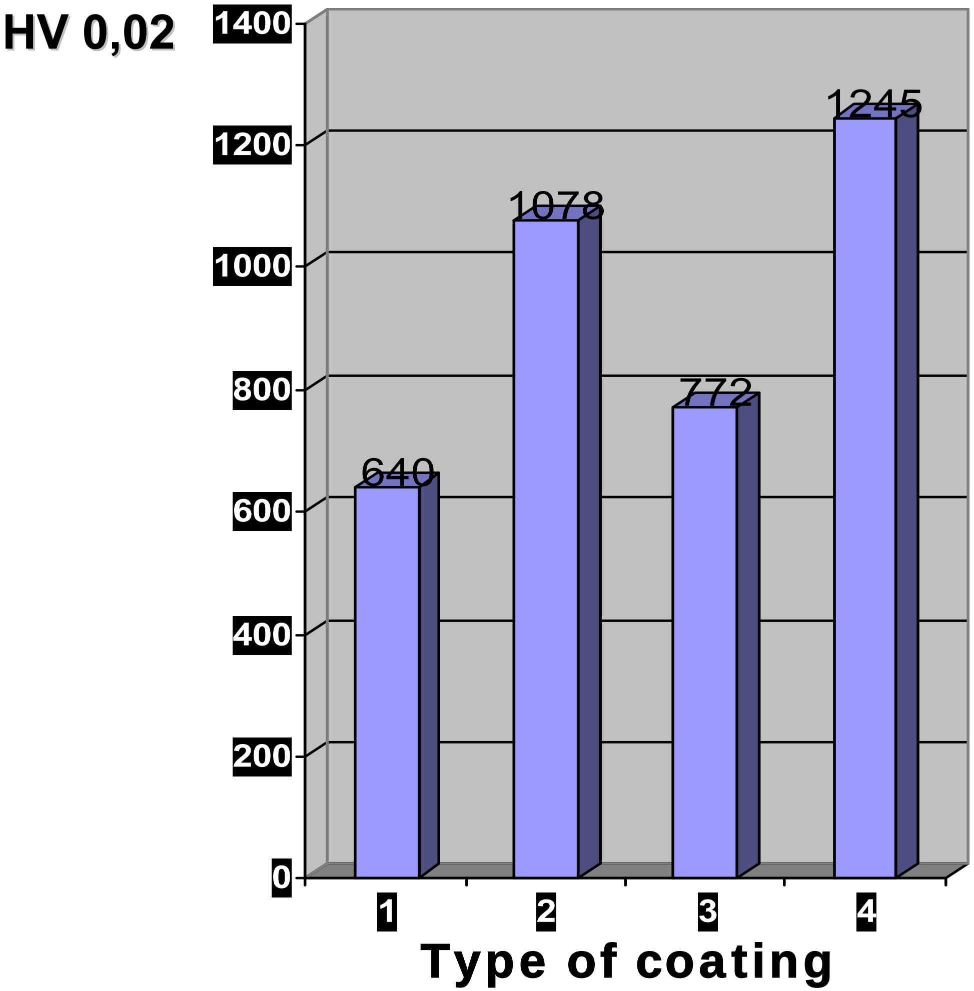


Figure 2: Averages of wear of samples after carburizing and coating with chemical method (under a load of 400 MPa all samples underwent galling) (ND is marked as UDDP)

Microhardness Measurements

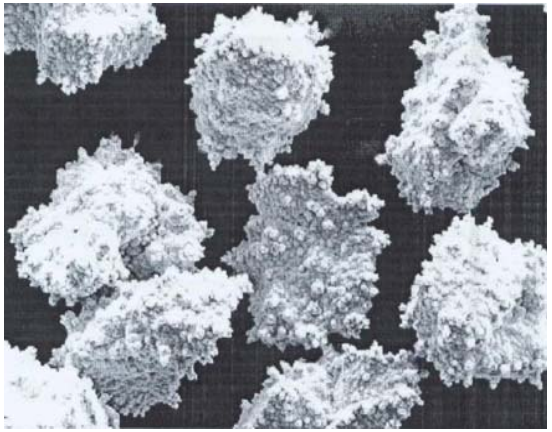


Among all the coating variants, the highest values of hardness were obtained with Ni+ND layer with next thermal processing. It was determined a considerable increase in surface hardness after thermal processing for all specimens coated.

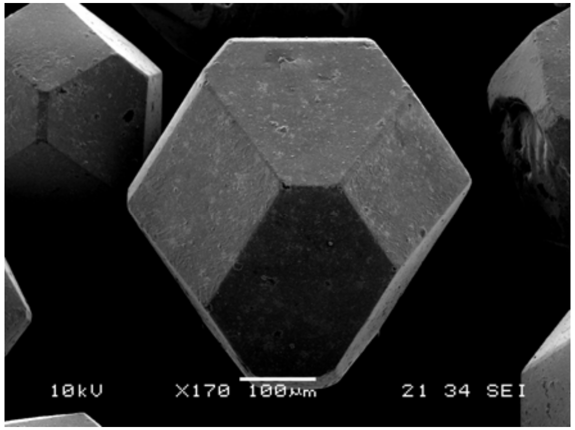
Figure 3: Microhardness of the samples with: **1-Ni+cBN, 2- Ni+cBN (TP), 3- Ni+ND, 4- Ni+ND (TP)**

SEM of Nickel Coated ND

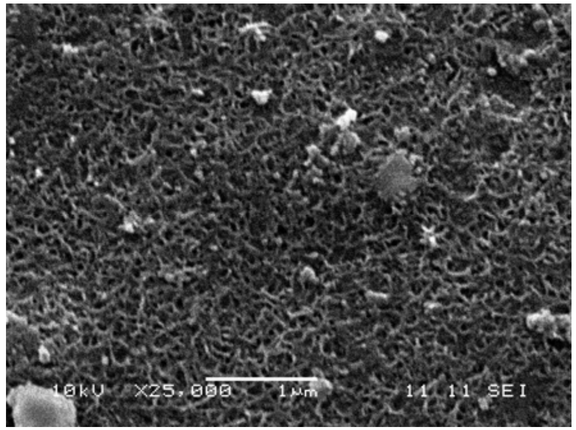
Electroless nickel coating on nano- and microsized particles
a – nanodiamond; b – microdiamond; c – SEM of nickel coating



a

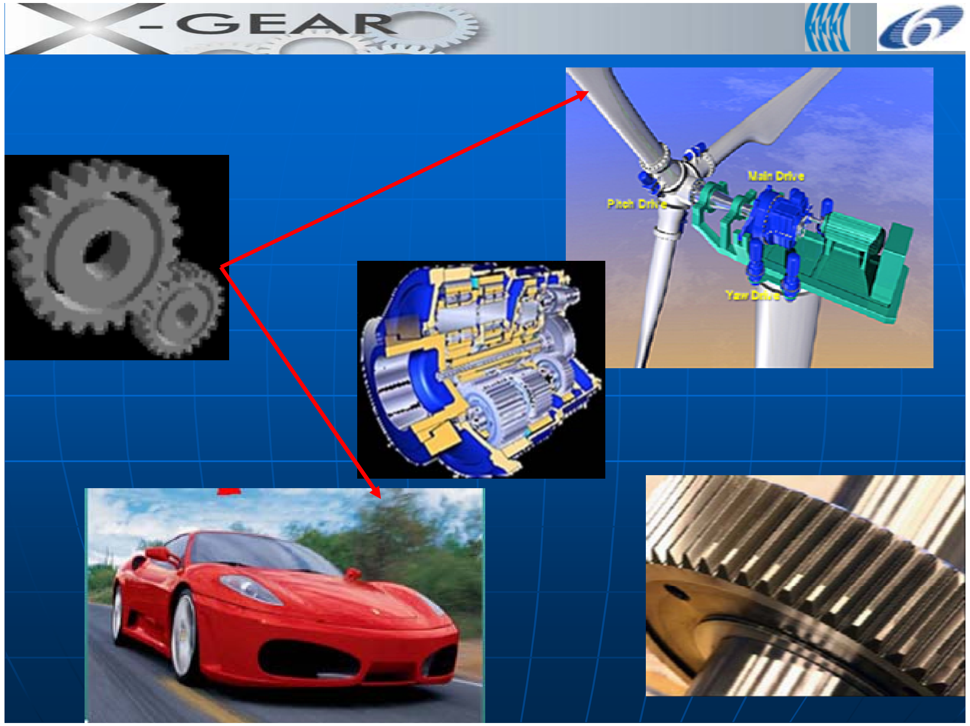


b



c

Applications in Industry



Composite nickel coatings

BIOMEDICAL APPLICATIONS OF NANODIAMONDS:

New Biodegradable Nanostructured Materials Enhancing Osteogenesis

Project ТК-Х-1704/2007, contract ДО-1-1126
with Scientific Research Fund, nanotechnology
Program of MES

Julian Karadjov, PhD, SRTI-BAS,
email: doctorka@abv.bg

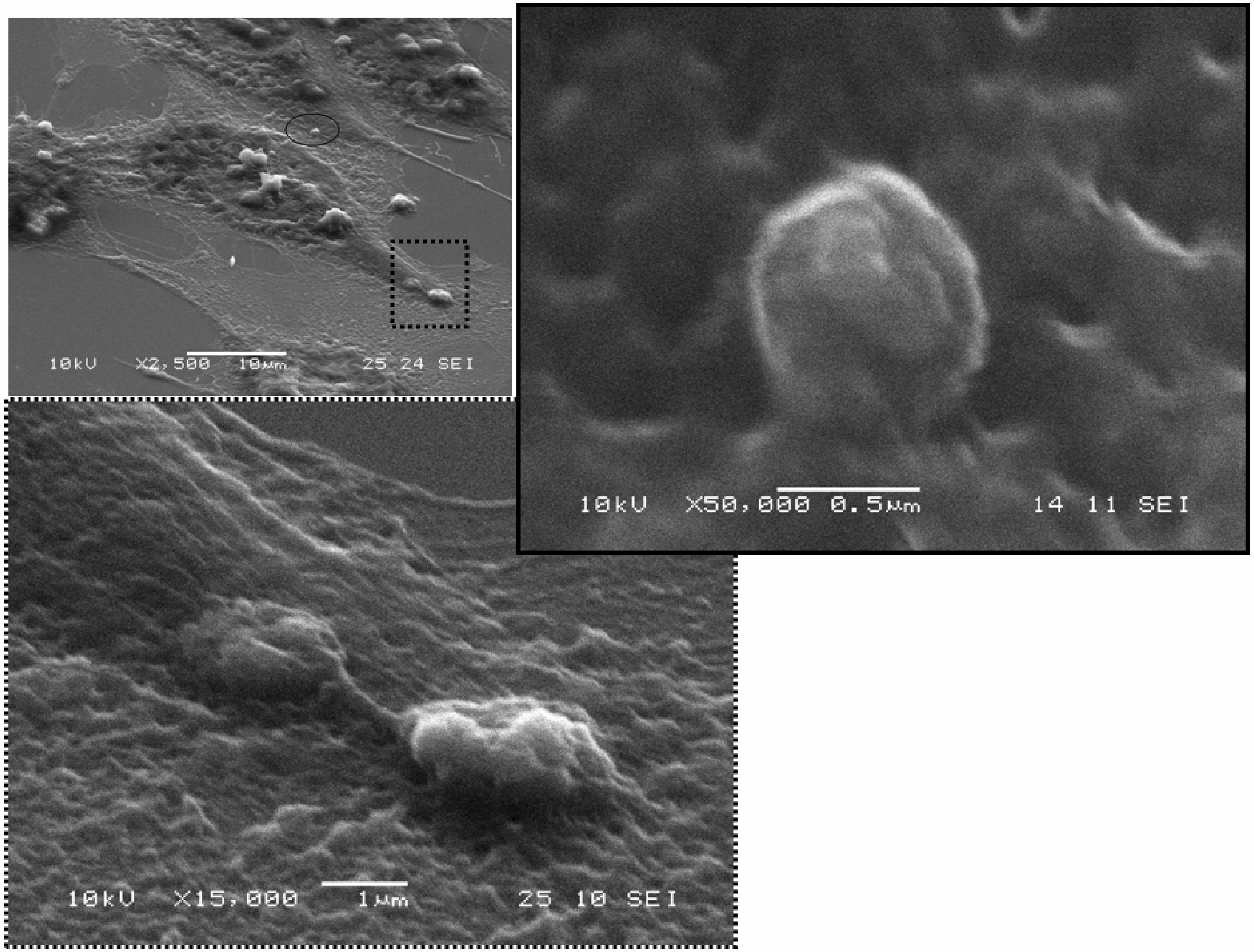
BIOMEDICAL APPLICATIONS OF NANODIAMONDS

New 3D biodegradable nanostructured materials were developed, charged with progenitor cells, with the aim to help the regeneration of bone tissue.

These materials are based on a **gel composite combining:**

Smart polymers – their water solutions display an exotic phase behaviour, which makes them suitable for biomedical applications

Nanodiamonds – they serve as crystallyzation centers for calcium phosphates crystals growth



SEM microphotograph of the interaction of endothelial cells
with nanodiamond particles

Experiments on female rats with a model of osteoporosis show that **smart polymer / nanodiamond composites, when injected into injured bone, serve as a basis for the growth of a healthy bone tissue**.

It seams, nanodiamonds play a crucial role as centers where the growth of new bone tissue begins.

When nanodiamond concentration was too high, an excessive growth of bone tissue was observed!

Results: The so proposed smart polymer – nanodiamond composite gels can be further developed as a promising new therapy for osteoporosis.

On the Response of Solids, Powders, and Powder Mixtures to Shock-wave Loading

Valentin Gospodinov, SRTI-BAS
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Introduction

- The study of the response of solids, powders, and powder mixtures to shock-wave loading, has added significantly to our understanding of physical processes which take place at high pressures, high temperatures and very short times

- The response contains valuable information about the thermophysical properties of solids and disperse media

- One particular aspect of these studies is to determine the equation of state for different materials from shock-wave experiments

Main results

- **Solids**
  - **Complete equation of state for solids, expresses in term of the material constants and the parameters of the shock Hugoniot**
  - **Expression for the temperature of the shock Hugoniot of a solid**

- **Powders and powder mixtures**
  - **The shock Hugoniot of a single component monodisperse system in which porosity appears as a parameter**
  - **Inverse shock Hugoniot (the shock volume expresses as a function of pressure)**
  - **The inverse shock Hugoniot of a two component monodisperse powder mixture**

Inverse Shock Hugoniot

Single component system :

Shock Hugoniot in variables P and V

$$P_H = \frac{(V_0 - V)c_0^2}{[V_0 - s(V_0 - V)]^2}$$

Inverse shock Hugoniot

$$V_H = V_0 \exp\left[\frac{1-(1+\beta P_H / B_0)^{1-x}}{\beta(1-x)}\right]$$

Multicomponent system

$$V_H = \sum_{i=1}^{n} \alpha_i V_{Hi}$$

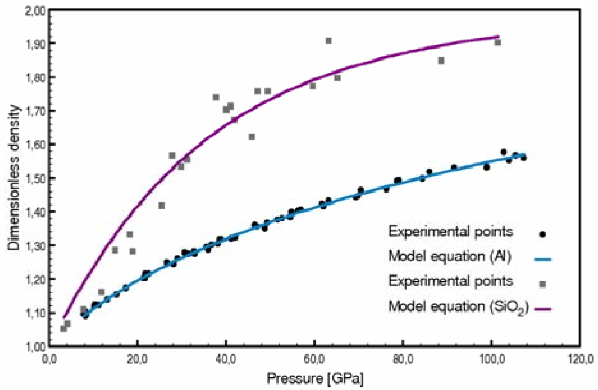
Two-component system $Al - SiO_2$

$$V_H = \alpha_{Al} V_{H,Al} + \alpha_{SiO_2} V_{H,SiO_2}$$

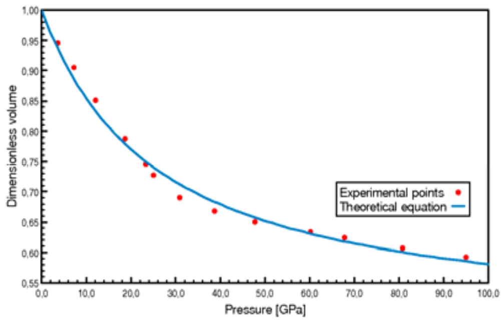
Examples

Experimental points and inverse shock Hugoniots for Al and SiO_2

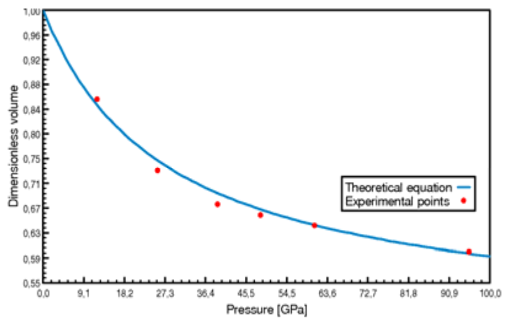
Single component systems : Al and SiO_2



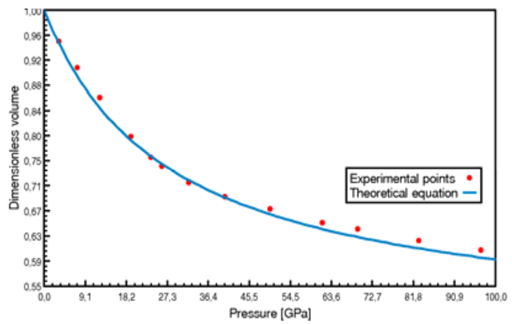
Multicomponent system : aluminum – quartz



aluminum – quartz: wt% SiO_2(50) Al(50)



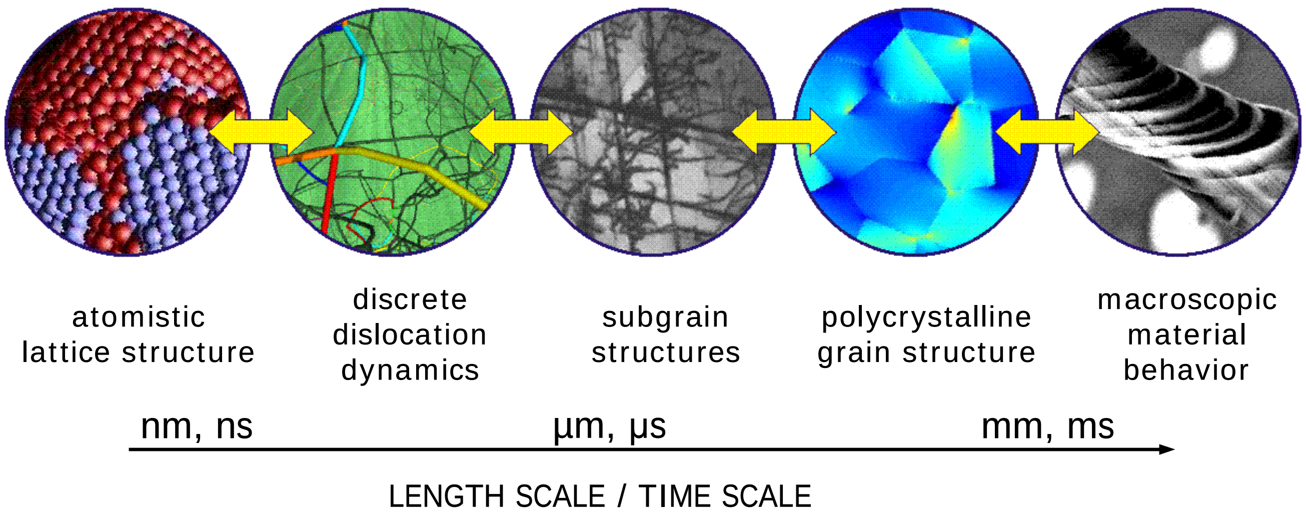
aluminum – quartz: wt% SiO_2(40) Al(60)



aluminum – quartz: wt% SiO_2(30) Al(70)

Multiscale Modeling of Space Materials

Roussislava Zaharieva, PhD
email: rsz@space.bas.bg



Atomistic to Continuum Models
MODEL → TEST → DESIGN

Approach

- Quantum Mechanics (**Ab-Initio**) Models
- **Continuum Theory** Models
- Advanced **Synthesis and Test** Methods

Materials of interest

- ❑ **Novel materials** operating under **extreme conditions**
- ❑ Multifunctional materials (**MESM**)
- ❑ Metal oxidation; Combustion
- ❑ Gas-metal surface phenomena

Research goal

→ **predict** the mechanical behavior of engineering materials;
design **novel materials** with exceptional performance

→ **improve** already existing materials:
metals, metal alloys and composites with nano reinforcements (i.e. CNT)

Computing: *Bulgarian GRID Portal*

- **Clusters at BAS (** 9 grid-clusters, CERN initiative)
  - **Madara cluster at IICT*, IOCCP****

    Linux based system
    102x4 microprocessors (Intel XEON HyperThreading E5520)
    Location: Supercomputing Center of the IOCCP-BAS**

- **IBM Blue Gene/P super computer** (since 2008)

    Linux based system :
    8192 microprocessors: 23.42 trillion operations per sec (TFLOPS)
    Location: Supercomputing Center of the SAITC***

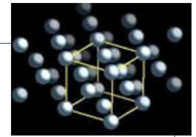
BG08-MADARA
Grid Cluster

Physical CPU	800
Logical CPU	800
Spec CPU 2006	21440
SI2K	1600
Storage	24 TB
Location	IOCCP-BAS

* IICT – Institute of Information and Communication Technology
** IOCCP – Institute of Organic Chemistry with Center of Phyto Chemistry
*** SAITC – Bulgarian State Agency for Information Technology and Communications

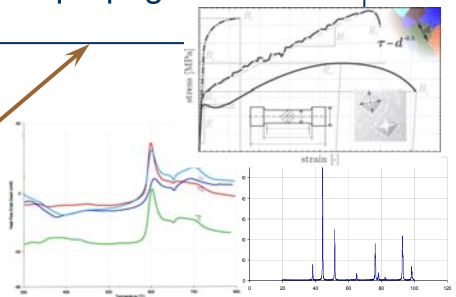
Novel materials, Development

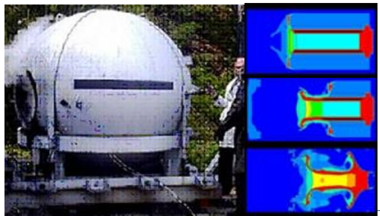
Material Tests and
Model Validation Tests



Multiscale Modeling:
- *First-Principles,* MD, Meso scales and continuum scale models.
- Constitutive Equations, dual branches of Failure criteria
- Bridging scales to continuum

Critical experiments to validate constitutive equations, strength, toughness, reaction Initiation, and Reaction propagation



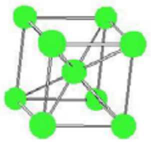


- Synthesis
- Binder + Gas phase materials
- Reinforcement
- Fracture characteristics and improvement of fracture toughness

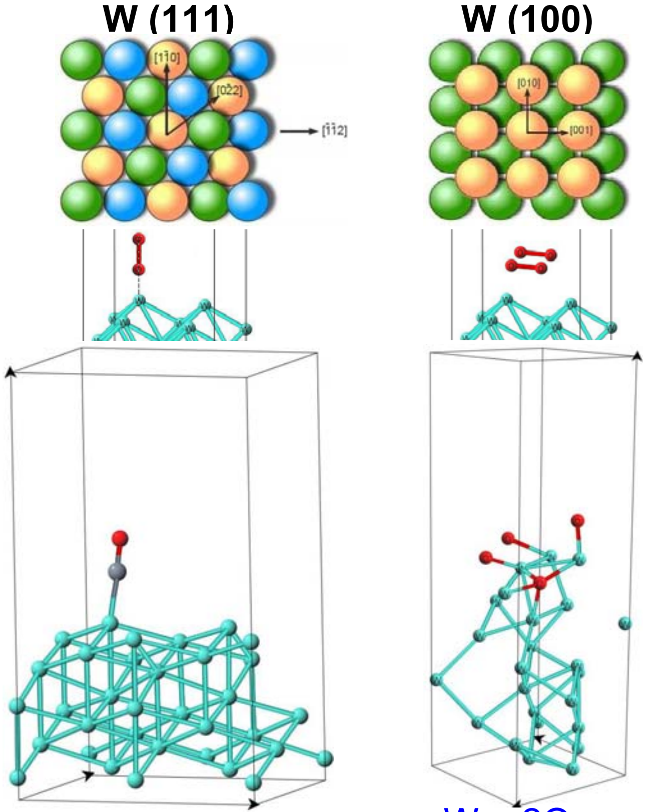
APPLICATIONS
Design, Analysis to replace Conventional materials with Advanced function materials; demonstration of an application; Hybrid Designs

Ab-Initio Chemical Reaction Models

Metal – Gas



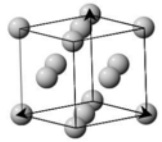
W (bcc), #74: [Xe] $4f^{14}\,5d^{4}\,6s^{2}$



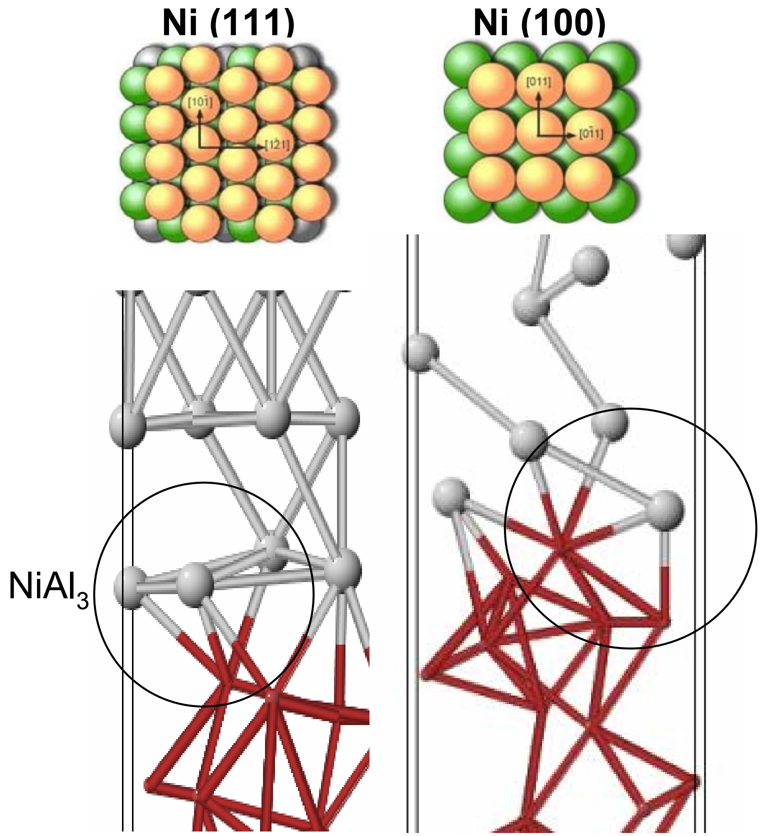
W + CO
0 K
“ontop” site

W + $2O_2$
950 K
“lying down”

Metal – Metal

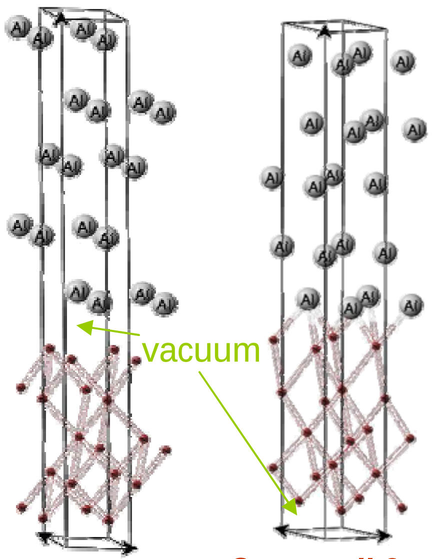


Al (fcc), #13: $1s^2\,2s^2\,2p^6\,3s^2\,3p^1$
Ni (fcc), #28: $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2 3d^8$



Ni + Al mixture, 660 C

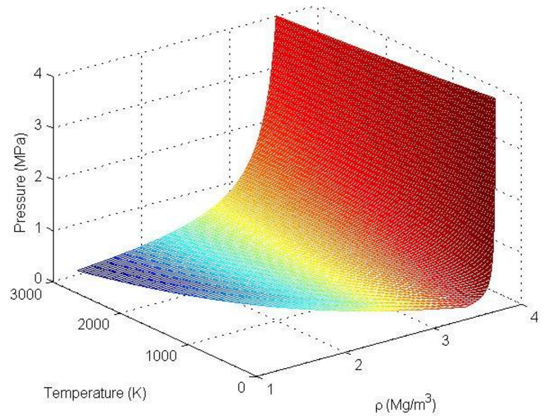
MESM, Equation of State

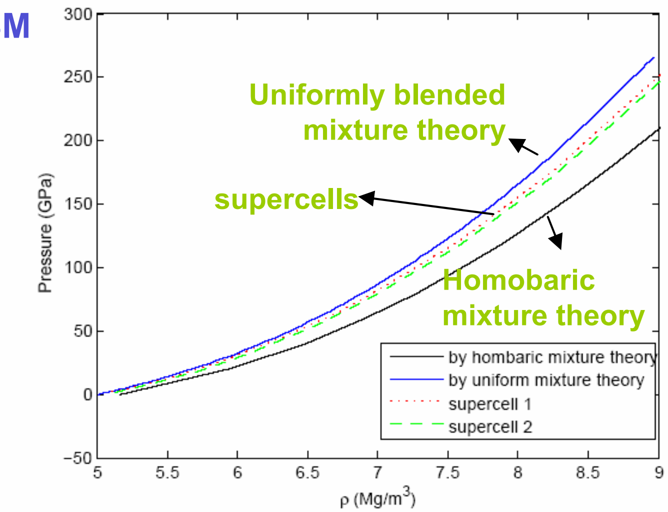


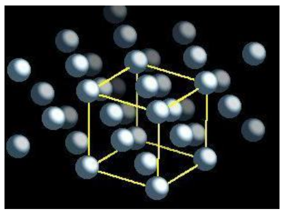
Supercell 1 **Supercell 2**

By Mixture Theories
By Supercell Approach

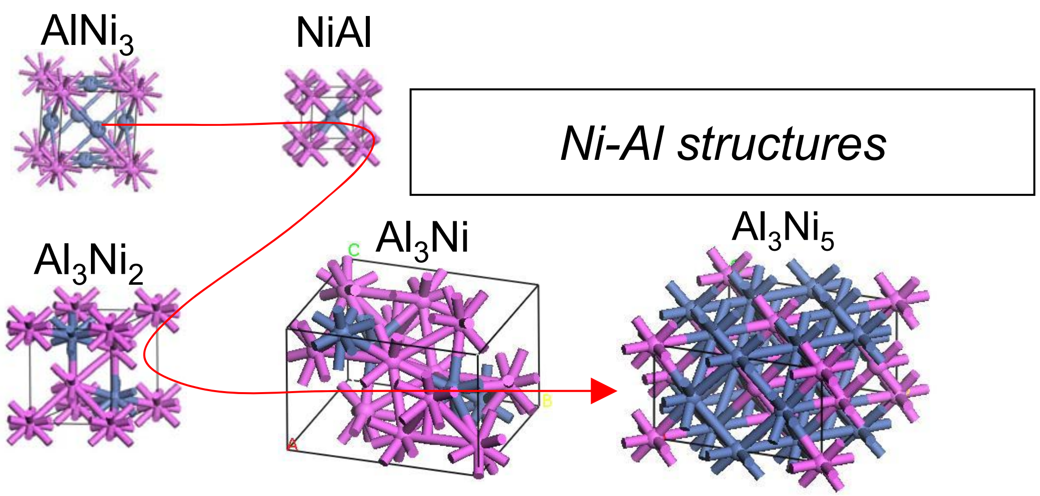
EOS of 3Al+Ni+15%porosity MESM





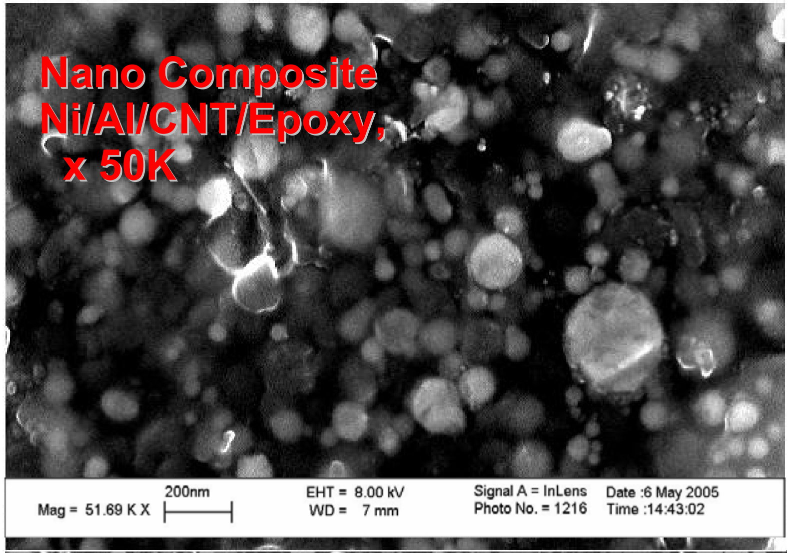


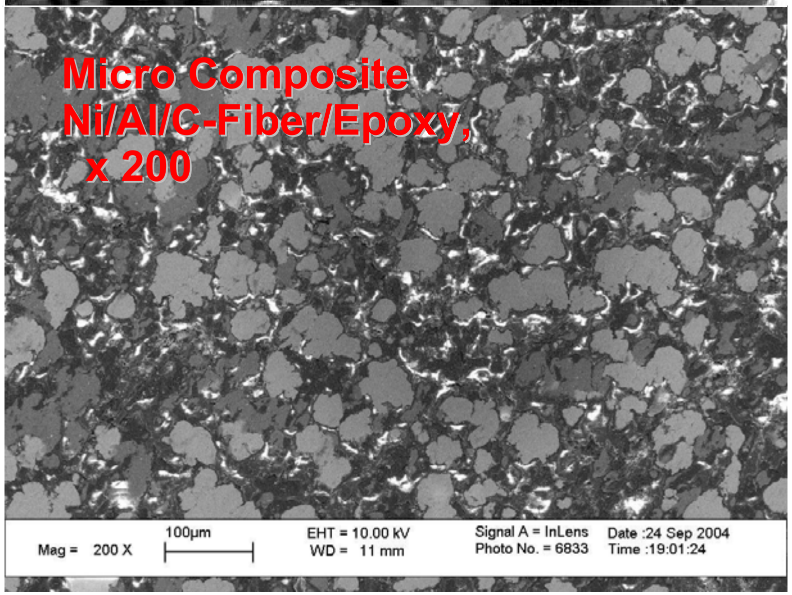
Al, Ni (fcc)



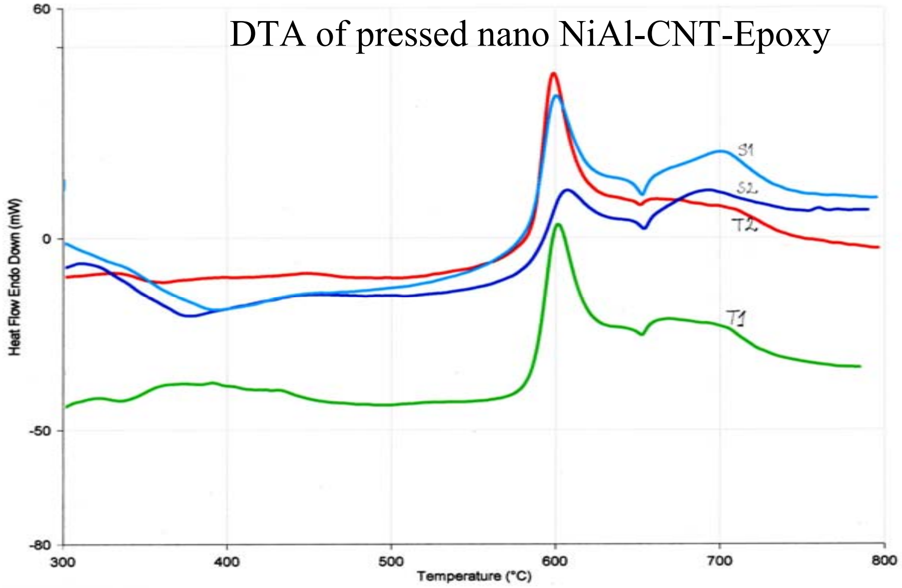
Characterization

SEM of pressed nano and micron powder samples

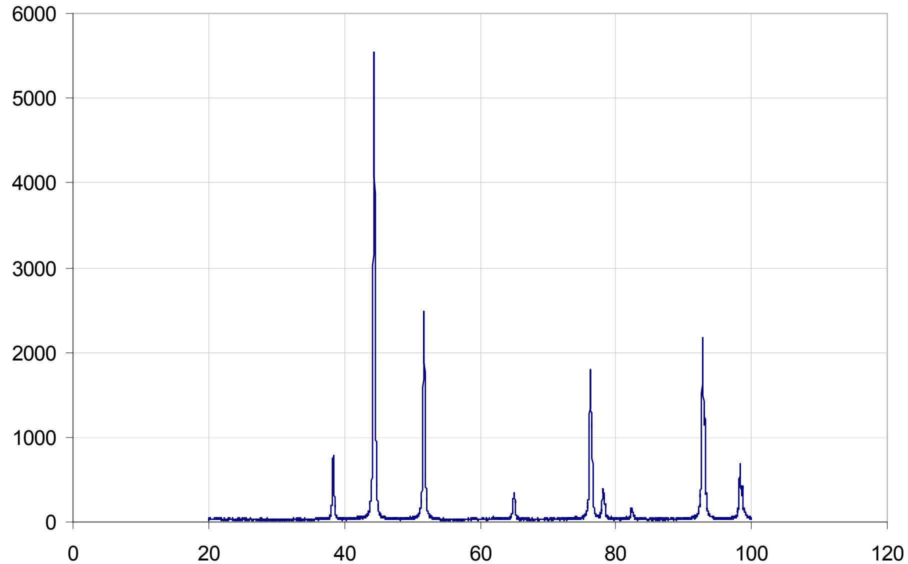




DTA of pressed nano NiAl-CNT-Epoxy



XRD of pressed nano NiAl-CNT-Epoxy



VITREOUS CARBON TECHNOLOGY

Assoc. Prof. Dimitar Teodosiev, PhD, SRTI-BAS
email: dteod@space.bas.bg

Spherical probes for measurements of electric fields aboard satellites

Use of a double probe -

measuring DC and AC electric fields in space plasma aboard satellites, rockets, and space stations

1980: Original method of glass-carbon coating on surfaces of graphite and ceramic materials

- for exploitation of the probes for measurements of electric fields in the ionosphere-magnetosphere plasma on board of satellite "IK-Bulgaria 1300"
- created by a group at SRTI and Institute of Metal Science - BAS

The method is protected by a patent in Bulgaria.

Satellite IK-Bulgaria 1300, launched 1981

Technological process for obtaining Vitreous Carbon Layers

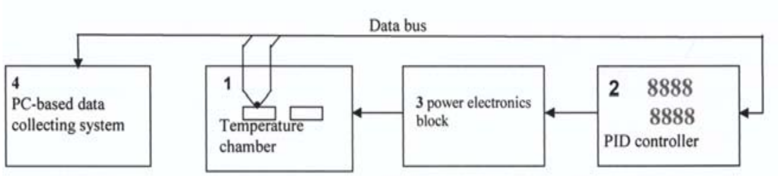
❑ Production of carbon-hydrogen substance (CHS)

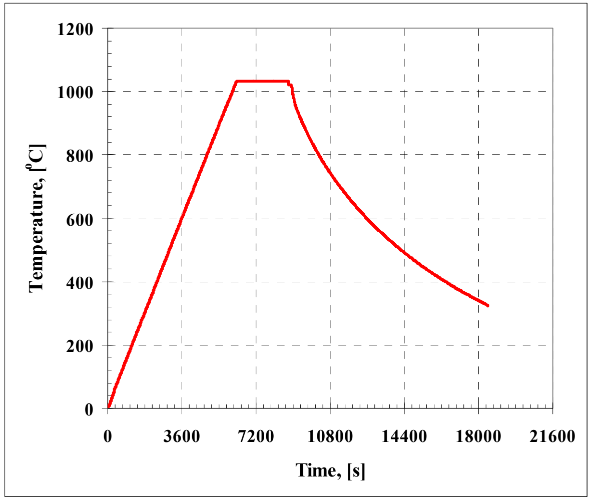
- ➢ Obtaining of Starting material for probe surface coating:
  - ✓ Polyvinyl chloride (PVC) powder was decomposed in an atmosphere of pure Ar or N_2 by holding for 30 min at temperatures 390-400°C. A black shining substance was obtained; analysis showed only the presence of C and H and it could be represented by the generalised formula C_8H_7.
- ➢ Coating procedure:
  - ✓ Thus, the obtained material is thermally treated in vacuum or argon atmosphere at temperature 1000 °C with rate of heating 15-20 °C /min and duration 5-10 minutes. After cooling, the process of the precipitation of the polymer materials is repeated several times until obtaining of surfaces with max thickness 20 μm.

Laboratory Equipment for Vitreous Carbon Technology

Four vacuum high-temperature furnaces with temperature regime control with accuracy of 1°C and data collection:

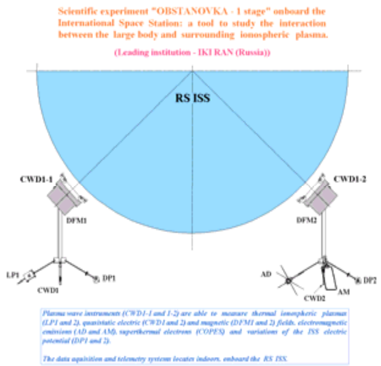
- Up to 1000 °C; Up to 1300 °C; Up to 1500 °C; Up to 2000 °C



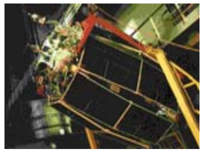


VITREOUS CARBON TECHNOLOGY ABOARD SATELLITE EXPERIMENTS

"IC Bulgaria 1300" 1981

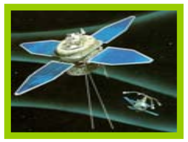


- Project "Potential"- body charge of space vehicles, Russia;
- Experiment "Obstanovka" on-board the International Space Station ("ISS , 2012)

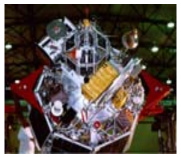


"IC 24", 1989

"IC 25", 1992



"Interball-2", 1996

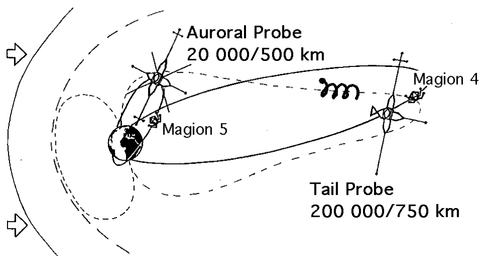


"Magion 2", 1989

"Magion 3", 1992

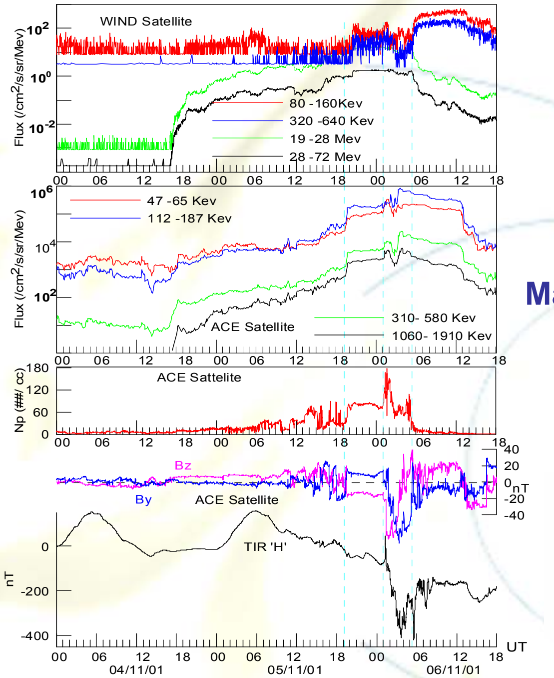
"Magion4", 1995

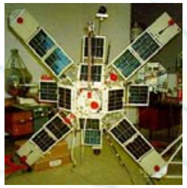
"Magion 5", 1996



The Interball Mission

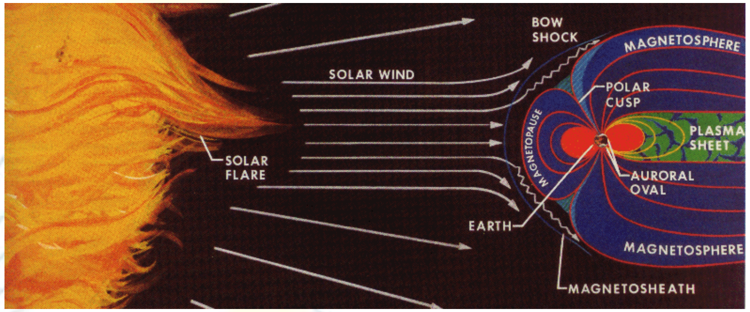
Use of the results from Electric Field measurement to Space Physics and Space Weather problems





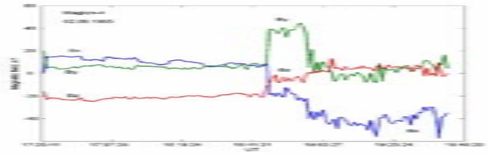
Magion-4 Satellite

Magion-5 Satellite



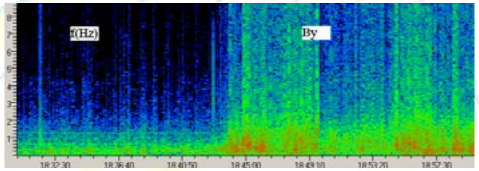
The following results are expected:

- To clear up the basic physical relations between generation of FAC and ELF/ULF waves in the magnetosphere.
- To have more adequate knowledge on the microstructure of wave processes in the boundary region of the magnetosphere (magnetosheath, magnetopause, cusp) on the base of multi component wave measurements.
- To receive a better estimation of the transfer of MHD energy from the magnetosphere towards the atmosphere of the Earth.



Magnetic field measurements in the magnetosphere.

The resuts of this project are presents at international scientific meetings and conferenses and published in scientific journals: *35th COSPAR, Paris, France 2004; 36th COSPAR, Beijing, China, 2006; ISROSSES, Varna Bulgaria 2007; PLASMA - 2006, Jaipur, India 2006; WDS 2007, Praha , Czech Republic,2007; Journals ASR*, *JASTP end ad.*

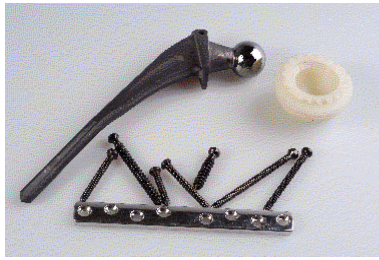


ULF waves in the magnetopause region

VITREOUS CARBON TECHNOLOGY in other AREAS

Medical Implementation :

-Composite ceramic materials based on vitreous carbon as transplanting materials in the human organism.

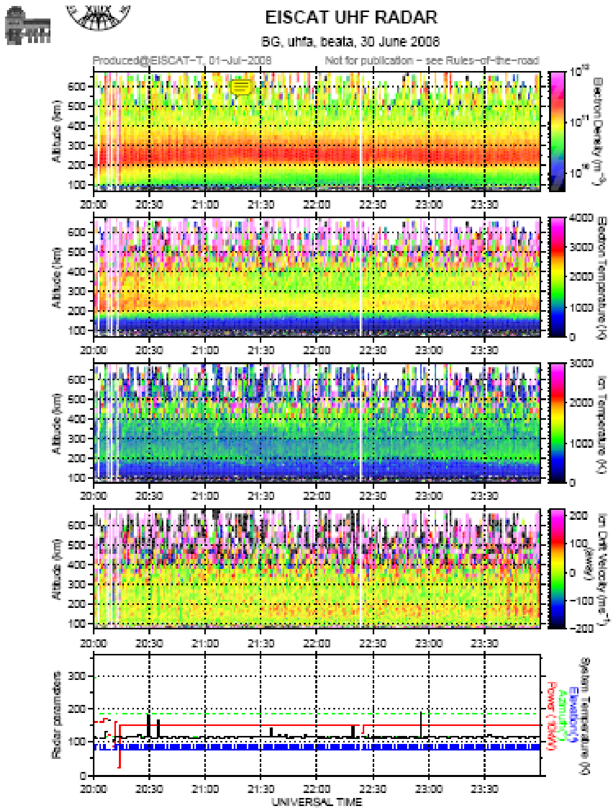


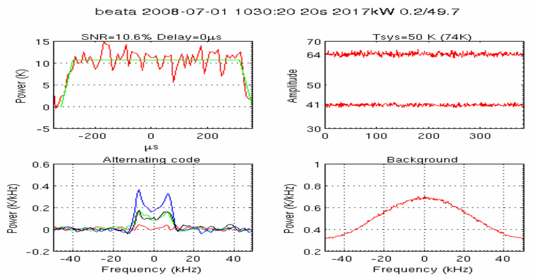
Implementation in Industry (mechanical, chemical and other) :

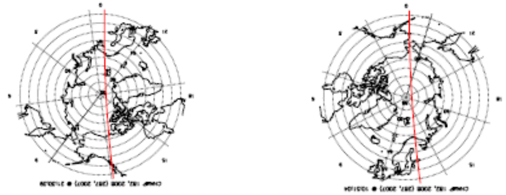
-Supports, crucibles, fiberguide, elements and the details used at receptions the pure substances.

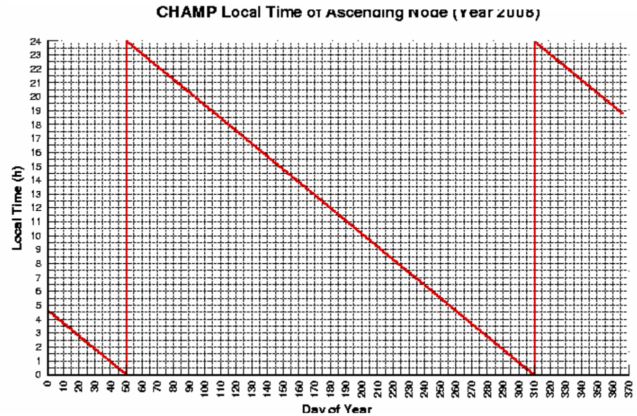
Implementation in Powder Metallurgy :

-Carbon hydrogen containing substance as donor of carbon for Powder Metallurgy (PM)

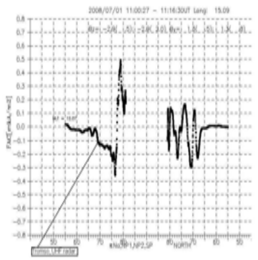


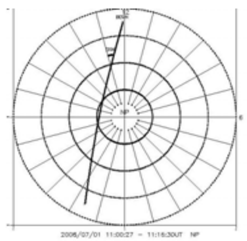


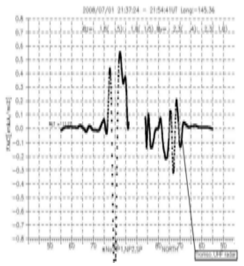


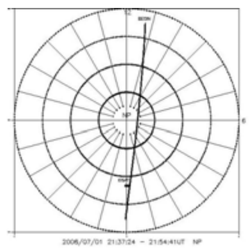


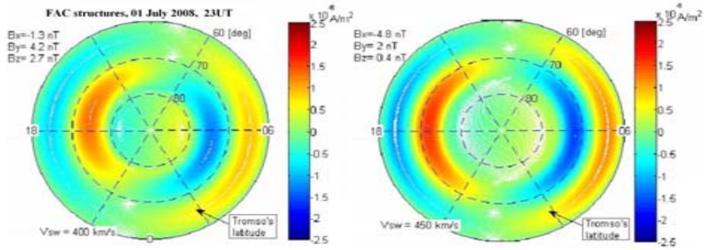
EC EISCAT TNA Program (2008 – 2011) "Magnetosphere/Ionosphere Coupling: Large Scale and Small Scale FAC Structure Interactions and Energy Transfer in the System" PI - Dr. D. Teodosiev











D. Teodosiev, et all, (2011), *Comptes rendus de l'Académie Bulgarie des Sciences* , vol. 64, № 5, pp. 729-736, 2011

BULGARIAN ACADEMY OF SCIENCES

SPACE RESEARCH AND TECHNOLOGIES INSTITUTE

Laboratory “Vacuum Investigations”

Tinka Grozdanova

Senior Research Associate

History and Main Activities of the Laboratory

- **Created in 1987**
- **Research Area**
  - ❑ Processes, materials and devices, related to space applications
  - ❑ Vacuum Tribology and Materials Science
  - ❑ Development of new composite materials with improved anti-frictional properties
- **Collaborations**
  - ✓ Institute of Materials Science,
    National Academy of Sciences of Ukraine
  - ✓ Austrian Research Centre Seibersdorf,
    Aerospace Materials Department

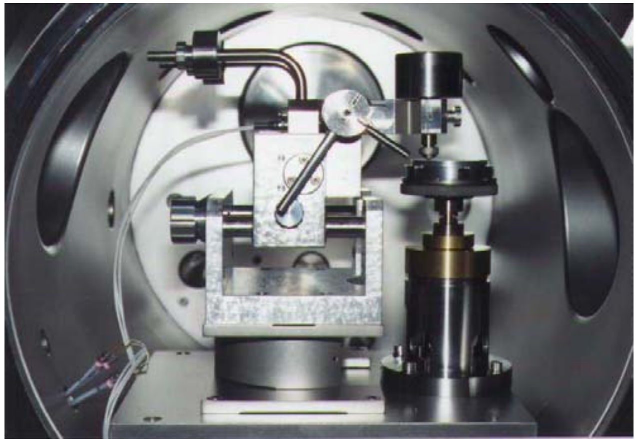
New Composite Materials with improved anti-frictional properties of the type “IPM”

Functionality

- **new class** of highly effective composite anti-frictional materials
- work flawlessly
    - ➢without lubrication
    - ➢in the absence of oxygen, moisture and in vacuum
    - ➢Without formation of centers of tear, gearing and cold welding at the tribocontact

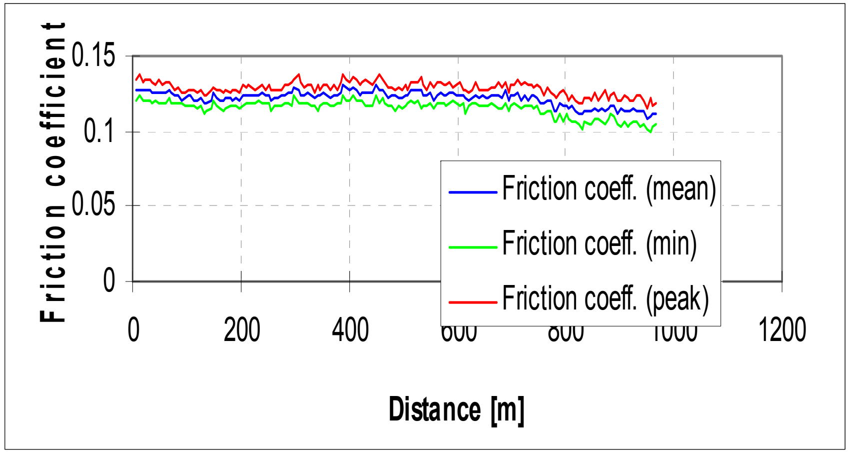
Tribological Characteristics

- Small stable coefficient of friction during long exploitation
- High wear sustainability at increased loading at the point of contact
- Adaptivity of the frictional surface to the regime of friction

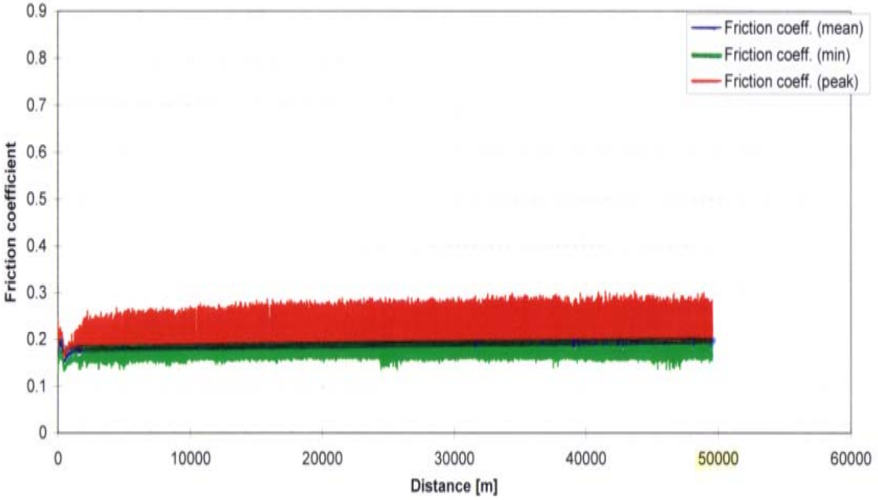


Изследване с UHV- трибометрична апаратура

Material IPM-304



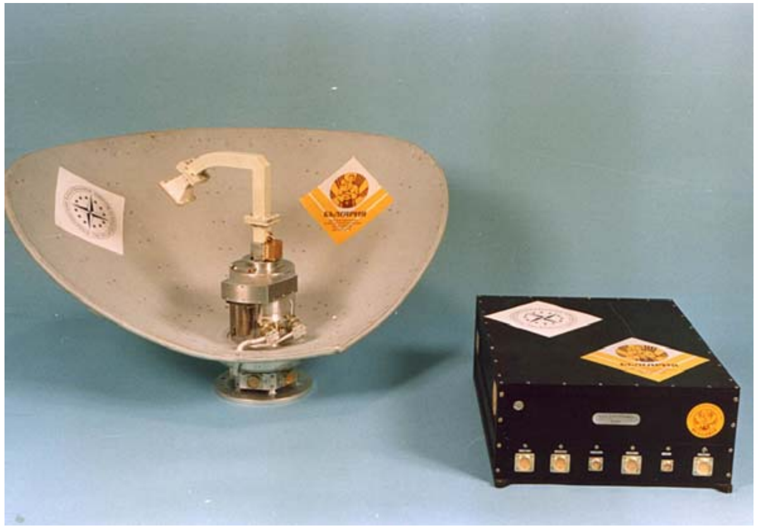
Variation of the coefficient of friction during 1000 meters for a gearing in dry friction and in vacuum with speed 1.0 m/s and load 2 N (IPM-304)

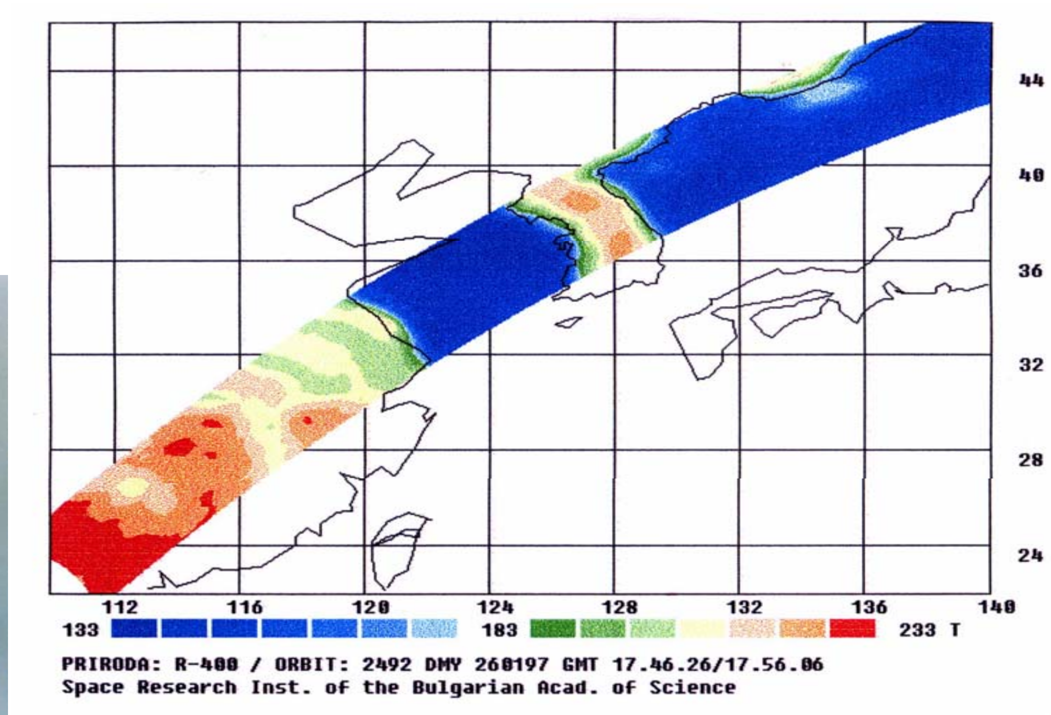


Variation of the coefficient of friction during 50 000 meters for a gearing in dry friection and in vacuum with speed 0.2 m/s and load 20 N (IPM-304)

Material IPM-301

Material **IPM-301** is used in the gears of the starting module of the system **"P-400"**, installed on the Orbital station **"MIR"** (1996 – 2001)





View of part of the Earth surface in the trajectory of the station "MIR" in the region of **Indo-China – Korean Peninsula**, obtained by the radio-metric system "**P - 400**" in space

QUANTUM CONFINED STARK EFFECT IN SOME NANOSTRUCTURES (QWs- QUANTUM WELLS)

A. M. Miteva

MODELLING STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF SEMICONDUCTOR NANOSTRUCTURES AND NANOSTRUCTURED DEVICES WITH NUMERICAL SEMI-EMPIRICAL TIGHT-BINDING METHOD.

THE ELECTRIC FIELD EFFECTS (HEREAFTER TERMED STARK EFFECTS) ON DIFFERENT QW STRUCTURES ARE VERY IMPORTANT FOR SEVERAL REASONS:
-DUE TO THE POSSIBILITY OF MAKING VARIOUS FAST ELECTRO-OPTICAL DEVICES;
-MANY SEMICONDUCTOR DEVICES BASED ON QWS WORK UNDER AN APPLIED ELECTRIC FIELD;
- IN ANY REAL TRANSPORT EXPERIMENT, EXTERNAL ELECTRIC FIELDS ARE APPLIED TO THE SYSTEM.

AS A RESULT OF SUCH CALCULATIONS IT IS POSSIBLE TO STUDY THE STARK SHIFTS OF THE QW ELECTRONIC STATES AND THEIR SPATIAL DISTRIBUTIONS. WITH THIS ESSENTIAL AND NEW INFORMATION WE CAN LOOK FOR A POTENTIAL PROFILE THAT PROVIDES GOOD STARK EFFECT CHARACTERISTICS OF A GIVEN QW. THIS WILL FACILITATE THE SEARCH FOR NEW MATERIALS POSSESSING UNIQUE ELECTRON AND OPTICAL PROPERTIES

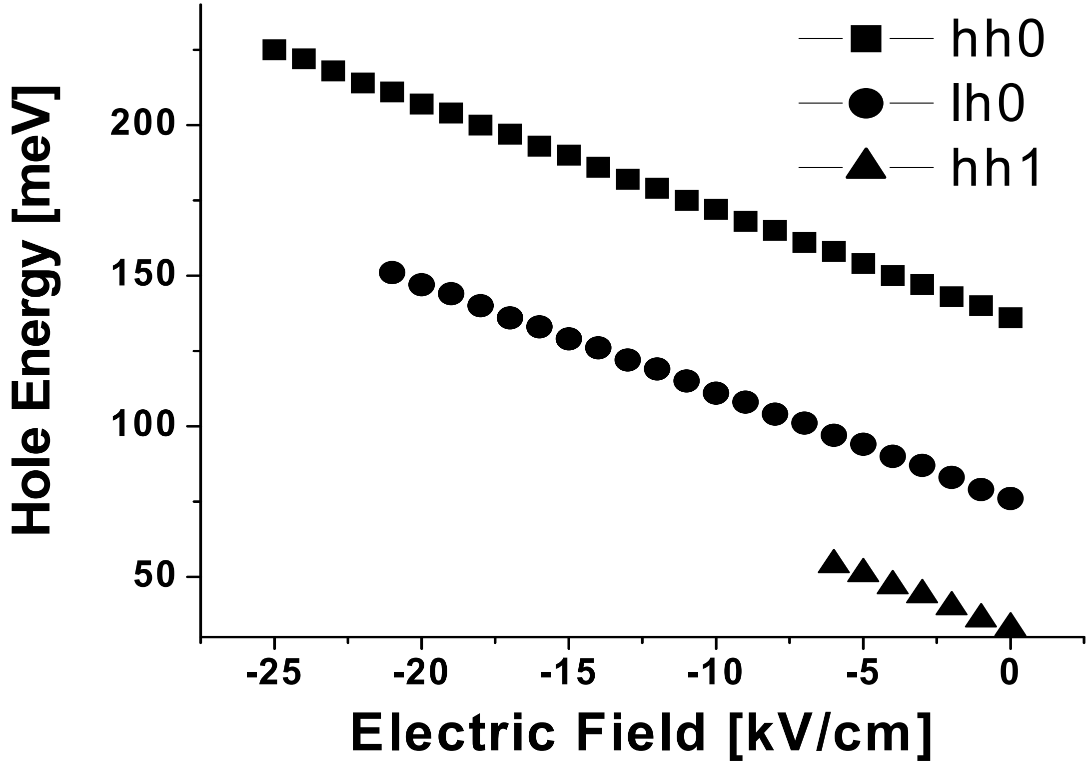


Figure 1. The dependence of the hole energy (hh0, lh0 and hh1) on the applied electric field intensity as a function of the acceptor concentration *p2D*, for a p-type Be *δ*-doped GaAs QW. The impurity concentration *p2D* is 50.1012 cm-2. (a) – first heavy hole energy level – hh0 (rectangles), (b) - first light hole energy level – lh0 (circles), (c) – second heavy hole energy level – hh1 (triangles).

We can say that the obtained results from such TB calculations would help to study more profoundly the physics of the doping at different impurity densities and at different electric field intensities. Such investigations that make possible to study in detail the Stark shifts of the hole energy states and their spatial distributions, and consequently the hole subband spectra and intersubband transitions, are very promising in looking for δ-doped structures for potential device applications, namely the devices based on the hole intersubband and intrasubband transitions (e.g. photodetectors and optical modulators).

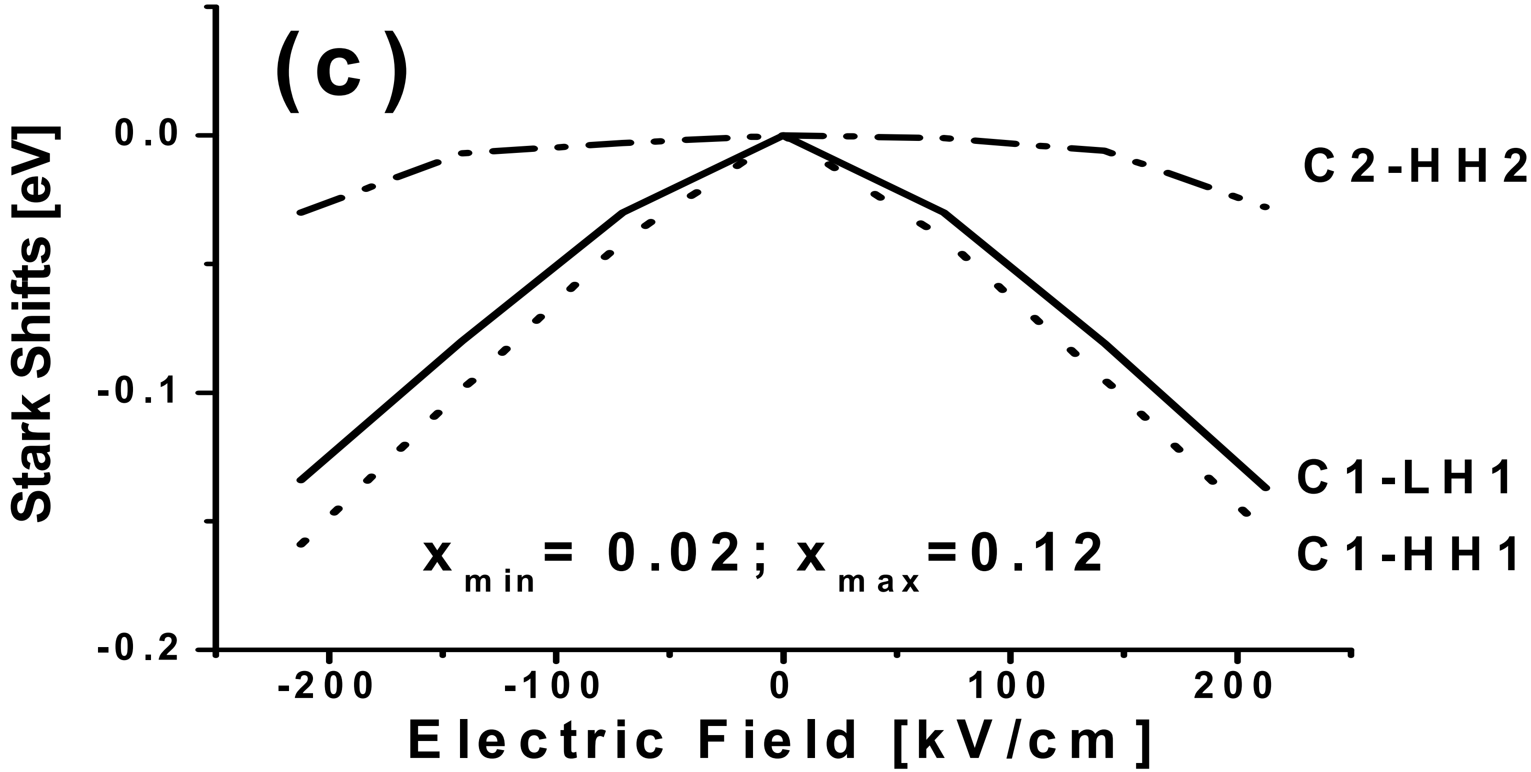


Figure 2. The dependence of the Stark shifts of the main optical transition energies E(C1-HH1), E(C1-LH1) and E(C2-HH2) for the PQW (Parabolic Quantum Well) on applied electric field. Al concentration is x. In the PQWs x varies parabolically from xmin = 0.02 at the barriers to xmax in the middle of the well. The growth direction is [100].

The Al concentration x in the barriers for all parabolic QWs (PQWs) is x=0.36.

We present the TB calculations of the quantum confined Stark effect in PQWs with parabolic potential and with QW width of 44 MLs. We can say that the results from the TB calculations, such in this work, help to study the physics of the electric field effects at different concentrations and electric field intensities. Such investigations that make possible to study in details the Stark shifts of the electronic states and their spatial distributions, are very promising in looking for PQW structures that provides good Stark effect characteristics for potential device applications. Such investigation will help us to find a QW potential profile with better Stark effect characteristics for application in QW-based devices.