

European Science Foundation
Standing Committee for Physical and Engineering Sciences (PESC)

ESF PESC EXPLORATORY WORKSHOP

Novel Superhard Materials



SCIENTIFIC REPORT

Bayreuth, Germany, 16-20 November 2005

Convened by:
Leonid Dubrovinsky and Natalia Dubrovinskaia

Universität Bayreuth



The European Science Foundation (ESF) acts as a catalyst for the development of science by bringing together leading scientists and funding agencies to debate, plan and implement pan-European scientific and science policy initiatives.

ESF is the European association of 78 major national funding agencies devoted to scientific research in 30 countries. It represents all scientific disciplines: physical and engineering sciences, life and environmental sciences, medical sciences, humanities and social sciences. The Foundation assists its Member Organisations in two main ways. It brings scientists together in its EUROCORES (ESF Collaborative Research Programmes), Scientific Forward Looks, Programmes, Networks, Exploratory Workshops and ESF Research Conferences to work on topics of common concern including Research Infrastructures. It also conducts the joint studies of issues of strategic importance in European science policy.

It maintains close relations with other scientific institutions within and outside Europe. By its activities, the ESF adds value by cooperation and coordination across national frontiers and endeavours, offers expert scientific advice on strategic issues, and provides the European forum for science.

European Science Foundation

1 quai Lezay Marnésia
BP 90015
F-67080 Strasbourg Cedex
Fax: +33 (0)3 88 37 05 32
<http://www.esf.org>

ESF Physical and Engineering Sciences:

Neil Williams
Head of Unit

Patricia Arsene
Scientific Secretary

Marie Gruber
Senior Administrative Assistant

Céline Quedrue
Administrative Assistant

Tel: +33 (0)3 88 76 71 07
Email: pesc@esf.org
<http://www.esf.org/pesc>

ESF Exploratory Workshops:

Nina Kancewicz-Hoffman
Scientific Coordinator

Valerie Allspach-Kiechel
Administrator

Tel: +33 (0)3 88 76 71 36
Email: vallspach@esf.org
<http://www.esf.org/workshops>



ESF PESC Exploratory Workshop:
Novel Superhard Materials
Bayreuth, Germany, 16-20 November 2005

Convenor:

Leonid Dubrovinsky

leonid.dubrovinsky@uni-bayreuth.de

Tel: +49 921 55 3736

Fax: +49 921 55 3769

<http://www.bgi.uni-bayreuth.de/>

Co- Convenor:

Natalia Dubrovinskaia

[Natalia.Dubrovinskaia@Uni-](mailto:Natalia.Dubrovinskaia@Uni-Bayreuth.de)

[Bayreuth.de](mailto:Natalia.Dubrovinskaia@Uni-Bayreuth.de)

Tel: +49 921 55 3739

Fax: +49 921 55 3769

Universität Bayreuth
Bayerisches Geoinstitut
95440 Bayreuth
Germany

Local Organiser:

Stefan Keyssner

Stefan.Keyssner@uni-bayreuth.de

Tel: +49 921 55 3704

Fax: +49 921 55 3769



1. EXECUTIVE SUMMARY

Interest in developing and studies of superhard materials (those approaching in hardness diamond and cubic boron nitride, c-BN) is driven by the two main objectives. From one side, hardness, as a mechanical property of materials, is still neither fully understood nor unambiguously characterized. Thus, hard materials attract scientific attention in attempts to understand their structure and bonding.

Like the traditional ones, diamond and c-BN, most novel superhard materials are high pressure-high temperature (HPHT) phases. High pressure allows tuning the volume and many other properties of solids, giving scientists a tool for controllably changing properties and for designing new materials with desirable properties. High pressure significantly affects the chemical potentials of substances, opening the way to synthesize, for example, new hard nitrides, oxides, and oxinitrides. Modern technologies require such very robust materials for use as abrasives, cutting tools and coatings where wear prevention, scratch resistance, surface durability and chemical stability are priorities. That is, development of HPHT methodology of synthesis of novel superhard materials is also driven by industrial needs.

The ESF Exploratory Workshop gathered 22 scientists from 12 countries (Austria, France, Germany, Japan, Romania, Russia, South Africa, Spain, Sweden, Ukraine, United Kingdom, USA; see the Workshop group photo), who came to Bayreuth to discuss recent achievements in design, synthesis and function of Novel Superhard Materials.

The program of the workshop included 20 talks lasting 35 minutes each + 10 minutes devoted to discussions. There were three very fruitful general and round table discussions on the various topics addressed by the Workshop.

The symposium covered fundamental issues of high-pressure, high-temperature synthesis and characterization of advanced superhard materials, thus making its topics highly relevant for presenting in the *High Pressure Research- an International Journal*. We would like to thank the Editor in Chief of the Journal, Dr. Stefan Klotz, for giving us an opportunity of preparing a special issue dedicated to the main problems discussed at the Workshop. This volume will be interesting not only for high-pressure physicists, chemists, material scientists, but also for engineers and scientists working on the development of new hard materials and their applications in science and technology.



The workshop was convened by Leonid Dubrovinsky and Natalia Dubrovinskaia (the Bavarian Geoinstitute, University of Bayreuth) The Bavarian Geoinstitute supported our initiative and provided the institution's resources that contributed to the success of this scientific forum. Personal help of Dr. S. Keyssner, Mrs. P. Buchert and Mrs. L. Kison- Herzing in the Workshop local organization is highly appreciated.

2. SCIENTIFIC CONTENT OF THE EVENT

The symposium covered fundamental issues of high-pressure, high-temperature synthesis and characterization of advanced superhard materials. The new fields of their application have been discussed. Special emphasis has been given to novel phases, such as nanodiamond, diamond-like phases of the B–C–N system, spinel nitrides, oxides, borides, carbides, etc. The topics covered are synthesis, crystal structure, testing of chemical, thermophysical and mechanical properties, as well as theoretical prediction and computer simulation of hard and superhard materials.

The scientific topics discussed during the workshop can be divided into several mutually related areas:

Carbon and Light Elements Superhard Materials

Diamond is the hardest known material followed by cubic boron nitride (c-BN). c-BN does not have a natural counterpart on the Earth. Despite both these materials are presently synthesized in huge amounts for industrial applications using high-pressure technology, there is still a lack of fundamental knowledge on their equilibrium phase diagrams, effects of impurities on the materials properties, new phases possible in the C-N-B system. Many of properties of the phases in this system, like, for example, recently observed superconductivity of B-doped diamond, still require scientific explanation. Thus, any contribution in the field serves to fundamental understanding of superhard materials physical phenomenon. It has been shown that the results of HPHT synthesis strongly depend on precursors used (not only on their chemical composition, but also on their structure and crystal state, which determine the mechanism involved into the phase transformation). **Vadim Brazhkin**, reported "hard regions" on P,T-transitional phase diagram of C₆₀. Graphite-like BN-C solid solutions are promising precursors for the high-pressure synthesis of novel superhard phases in the B–C–N system. **Vladimir L. Solozhenko** presented a new family of superhard phases, cubic boron carbonitrides with stoichiometries from



BCN to BC₈N, synthesized by solid state phase transitions of graphite-like BN–C solid solutions at pressures up to 30 GPa and temperatures up to 3500 K using a laser-heated diamond anvil cell, a multianvil press and shock compression. The BC₂N phase has an unusual combination of mechanical parameters: its elastic moduli are slightly lower than those of cubic boron nitride, whereas its Vickers hardness (76 GPa) is 1.5 times higher than that of single-crystal cBN and is second only to diamond. The results of investigations presented by **Olexander O. Kurakevych** have shown that in the course of phase transitions of turbostratic graphite-like BC₂N, which have been studied up to 30 GPa in a diamond anvil cell (DAC) using X-ray diffraction with synchrotron radiation, a reversible diffusionless transformation of the initial turbostratic structure into disordered layered high-pressure phase takes place at pressures above 20 GPa. The general mechanism of the process includes disordering in interlayer spacings, buckling of layers and abrupt change of interlayer spacings attributed to the formation of the disordered high-pressure phase consisting of close-packed buckled layers with a diamond-like structure. The transformation was found to be completely reversible, so the formation of interlayer bonds did not occur.

In situ studies of processes of crystallisation are always challenging. The work presented by **Yann Le Godec** was the first attempt to study *in situ* the crystallization of cubic boron nitride from BN solutions in supercritical N–H fluid at pressures up to 5.2 GPa and temperatures up to 1600 K using angle- and energy-dispersive X-ray diffraction with synchrotron radiation. Low-pressure crystallization of cBN in the region of its thermodynamic stability is kinetically restricted. However, for a rich variety of systems, the threshold pressure of cBN spontaneous crystallization is about 4 GPa irrespective of the temperature. In cooling of the BN solution in supercritical N–H fluid, the disappearance of short-range order in the solution is observed which is accompanied by the precipitation of solid phases (cBN or hBN and BN–NH₃ intercalation compound depending on the pressure, temperature and concentration). Spontaneous crystallization of cubic boron nitride has been observed down to 1.9±0.2 GPa, which is the lowest pressure of the cBN crystallization reported so far.

In order to utilize the full potential of boron nitride crystals in optical and mechanical applications, the systematic quantitative study of defects and impurities and their influence on properties of c-BN crystals is of a great importance. **Takashi Taniguchi** reported the effect of oxygen and carbon impurities on the properties of single- and polycrystalline cBN synthesized under high pressure. In particular, he showed that fine c-BN crystals with oxygen content less than 10¹⁷ cm⁻³ exhibit band edge optical properties such as free exciton luminescence and optical absorption. Oxygen impurity near the grain boundaries of polycrystalline c-BN also affects



mechanical properties of the sintered binder-less cBN. Control of impurities in c-BN crystals must be essential and important issue for the application of c-BN as the wide band gap semiconducting materials. Some trials for the artificial doping by lanthanide elements have been done, and typical optical luminescence originated by the lanthanide element was found in the BN crystals grown under HP, suggesting a formation of a new type of luminous c-BN crystals. **Sergiu V. Nistor** gave a review of the actual status of knowledge concerning the presence, nature and atomic properties of point defects in c-BN resulted from recent multifrequency Electron Spin Resonance and optical studies on crystalline powders and single crystals. These investigations allowed identification of several intrinsic paramagnetic point defects in undoped superabrasive cBN crystalline powders.

To complete the picture of modern state of hard materials synthesis, in particular diamond, **Roland Haubner** gave an overview of low-pressure diamond deposition.

Novel Superhard Phases

The ultra-high pressure and temperature synthesis of novel crystalline phases of silicon nitride, germanium nitride and sialons with spinel structure have caused an enormous impact around the world on both the basic science and the technological development of advanced nitrides. Since the discovery of spinel nitrides in 1999, there is presently much effort in basic science to work on advanced nitrides and their applications in electronics. Aim and scope of the research in this field is to develop novel nitrides for structural and functional applications. Silicon-based spinel nitrides are expected to show ultra-hardness and optoelectronic properties suitable for applications as cutting tools and light emitting diodes, respectively.

The lecture of **Ralf Riedel** highlighted the scientific efforts and issues associated with the high pressure synthesis, structure, properties, and modeling of novel nitrides including group 13 and 14 element nitrides, transition metal nitrides, carbide nitrides, oxide nitrides and others. **Paul F. McMillan**, reported new data on spinel-structured nitrides formed in the $\text{Si}_3\text{N}_4\text{-Ge}_3\text{N}_4$ system and characterised a solid solution between the two phases. He also emphasized that despite much is known about mechanical engineering parameters of transition metal nitrides and carbides (TiN, WC etc.), well-known high-hardness materials, their microscopic properties have not been determined. New experimental data on the bulk modulus for several metallic nitrides using synchrotron X-ray techniques in the diamond anvil cell were reported.



Nanomaterials and Nanocomposites

High-purity polycrystalline diamond has unique potential for industrial applications as an abrasion-resistant material because of its extremely high hardness, no cleavage feature and high thermal stability. Natural polycrystalline diamond (carbonado) is rather rare. Recently there have been reports on synthesis of superhard polycrystalline diamonds, nanodiamonds, and aggregated diamond nanorods (ADNRs) from various precursors. Nanodiamonds (polycrystalline diamonds with nanosized grains) show extremely high hardness ranging from 70 to 145 GPa depending on synthesis conditions. Nanocomposites show enhanced mechanical properties in comparison with those of their constituents. During numerous discussions at the Workshop, the participants concluded that synthesis of nanocrystalline superhard materials is one of the most realistic and promising ways for enhancement of superhard materials properties, such as hardness, fracture toughness, thermal stability, and as a result, their wear resistance. In order to realize industrial synthesis of nanocrystalline diamonds, it is important to learn mechanisms of their formation at various HPHT conditions.

Hitoshi Sumiya reported the results of experimental exploration of a broad PT field of the diamond phase diagram aiming to establish formation conditions of nano-polycrystalline diamonds from graphite and non-graphitic carbons (carbon black, glassy carbon, C₆₀, and carbon nanotubes). On the basis of investigation of their microstructure using transmission electron microscopy, it was concluded that the onset temperature for diamond formation at P>15 GPa is 1500-1600 °C for all carbon materials, although the required temperature conditions for pure polycrystalline diamond are >2200 °C for graphite and >1600 °C for non-graphitic carbons. Polycrystalline diamond forms as a result of simultaneous the diffusion and two-step martensitic processes from graphite, while it forms only due to diffusion without graphitization or formation of intermediate phases from non-graphitic carbon. Nano-polycrystalline diamonds consisting only of very fine particles (less than 10 nm in size) can be obtained from non-graphitic carbons at 1600-2000 °C under pressures higher than 15 GPa.

Natalia Dubrovinskaia described the results of measurements of mechanical properties (hardness, fracture toughness, and Young's modulus) of aggregated diamond nanorods synthesised as a bulk sample. The investigation has shown that this nanocrystalline material has the fracture toughness $11.1 \pm 1.2 \text{ MPa m}^{0.5}$, which exceeds that of natural and synthetic diamond (that varies from 3.4 to 5.0 MPa m^{0.5}) by 2-3 times. At the same time, having a hardness and Young's modulus comparable with that of natural diamond and suppressed because of the random orientation of nanorods 'soft' directions, ADNR samples show the enhancement of wear



resistance up to 300 % in comparison with commercially available polycrystalline diamonds (PCDs). This makes ADNRs extremely prospective materials for applications as superabrasives, reinforcements in nanocomposites, and for high speed and precision machining. She also reported synthesis and characterization of heavily B-doped diamonds.

Stan Veprek reported recent progress in the understanding of the origin of hardness enhancement in superhard nc-TiN/a-Si₃N₄ nanocomposites (“nc-“ stands for “nanocrystalline, “a-“ for “X-Ray amorphous”). “Ti-Si-N” coatings were reported to have hardness of about 60 GPa. The recent results of the first principle DFT calculations as well as the experimental work on the TiN/Si₃N₄ heterostructures of a high quality confirmed that the strong enhancement of the hardness in superhard nc-TiN/a-Si₃N₄ nanocomposites is due to a strong nanostructure with an optimum thickness of about one monolayer of the interfacial Si₃N₄. The theoretical calculations revealed that this configuration displays an enhanced decohesion energy of the TiN/Si₃N₄/TiN sandwich which is higher than that of bulk Si₃N₄.

Hardness of Superhard Materials

The synthesis of new classes of hard and superhard materials makes the problem of measuring hardness of materials especially acute. Quantitative claims and appropriate criteria for hardness measurements of these materials generate hot discussions among the specialists in fundamental aspects of superhard materials. Hardness measurements (Vickers, Brinell and Knoop) belong to standard methods to characterise materials. Classical hardness measurements use a defined test body to make an indent into the material surface. The image of the indent is visible in the microscope and the indented area is determined. Hardness is defined as the value of maximum applied load divided by the indentation area.

Asta Richter emphasized that this method cannot be applied easily to superhard materials, because for them elastic deformation and crack formation is more important than plastic deformation with the generation and motion of dislocations characteristic for metals. Depth sensing nanoindentation differs from classical hardness measurements. Load and penetration depth are simultaneously recorded during both loading and unloading, resulting in a load-displacement diagram. This diagram provides much more information than a microscopy image of the impression since it tells us the “story” of the elastic and plastic deformation with increasing and decreasing load and permits to extract hardness (contact pressure) and Young’s modulus (indentation modulus) in dependence on penetration depth. Within depth sensing nanoindentation it is possible to develop special force-time functions to test the material by



dynamical and repeated loading and unloading processes. These intelligent load functions result in multi-cycling indents at the same place on the sample surface. Hysteresis loops during this type of materials testing represent either phase transformations or visco-elastic materials response.

Roger Smith described molecular dynamics computer simulations of the nanoindentation process by a cube-corner diamond indenter into a {100} oriented diamond crystal, which showed that the contact pressure of the tip on the surface approaches the classical hardness value of diamond after indentation of only 2 nm, with only a small observable indentation size effect. Experiments carried out on both silicon and diamond also show no indentation size effect for the measured contact pressure. Metals on the other hand exhibit a large indentation size effect with the measured nanohardness value only approaching the classical hardness values after indentation of several hundred nanometers. This investigation suggests an extension to the engineering definition of hardness for superhard materials by using the concept of nanohardness or contact pressure which is more physically well-defined and applicable over all length scales.

Sergey Dub reported a new approach to determination of Young's modulus of superhard materials by means of measuring of elastic surface deformation during nanoindentation. With the known tip radius, the elastic moduli have been determined for ZrC, B₄C, nanocrystalline cBN compact and a type Ia natural diamond based on elastic loading data and the Hertz equation. The resulted values of the Young's modulus were depth-independent and in good agreement with the reference data. The proposed technique allows more local and more precise measurement of elastic modulus in comparison with traditional technique due to use of the exact solution of the elastic problem which not includes empirical coefficients.

Computer Simulation Of The Novel Superhard Materials

Hard compounds that are made of light elements are important for a large number of commercial applications. They can be used as protective coating on hard discs and recorder heads and can also play a crucial role in some medical area. For instance, the recovery of orthopedic substrates has already been tested for joint arthroplasty in human implants. The characterization and the development of bio-compatible hard phases represent nowadays an important growing field that has recently provoked the interest of many scientists. Considering the cost and the complexity of the synthesis/characterization procedure, computer-modeling investigation has turned out in an indispensable tool for discovering new phases and for predicting material properties in a faster and cheaper way.



Density-functional calculations of novel bio-compatible hard materials were presented by **Maurizio Mattesini**. The purpose of his study was twofold: 1) to achieve a quantitative prediction of the hardness and stability of a wide variety of carbon-based systems by computing athermal elastic constants, bulk and shear moduli, cohesive energies and enthalpy of formations; 2) to extract modeled spectroscopic quantities (XANES, EELS and ^{13}C NMR chemical shifts) in order to help experimentalists assessing the properties of the synthesized amorphous carbon- and boron carbon-nitrides samples. The electronic band structures of three different stoichiometries (C_3N_4 , C_{11}N_4 and BC_2N) have been deeply investigated by using up-to-date first principles computational methods based on the well-known density functional theory (DFT). As a matter of fact, one of the problems that limit the development of these compounds resides on the lack of pure crystalline samples, which has heavily restricted their experimental characterization. Nevertheless, an important understanding of the relationship between composition and electronic structure properties can be achieved by combining together experimental results and computational outcomes.

J. E. Lowther discussed the role of computational modeling to indicate potential ways that the binary oxides could have their properties enhanced, as well as some recent measurements on nano-particle oxides. He also presented a model as to why in the nano-structure evident in the nano-particle could enhance the properties.

MAX phase materials (compounds based on the $\text{M}_{n+1}\text{AX}_n$ formula - named for short "MAX phases" - where M is an early transition metal, A is an A-group element (mostly III A and IV A) and X is C and/or N and $n = 1$ to 3, representing a very specific new class of solids) and their relation to hard transition metals carbides and nitrides were characterized by **Rajeev Ahuja**. Electronic and mechanical properties of these materials were evaluated by means of *ab initio* calculations.

***In situ* studies of superhard materials**

Pierre Bouvier's talk was concentrated on the examination of chemical and thermophysical properties of boron-doped diamond electrodes using *in situ* Raman spectroscopy and photoelectrochemistry either at macro- or microscopic scales. The potential of use of scanning electrochemical microscopy (SECM) for the determination of boron concentration in diamond films was shown. This complex approach is very important, since the electrochemical response of polycrystalline boron-doped diamond films seems to be dependent on several factors such as: (1) non-diamond carbon impurity phases, (2) surface termination (hydrogen versus oxygen), (3)



dopant level and distribution inside the film, (4) grain boundaries and other morphological defects, and (5) crystallographic orientation.

A new state-of-the art synchrotron beamline ID27, fully optimized for monochromatic X-ray diffraction at high pressure and high (or low) temperature, was presented by **Wilson Crichton**. In comparison with the old high-pressure beamline ID30, this new beamline exhibits outstanding performance in terms of photon flux and focusing capabilities. Current experimental possibilities include *in situ* laser heating at high pressure, single-crystal data collection, and total scattering from large-volume apparatus.

The conditions normally employed to synthesize superhard materials require extreme pressures and temperatures, or chemical vapor deposition technique (the latter, however, does not provide bulk superhard materials). Recent developments in large-volume high-pressure apparatus, laser- and electrically-heated diamond anvil cell (DAC), as well as in powder X-ray diffraction with synchrotron radiation, have provided a unique combination of tools not previously available to researchers in this area. All this provides the capability to tackle the synthesis, recovery and characterization of new high-pressure phases. The unique, state of the art equipment and facilities are spread all over Europe, and the common politic in their collaborative use is very important to make the efforts in the development of novel materials more effective.

3. ASSESSMENT OF THE RESULTS, CONTRIBUTION TO THE FUTURE DIRECTION OF THE FIELD

Scientific conclusions

The workshop provided a platform for discussion among the leading European scientists working in the field of design, synthesis and function of Novel Superhard Materials. The talks presented during the workshop provided a very up-to-date overview of the state of the art in this dynamically developing research area in Europe, which greatly helped to identify and pinpoint the main challenges in the field.

Workshop participants concluded that (1) the search for superhard substances with high elastic moduli is shifting now to non-traditional compositions (like $C_{11}N_4$ and TaON, for example), in binary (B-C, C-N, etc.) or ternary (Ta-O-N, Ti-O-N) systems. (2) The synthesis of new classes of hard and superhard materials makes the problem of measuring hardness of materials especially acute. Quantitative claims and appropriate criteria for hardness measurements of these materials generate hot discussions among the specialists in fundamental aspects of superhard materials. It was emphasized that for hardness tests of superhard materials (especially nanocrystalline and



amorphous ones), it is very important to study their multi-indent dynamic behaviour reflecting their visco-elastic properties. (3) The future of fabrication of novel superhard materials is highly connected to a smart control of the grain size and morphology as well as the defect state of already existing hard materials like diamond, c-BN, SiC, B₄C, etc. Such an approach will allow achieving the "ideal" values of mechanical properties in the two opposite cases: (a) for materials in the nanocrystalline (or multilayered) state with the optimal correlation grain size around 10nm (like in nanodiamond) and (b) for materials in the single crystal state without defects (like in synthetic II-a diamond).

During numerous discussions at the Workshop, the participants concluded that synthesis of nanocrystalline superhard materials is one of the most realistic and promising ways for enhancement of superhard materials properties, such as hardness, fracture toughness, thermal stability, and as a result, their wear resistance.

Based on the participants' opinion, the workshop was a great success. That is, new ideas discussed at the Workshop will motivate scientific and technological searches for novel superhard materials.

Organizational conclusions

Workshop participants agreed that the benefits of development of novel superhard materials could best be realised through cooperative international programs involving universities, industry, and government agencies at all levels. The unique, state of the art equipment and facilities are spread all over Europe, and the common politic in their collaborative use is very important to make the efforts in the development of novel materials more effective.

It was decided to search for networking both inside Europe and with overseas partners (Japan, USA, South Africa, Russia, Ukraine). A group of four scientists (Leonid Dubrovinsky, Natalia Dubrovinskaia, Germany; Paul McMillan, UK; Vladimir Solozhenko, France) was elected to work as an informal committee and to coordinate efforts for establishing close collaboration using existing or newly coming ESF programs (FP7, for instance). It was agreed to submit a EUROCORES theme proposal on Novel Superhard Materials.



4. FINAL PROGRAMME

Wednesday 16 November 2005

Afternoon/Evening *Arrival*

Thursday 17 November 2005

- | | |
|---------------|--|
| 09.00 | Presentation of the European Science Foundation (ESF)
Bozidar Liscic (Standing Committee for Physical and Engineering Sciences) |
| 09.15 | Opening remarks |
| 09.30 | Session 1: Carbon and Light Elements Superhard Materials
Chairman: Malcolm Nicol |
| 09.30 - 10.15 | Yann Le Godec , Cubic boron nitride crystallization in fluid systems - in situ studies |
| 10.15 - 11.00 | T. Taniguchi , Effect of impurities on the properties of single- and polycrystalline cBN synthesized under high pressure |
| 11.00 - 11.15 | <i>Coffee Break</i> |
| 11.15 - 12.00 | O.O. Kurakevych , Reversible pressure-induced structure changes in turbostratic BN-C solid solutions |
| 12.00 - 12.45 | Sergiu V. Nistor , Atomic defects in superhard cubic boron nitride |
| 12.45 - 14.15 | <i>Lunch</i> |
| 14.15 | Session 2: Novel Superhard Phases
Chairman: Vladimir Solozhenko |
| 14.15 - 15.00 | Paul F. McMillan , Synthesis and Properties of Nitrides at High Pressure and High Temperature |
| 15.00 - 15.45 | Ralf Riedel , High Pressure Synthesis of Advanced Nitrides with Unusual Solid State Structures and Properties |
| 15.45 - 16.30 | H. Sumiya , Nano-polycrystalline diamonds synthesized directly from graphite and non-graphitic carbons under high pressure and high temperature |
| 16.30 - 16.45 | <i>Coffee Break</i> |
| 16.45 - 17.15 | General Discussion: New Trends in Light Elements Superhard Materials |
| 17.15 - 18.00 | <i>Visiting Labs at BGI</i> |



Friday 18 November 2005

Session 3: Hardness of Superhard Materials

Chairman: **Vadim Brazhkin**

09.00 - 09.45 **Sergey Dub**, Young modulus of superhard materials measured by elastic surface deformation during nanoindentation

09.45 - 10.30 **Asta Richter**, Mechanical Properties of Superhard Materials Investigated by Nanoindentation and Nanoscratching

10.30 - 11.00 *Coffee Break*

11.00 - 11.45 **Roger Smith**, Nanoindentation of diamond

11.45 - 12.15 **General Discussion: Hardness Measurements of Superhard Materials: Science or Art?**

12.15 - 13.30 *Lunch*

13.30 **Session 4: Computer Simulation Of The Novel Superhard Materials**

Chairman: **J E Lowther**

13.30 - 14.15 **Rajeev Ahuja**, MAX phase materials and its relation to hard transition metals carbide and nitride.

14.15 - 15.00 **Maurizio Mattesini**, Density-functional characterization of novel bio-compatible hard materials

15.00 - 15.30 *Coffee Break*

15.30 - 16.15 **J. E. Lowther**, Advancing the properties of metal oxides through computing: nano-scale structures to quaternary oxy-nitrides and beyond

16.15 **Session 5: In situ studies of superhard materials**

Chairman: **N. Dubrovinskaia**

16.15 - 17.00 **Wilson Crichton**, ID27 at the ESRF, a new state-of-the-art X-ray beam line optimized for monochromatic diffraction experimentation

17.00 - 17.45 **Pierre Bouvier**, Photoelectrochemistry on boron-doped diamond electrodes

19.00 *Workshop Dinner*



Saturday 19 November 2005

Chairman: **Leonid Dubrovinsky**

- 09.00 **Session 6: Carbon And Light Elements Superhard Materials-II**
- 09.00 –09.45 **Vadim Brazhkin**, "Hard regions" onto P,T-transitional phase diagram of C₆₀
- 09.45 - 10.30 **Stan Veprek**, Superhard Nanocomposites: Basic Science and Industrial Applications
- 10.30 - 10.45 *Coffee break*
- 10.45 - 11.30 **Roland Haubner**, Low-pressure diamond: preparation, applications, characterization and characterization
- 11.30 - 12.15 **Vladimir L. Solozhenko**, Superhard cubic boron carbonitrides-synthesis and properties
- 12.15 - 13.00 **Natalia Dubrovinskaia**, Synthesis and characterization of heavily B-doped diamonds and aggregated diamond nanorods
- 13.00 - 14.30 *Lunch*
- 14.30 - 16.00 **Round Table Discussion: Fundamentals and Trends in Novel Superhard Materials**
Chairman: **Malcolm Nicol**
- 16.00 - 16.30 **Closing Remarks**

Sunday 20 November 2005

Morning *Departure*



5. FINAL LIST OF PARTICIPANTS

Convenor:

1. **Leonid DUBROVINSKY**
Bayerisches Geoinstitut
Universität Bayreuth
95440 Bayreuth
Germany
Tel: +49 921 55 3736
Fax: +49 921 55 3769
Email: leonid.dubrovinsky@uni-bayreuth.de

Co-Convenor:

2. **Natalia DUBROVINSKAIA**
Bayerisches Geoinstitut
Universität Bayreuth
95440 Bayreuth
Germany
Tel: +49 921 55 3739
Fax: +49 921 55 3769
Email: Natalia.Dubrovinskaia@Uni-Bayreuth.de

ESF Representative:

3. **Bozidar LISCIC**
Dept. for Materials Science
Faculty of Mech. Engineering and Naval
Architecture
University of Zagreb
Ivana Lucica Street 5
10 000 Zagreb
Croatia
Tel: +385 1 61 68 360
Fax: +385 1 615 69 40
Email: bliscic@fsb.hr

Participants:

4. **Rajeev AHUJA**
Department of Physics
University of Uppsala
Box 530
75121 Uppsala
Sweden
Tel: +46 18 471 36 26
Fax: +46 18 471 35 24
Email: rajeev.ahuja@fysik.uu.se

5. **Vadim BRAZHKN**
Institute for High Pressure Physics
142190 Troitsk Moscow
Russian Federation
Tel: +7 095 334 00 11
Fax: +7 095 334 0012
Email: brazhkin@hppi.troitsk.ru

6. **Pierre BOUVIER**
Laboratoire d'Electrochimie et de
Physicochimie
des Matériaux et des Interfaces
LEPMI - ENSEEG
1130 rue de la Piscine
BP 75
38402 Saint Martin d'Herès Cedex
France
Tel: +33 4 76 82 66 82
Fax: +33 4 76 82 66 30
Email: Pierre.Bouvier@lepmi.inpg.fr

7. **Wilson CRICHTON**
ID30, ESRF
6, rue Jules Horowitz
BP220
38043 Grenoble
France
Tel: +33 4 76 88 22 69
Fax: +33 4 76 88 29 07
Email: wilson.crichton@esrf.fr

8. **Sergey DUB**
Department 11
Institute for Superhard Materials of the
National
Academy of Sciences
2, Avtozavodskaya Str.
04074 Kiev 74
Ukraine
Tel: +380-44-462 91 51
Email: lz@ism.kiev.ua

9. **Roland HAUBNER**
CT - Chemical Technologies
Institute for Chemical Technologies and
Analytics
Vienna University of Technology
Getreidemarkt 9/164
1060 Vienna
Austria
Tel: +43-1-58801 16128
Email: rhaubner@mail.zserv.tuwien.ac.at

10. **Oleksandr KURAKEVYCH**
LPMTM-CNRS
Université Paris Nord
99, avenue J.B. Clement
93430 Villetaneuse
France
Tel: +33 1 49 40 30 00 (secr)
Fax: +33 1 49 40 39 38
Email: kura@galilee.univ-paris13.fr



11. Yann LE GODEC

UMR 7602 CNRS
Laboratoire de Physique des Milieux
Condensés
Université Pierre et Marie Curie
140 rue de Lourmel
75252 Paris Cedex
France
Tel: +33 1 44 27 44 56
Fax: +33 1 44 27 44 69
Email: yann.legodec@pmc.jussieu.fr

12. J.E. LOWTHER

DST/NRF Center of Excellence in Strong
Materials
School of Physics
University of the Witwatersrand
Private Bag 3
PO Box Wits
2050 Johannesburg
South Africa
Email: lowther@physnet.phys.wits.ac.za

13. Maurizio MATTESINI

Modulo C-III/503-2
Departamento de Física de la Materia
Condensada
Facultad de Ciencias
Universidad Autónoma de Madrid
28049 Madrid
Spain
Tel: +34 91 497 3805
Fax: +34 91 497 4740
Email: maurizio.mattesini@uam.es

14. Paul MCMILLAN

Department of Chemistry
Christopher Ingold Laboratories
University College London
20 Gordon Street
London WC1H0AJ
United Kingdom
Tel: +44 20 7679 4610
Fax: +44 20 7679 7463
Email: p.f.mcmillan@ucl.ac.uk

15. Malcolm NICOL

Department of Physics
University of Nevada Las Vegas
Las Vegas NV 89154-4002
United States
Tel: +1-702-895-1725
Fax: +1-702-895-0804
Email: nicol@physics.unlv.edu

16. Sergiu V. NISTOR

Laboratory 190 "Microstructure of Defects
in Solids"
National Institute for Materials Physics
Atomistilor Street 105bis
PO Box MG-7
77125 Magurele-Bucharest
Romania
Tel: +40 21 493 0195
Fax: +40 21 493 0267
Email: snistor@infim.ro

17. Asta RICHTER

Fachbereich Physikalische Technik
University of Applied Sciences Wildau
Bahnhofstrasse 1
15745 Wildau
Germany
Tel: +49 3375 507 219
Fax: +49 3375-508 238
Email: richter@pt.tfh-wildau.de

18. Ralf RIEDEL

Fachbereich Material- und
Geowissenschaften
Technische Universität Darmstadt
Petersenstr. 23
64287 Darmstadt
Germany
Tel: +49-6151-16-634
Fax: +49-6151-16-6346
Email: riedel@materials.tu-darmstadt.de

19. Roger SMITH

Math. Sciences Dept
School of Physics & Mathematics
Loughborough University
Ashby Road
Loughborough LE11 3TU
United Kingdom
Tel: +44 1509 223 192
Fax: +44 1509 223 969
Email: R.Smith@lboro.ac.uk

20. Vladimir SOLOZHENKO

LPMTM-CNRS
Université Paris Nord
99, avenue J.B. Clement
93430 Villetaneuse
France
Tel: +33 1 49 40 34 89
Fax: +33 1 49 40 39 38
Email: vls@lpmtm.univ-paris13.fr



ESF PESC Exploratory Workshop:

Novel Superhard Materials

Bayreuth, Germany, 16-20 November 2005

21. Hitoshi SUMIYA

Sumitomo Electric Industries, Ltd.
Electronics Materials R&D Laboratories
1-1-1, Koya-kita
664-0016 Itami, Hyogo
Japan
Tel: +81 727.72.4804
Fax: +81 727.70.6727
Email: sumiya@sei.co.jp

22. Takashi Taniguchi

National Institute for Materials Sciences
Advanced Materials Laboratory
1-1 Namiki Tsukuba Ibaraki 305-0044
Japan
Tel: +81-29-860-4413
Fax: +81-29-851-2768
Email: taniguchi.takashi@nims.go.jp

23. Stan VEPREK

Department of Chemistry
Institute for Chemistry of Inorganic
Materials
Technical University Munich
Lichtenbergstrasse 4
85747 Garching
Germany
Tel: +49-89-2891 3624
Fax: +49-90-2891 3626
Email: veprek@ch.tum.de



6. STATISTICAL INFORMATION ON PARTICIPANTS

Age structure of participants (Young Scientists)

6 participants out of 22 were under the age of 40 with less than 5 years in a permanent position

Countries of origin, see also point 5 above

ESF:

Austria (1)
France (5)
Germany (5)
Romania (1)
Spain (1)
Sweden (1)
United Kingdom (2)

Non-ESF:

Japan (2)
Russia (1)
South Africa (1)
Ukraine (1)
USA (1)

Gender Distribution

Male: 20, Female: 2

Industrial/ Academic Split

Industry: 1

Academe: 21