

Programme & The Book of Abstracts

Twenty-first Annual Conference

YUCOMAT 2019

&

Eleventh World Round Table Conference

on Sintering –

Science of Sintering & Its Future: Fifty Years Later

WRTCS 2019

Herceg Novi, Montenegro September 2 - 6, 2019

Organised by



Twenty-first Annual Conference
YUCOMAT 2019
&
Eleventh World Round Table Conference
on Sintering
WRTCS 2019

Programme and The Book of Abstracts

Organised by:
Materials Research Society of Serbia
&
International Institute for the Science of Sintering

Hunguest Hotel Sun Resort Herceg Novi, Montenegro,
September 2-6, 2019, <http://www.mrs-serbia.org.rs>

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WRTCS 2019
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WELCOME SPEECH BY THE PRESIDENT OF IISS AND MRS – SERBIA:

Dear Attendees,



It is my great pleasure to welcome you on behalf of the International Institute for the Science of Sintering (IISS) and the Materials Research Society of Serbia (MRS-Serbia) to the 11th World Round Table Conference on Sintering (WRTCS) and the 21st YUCOMAT. This year marks the 50th anniversary since the first International Conference on Sintering was held in this very same hall, in 1969. As for YUCOMAT, the first one in this series of conferences was organized 24 years ago, in 1995, also in Herceg-Novı. The more seasoned amongst you may remember that YUCOMAT was initially a “spinoff” of the WRTCS. The last WRTCS held in Herceg-Novı took place here in 1989, not long before the onset of the Yugoslav Civil War. Here, for the first time, they are being held together.

While developing the concept of the conference, we had some concerns about the fit of the two topics within a single conference. Eventually, we concluded that these are two very similar, complementary disciplines and that all the participants should be able to benefit from the simultaneous exposure to both topics. Unfortunately, we did not have a significant number of papers submitted for the WRTCS this year. Nonetheless, it is very encouraging that all the members of the International Institute on the Science of Sintering (IISS), including both the ones present here and those who were unable to attend, have accepted the idea of the renewal of the IISS activities. Considering the recent expansion of the activities within the IISS, I am certain that we will have more participants next time around and that we will exceed the record numbers set in the previous years.

As in the previous years, this year’s conference will be well-attended. A total of 170 abstracts were accepted for presentation: 140 for YUCOMAT and 30 for WRTCS. Specifically, we have 32 lectures by invited plenary speakers (23 for YUCOMAT, 9 for WRTCS), 70 oral lectures (58 for YUCOMAT and 12 for WRTCS), and 70 poster papers (63 for YUCOMAT, 7 for WRTCS). I will let these numbers alone speak about the continuous rising track that YUCOMAT has been on since its inception. As for the international participants, this year they come from more than 30 countries, with the most numerous delegations being from Russia, Japan, Slovenia, USA, Ukraine and Romania. Serbian researchers are very well represented too, with a total 36 presentations, as well as the researchers from the region of the former Yugoslavia. As it has been the case in the past, 5 plenary speakers who will speak at the First Plenary Session participate at YUCOMAT for the first time. More than half of all YUCOMAT plenary speakers are here for the first time too.

I am pleased to announce that the laureate of the 2019 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering is Prof. Danilo Suvorov of Jožef Stefan Institute in Ljubljana, Slovenia. He is awarded for his achievements in the

investigation of microwave ceramic materials for wireless applications. It is also a great pleasure to be granting this award at this moment, when both conferences are held at the same time, along with the 50th anniversary since the first WRTSC. Prof. Suvorov has been a true follower and admirer of the work of Prof. Drago Kolar, one of the founders of the IISS and a scientist who had done enormously much for Slovenian ceramics and the science of sintering. This is also the last award which will have been limited to scientists from the former Yugoslavia or scientists who originated from this region, but who may have worked in foreign laboratories. The Society decided that from the following year the Grand Prize of the Society would be fully "open" and internationalized and all of its members will be eligible for it, provided that they have contributed significantly to the goals and the interests of the MRS-Serbia. Moreover, there will be the possibility of choosing the Honorary President of the Society and a Honorary Member of the Society, who will be announced for the first time at the next YUCOMAT, in 2020, also here in Herceg-Novı.

As in the last few years, the Diamond Sponsors of the Conference are Thermo Fisher Scientific, their subsidiary FEI and Dove Press (International Journal of Nanomedicine). We are incredibly grateful to them for their continuous help in overcoming our financial difficulties. Long-standing members of the International Advisory Board must be acknowledged for their assistance in helping us secure these sponsorships. We also highly appreciate the financial support by the gold, silver and other sponsors, the names of which could be found on the list of sponsors in the Book of Abstracts. This has helped us to fulfill our main goal of promoting the areas of competence to which our MRS is dedicated and also to support young researchers through the awards given at the Young Researchers' Conference in December and YUCOMAT in September. This year, the list of awardees has expanded because of a large number of young participants with financial problems, not only from Serbia, but from other countries too. We are already thinking about the best candidate(s) who would be representing us at the EUROMAT Junior Conference, which will be held in Granada, Spain, July 5-9, 2020.

All in all, I wish you a pleasant stay and a lot of unforgettable moments from this year's YUCOMAT and WRTCS joint events.

Sincerely Yours,

Dragan Uskoković

President of IISS and MRS-Serbia

2019 MRS-SERBIA AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

We are pleased to announce that the laureate of the 2019 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering is Prof. Danilo Suvorov of the “Jožef Stefan” Institute from Ljubljana, Slovenia. He is awarded for his achievements in investigation of microwave ceramic materials for wireless application.



This is the decision of the MRS-Serbia Executive Board:

The Executive Board of the MRS-Serbia Presidency, at their meeting on April 2, 2019, considered the submitted nominations for the MRS-Serbia's 2019 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering and concluded that the procedure was conducted in accordance with the Awarding Rulebook, that the Call was announced on the MRS-Serbia's website on January 1, 2019, and that in the stipulated period of 45 days two nominations were submitted. Prof. Suvorov was nominated by Prof. Dragan Uskoković, strongly supported by Prof. Mamoru Senna, Prof. Enrico Traversa,

Prof. Stane Pejovnik, Dr. Slobodan Milonjić, Prof. Biljana Stojanović, Prof. Vuk Uskoković, Asst. Prof. Srečo Škapin and Dr. Smilja Marković.

Having received the opinion from the Expert Committee members, Prof. Dr. Robert Sinclair (Chair of YUCOMAT Conferences International Advisory Board), Prof. Dr. Ivan Božović (2015 Laureate), Prof. Dr. Gordana Vunjak-Novaković (2016 Laureate), Prof. Dr. Velimir Radmilović (2017 Laureate), and Prof. Dr. László Forró (2018 Laureate), the Executive Board of the MRS-Serbia Presidency took the decision that Prof. Danilo Suvorov should be granted MRS-Serbia's 2019 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering.

Prof. Danilo Suvorov's invited plenary lecture "Epitaxial integration of oxides with silicon" will be presented during the Opening Ceremony of the 21st MRS-Serbia Annual Conference YUCOMAT 2019 and the 11th IISS World Round Table Conference on Sintering, starting at 9.00 h on Monday, September 2, 2019.

President of IISS and MRS-Serbia, Prof. Dr. Dragan Uskoković

Vice-President of MRS-Serbia, Dr. Slobodan Milonjić

Vice-President of MRS-Serbia, Prof. Dr. Velimir Radmilović

Vice-President of MRS-Serbia, Prof. Dr. Dejan Raković

Materials Research Society of Serbia (MRS Serbia)

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History:

Materials science and engineering incorporate acquiring of knowledge on synthesis and processing of materials, their composition and structure, properties and behaviour, functions and potentialities as well as application of that knowledge to various final products. Economic prosperity, life quality, and healthy environment are tightly connected with the improvements in

the existing and the development of new materials and processing technologies. These improvements and development can contribute greatly to the national priorities: energy saving, environment and health protection, information and communication, infrastructure, transportation, etc.

The First Conference on materials science and engineering, including physics, physical chemistry, condensed matter chemistry, and technology in general, was held in September 1995, in Herceg Novi. An initiative to establish Yugoslav Materials Research Society was born at the conference and, similar to other MR societies in the world, the programme was made and objectives determined. The Yugoslav Materials Research Society (Yu-MRS), a non-government and non-profit scientific association, was founded in 1997 to promote multidisciplinary goal-oriented research in materials science and engineering. Main task and objective of the Society is to encourage creativity in materials research and engineering to reach a harmonic coordination between achievements in this field in our country and analogous activities in the world with an aim to include our country into the global international projects. Until 2003, Conferences were held every second year and then they grew into Annual Conferences that were traditionally held in Herceg Novi in September of every year. Following the political separation between Serbia and Montenegro, in 2007 Yu-MRS formed two new MRS: MRS-Serbia (official successor of Yu-MRS) and MRS-Montenegro (in founding). In 2008 MRS-Serbia became a member of FEMS (Federation of European Materials Societies)

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History:

The International Institute for the Science of Sintering (IISS) was established in 1968 in Belgrade, Yugoslavia, today the Republic of Serbia. It began as the International Team for Studying Sintering after the great initiative of late academician, Momcilo M. Ristic, who was its long-term General Secretary and President. Since 1973, the Team has changed its name to IISS and become an umbrella of the Serbian Academy of Sciences and Arts as well as other eminent institutions from membership countries. The IISS has thus far organized ten international conferences on sintering (World Round Table Conferences on Sintering, WRTCS): Herceg Novi, Yugoslavia, 1969, 1971, and 1973; Dubrovnik, Yugoslavia, 1977; Portoroz, Yugoslavia, 1981; Herceg Novi, Yugoslavia, 1985 and 1989; and Belgrade, Yugoslavia, 1998 and 2002. Since 1975, the IISS has organized seven International Topical Symposia on Sintering: Herceg Novi, Yugoslavia, 1975; Warsaw, Poland, 1979; New Delhi, India 1983; Tokyo, Japan, 1987; Vancouver, Canada, 1991; Haikou, P.R. China, 1995; and New Delhi, India, in 2000. After the final WRTCS was held in Belgrade in 2002, IISS activity has drastically decreased.

With this Conference, we wish to re-establish the activity of the Institute, which had the important role in bringing scientists together from this field worldwide, having in mind that at the time, our country was the rare meeting place for the scientists from the East and scientists from the West.

GENERAL INFORMATION

DATE AND VENUE: The conference will be held on September 2-6, 2019, at the Hunguest Hotel Sun Resort, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, September 2, at 09.00 and end on Friday, September 6, 2019, at 12.00.

REGISTRATION: Registration, registration fee payment, conference materials distribution, etc, will take place at the conference desk (Conference Secretariat) open on Sunday, September 1, and Monday, September 2, from 8.00 to 19.00, on Tuesday, Wednesday and Thursday from 8.00 to 13.00 and from 19.00 to 20.00, and on Friday from 8.00 to 12.00. At registration, the participants are requested to submit a proof of their registration fee payment.

INSTRUCTION FOR AUTHORS: The conference will feature plenary sessions, oral sessions, poster sessions, and an Exhibition of synthesis and characterization equipment.

Time of papers' presentations to be given in ORAL SESSIONS is limited. Time available for delivery is 30 min for plenary and 15 min for other papers, including discussion. Video-beam is available. PowerPoint presentations, recorded on CD or USB flash-memory, should be given at registration, specifying the name of the speaker and the day and session number.

In POSTER SESSIONS, the authors are requested to display their posters minimum one hour before the session and to be present beside their posters during the session. Poster sessions' venue will be open Tuesday to Thursday, from 20.00 to 22.00.

Conference awards: Materials Research Society of Serbia will award the authors (preferably young members under 35) of the best oral and poster presentation at the conference, and also the authors of highly rated PhD theses defended between two conferences. Awarded researchers are granted free registration at the next YUCOMAT Conference.

Additional Activities: An Exhibition of synthesis and characterization equipment will be held during the Conference. Traditional Cocktail Party on Monday evening and excursion on Thursday afternoon (boat trip around Boka Kotorska Bay) will be organized again.

GENERAL CONFERENCE PROGRAMME

Sunday, September 1, 2019

08⁰⁰-19⁰⁰ **Registration**

Monday, September 2, 2019

08⁰⁰-19⁰⁰ **Registration**

09⁰⁰-10⁰⁰ **OPENING CEREMONY**

- Introduction and Welcome

Main Conference Hall

10³⁰-13⁰⁰ **First YUCOMAT Plenary Session**, Main Conference Hall

13⁰⁰ **Photo Session**

15⁰⁰-18³⁰ **First WRTCS Plenary Session**, Main Conference Hall

19³⁰-21⁰⁰ **Cocktail Party**

SYMPOSIUM A: Advanced Methods in Synthesis and Processing of Materials

SYMPOSIUM B: Advanced Materials for High-Technology Application

SYMPOSIUM C: Nanostructured Materials

SYMPOSIUM D: Eco-materials and Eco-Technologies

SYMPOSIUM E: Biomaterials

SYMPOSIUM F: WRTCS

Tuesday, September 3, 2019

09⁰⁰-13⁰⁰ **Second YUCOMAT Plenary Session**, Main Conference Hall

15⁰⁰-16³⁰ **Third YUCOMAT Plenary Session**, Main Conference Hall

17⁰⁰-18⁴⁵ **Second WRTCS Plenary Session**, Main Conference Hall

20⁰⁰-22⁰⁰ **Poster Session I** (Symposium A and B1), Villa MIMOZA

Wednesday, September 4, 2019

09⁰⁰-13⁰⁰ **Fourth YUCOMAT Plenary Session**, Main Conference Hall

15⁰⁰-17⁰⁰ **First WRTCS Oral Session**, Main Conference Hall

17³⁰-19³⁰ **Second WRTCS and First YUCOMAT Oral Session**, Main Conference Hall

20⁰⁰-22⁰⁰ **Poster Session II** (Symposium B2 and C1), Villa MIMOZA

Thursday, September 5, 2019

09⁰⁰-12⁴⁵ **Second YUCOMAT Oral Session**, Main Conference Hall

09⁰⁰-12³⁰ **Third YUCOMAT Oral Session**, Small Conference Hall

14⁰⁰-19⁰⁰ **Boat-trip around Boka Kotorska Bay**

20⁰⁰-22⁰⁰ **Poster Session III** (Symposiums C2, D, E and F), Villa MIMOZA

Friday, September 6, 2019

09⁰⁰-11¹⁵ **Fourth YUCOMAT Oral Session**, Main Conference Hall

09⁰⁰-11³⁰ **Fifth YUCOMAT Oral Session**, Small Conference Hall

11³⁰-12⁰⁰ **Awards and Closing Ceremony**

OPENING CEREMONY

Monday, September 2, 2019

Main Conference Hall

09⁰⁰-10⁰⁰

Welcome Speech

Dragan Uskoković, President of IISS and MRS-Serbia, Belgrade, Serbia

Welcome Address

Robert Sinclair, Chair of International Advisory Board

Presentation of YUCOMAT 2018 Awards

Slobodan Milonjić, Vice President of MRS-Serbia

MRS-Serbia 2019 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering

Epitaxial integration of oxides with silicon

Danilo Suvorov

Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia

Break: 10⁰⁰-10³⁰

FIRST YUCOMAT PLENARY SESSION

Main Conference Hall

Session I: 10³⁰-13⁰⁰

Chairpersons: Yoshio Bando, Elvira Fortunato and Andrea C. Ferrari

10³⁰-11⁰⁰

Stable perovskite solar cells by compositional and interface engineering

Sanghyun Paek, Hiroyuki Kanda, Yi Zhang, Hobeom Kim, Yonghui Lee, Kyung Taek Cho, Mousa Abuhelaiqa, Aron Joel Huckaba, Roldan Carmona Cristina and Mohammad Khaja Nazeeruddin

The Group for Molecular Engineering of Functional Materials, Ecole Polytechnique Fédérale de Lausanne, CH-1951 Sion, Switzerland

11⁰⁰-11³⁰

Graphene and related materials, from production to applications

Andrea C. Ferrari

Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 0FA, United Kingdom

- 11³⁰-12⁰⁰ **Next-generation large-area graphene for electronic devices**
Simon Thomas¹, Ivor Guiney¹ and Colin Humphreys²
¹Paragraf Ltd, Somersham, Cambridge, United Kingdom; ²School of Engineering and Materials Science, Queen Mary University of London, London E1 4NS, United Kingdom
- 12⁰⁰-12³⁰ **Functionality and versatility of metal oxides**
Elvira Fortunato
i3N/CENIMAT, Department of Materials Science from Faculty of Science and Technology, Universidade NOVA de Lisboa and CEMOP/UNINOVA, Campus de Caparica, 2829-516 Caparica, Portugal
- 12³⁰-13⁰⁰ **Boron nitride nanotube/nanosheet for energy applications**
Yoshio Bando^{1,2,3}
¹Institute of Molecular Plus, Tianjin University, Tianjin, China; ²International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), Ibaraki 305-044, Japan, ³Australian Institute for Innovative Materials (AIIM), University of Wollongong (UOW), NSW, 2522, Australia

13⁰⁰-13¹⁵ Photo session

Break: 13¹⁵-15⁰⁰

FIRST WRTCS PLENARY SESSION

Main Conference Hall

Session I: 15⁰⁰-16³⁰

Chairpersons: Suk-Joong L. Kang and Bernd Kieback

- 15⁰⁰-15³⁰ **Challenges and further developments in modeling of sintering**
Eugene A. Olevsky
College of Engineering, San Diego State University, San Diego, CA 92182, United States
- 15³⁰-16⁰⁰ **Micromechanics of sintering in particle scale**
Fumihiro Wakai
Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology, Yokohama, Japan

16⁰⁰-16³⁰ Coupled experimental and numerical investigation of evolution of anisotropic microstructures during stress-assisted and constrained sintering

Rajendra K. Bordia¹, Eugene A. Olevsky², Christophe Martin³

¹Clemson University, Clemson, SC 29634, United States; ²San Diego State University, San Diego, CA 92182, United States; ³Univ. Grenoble Alpes, CNRS, SIMaP, Grenoble F-38000, France

Break: 16³⁰-17⁰⁰

Session II: 17⁰⁰-18³⁰

Chairpersons: Eugene A. Olevsky and Fumihiro Wakai

17⁰⁰-17³⁰ Fundamentals of solid state sintering in multicomponent high entropy alloys

Bernd Kieback¹ and Nadine Eißmann²

¹Technische Universität Dresden, Institute for Materials Science, Dresden, Germany;

²Fraunhofer Institute for Manufacturing and Advanced Materials (IFAM), Dresden, Germany

17³⁰-18⁰⁰ What we should consider for full densification when sintering

Suk-Joong L. Kang

Korea Advanced Institute of Science and Technology (KAIST), Department of Materials Science and Engineering, Daejeon 34141, Republic of Korea

18⁰⁰-18³⁰ Increase of fracture toughness of transparent ceramics by functional, low thermal-expansion coatings

Marc Rubat du Merac², Martin Bram¹, Jürgen Malzbender¹, Mirko Ziegner¹, Marcin Rasinski¹, Olivier Guillon³

¹Forschungszentrum Jülich GmbH, Jülich, Germany; ²CeramTec GmbH, Plochingen, Germany; ³JARA-Energy, Aachen, Jülich, Germany

SECOND YUCOMAT PLENARY SESSION

Tuesday, September 3, 2019

Main Conference Hall

Session I: 09⁰⁰-11⁰⁰

Chairpersons: Robert Sinclair and Vladimir Torchilin

09⁰⁰-09³⁰ **Model based characterisation of magnetic moments and charge densities in the transmission electron microscope**

Rafal E. Dunin-Borkowski, Jan Caron, Patrick Diehle, Fengshan Zheng, Vadim Migunov and András Kovács

Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

09³⁰-10⁰⁰ **Using STEM-EELS to optimize gold nanoparticles for early cancer detection**

Robert Sinclair, Yitian Zeng and Steven Madsen

Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, United States

10⁰⁰-10³⁰ **Engineering of novel pharmaceutical drug delivery systems for combination therapy of multidrug resistant cancer**

Vladimir Torchilin

Center for Pharmaceutical Biotechnology and Nanomedicine, Northeastern University, Boston, MA 02115, United States

10³⁰-11⁰⁰ **Synthesis and applications of megamolecules**

Milan Mrksich

Department of Biomedical Engineering and Chemistry, Northwestern University, Evanston, IL 60208, United States

Break: 11⁰⁰-11³⁰

Session II: 11³⁰-13⁰⁰

Chairpersons: Sotiris E. Pratsinis and Milan Mrksich

11³⁰-12⁰⁰ **Combustion spray synthesis of nanostructured materials: from carbon black to breath sensors**

Sotiris E. Pratsinis

Particle Technology Laboratory, Institute of Process Engineering, Swiss Federal Institute of Technology (ETH Zurich), CH-8092 Zurich, Switzerland

12⁰⁰-12³⁰ Making the hospital a safer place by the sonochemical coating of all its textiles and medical devices with antibacterial nanoparticles

Aharon Gedanken

Bar-Ilan University Department of Chemistry, and the BINA center, Ramat-Gan 5290002, Israel

12³⁰-13⁰⁰ Earthlike and its discontents

Vuk Uskoković

Department of Mechanical and Aerospace Engineering, University of California, Irvine, CA, United States

Break: 13⁰⁰-15⁰⁰

THIRD YUCOMAT PLENARY SESSION

Main Conference Hall

Session I: 15⁰⁰-16³⁰

Chairpersons: Yuntian Zhu and Mamoru Senna

15⁰⁰-15³⁰ Heterostructured materials: a new paradigm for superior mechanical properties

Yuntian Zhu

Nano & Heterogeneous Materials Center, Nanjing University of Science and Technology, Nanjing, China; Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC 27695, United States

15³⁰-16⁰⁰ Optimizing the properties of titanium alloys processed using additive manufacturing

Brian Welk, Nevin Taylor, Samuel Kuhr, G.B Viswanathan, Hamish L. Fraser

Center for the Accelerated Maturation of Materials, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, United States

16⁰⁰-16³⁰ Hybridization of solid carbohydrates or hydrocarbon with metal oxides under mechanical stressing toward sustainable materials

Mamoru Senna¹, Chika Takai², Masayoshi Fuji³

¹Faculty of Science and Technology, Keio University, Hiyoshi, Yokohama, 223-8522, Japan; ²Faculty of Engineering, Gifu University, Yanagido, Gifu, 501-1193, Japan;

³Advanced Ceramics Research Center, Nagoya Institute of Technology, Honmachi, Tajimi, 507-0033, Japan

Break: 16³⁰-17⁰⁰

SECOND WRTCS PLENARY SESSION

Main Conference Hall

Session II: 17⁰⁰-18⁴⁵

Chairpersons: Heli Jantunen and Andrey V. Ragulya

17⁰⁰-17³⁰ Electroceramics without sintering

Heli Jantunen

Microelectronics Research Unit, Faculty of Information Technology and
Electrical Engineering, P. O. BOX 4500, University of Oulu, FI-90014 Oulu,
Finland

**17³⁰-18⁰⁰ The mechanisms behind solute-drag and solute-acceleration during
microstructural evolution of alumina**

Ruth Moshe, Rachel Marder, Leon Rudnik, Wayne D. Kaplan

Department of Materials Science and Engineering, Technion – Israel Institute of
Technology, Haifa, Israel

18⁰⁰-18³⁰ Understanding of sintering in Ukraine: overview of results

Andrey V. Ragulya, Mikhail Borisovich Shtern

Frantsevich Institute for Problems in Materials Science NAS of Ukraine, 3
Krzhizhanovsky str., 03142 Kiev, Ukraine

18³⁰-18⁴⁵ Field assisted reaction sintering of ceramic materials

Andrey V. Ragulya

Frantsevich Institute for Problems in Materials Science NAS of Ukraine, 3
Krzhizhanovsky str., 03142 Kiev, Ukraine

FOURTH YUCOMAT PLENARY SESSION

Wednesday, September 4, 2019

Main Conference Hall

Session I: 09⁰⁰-10³⁰

Chairpersons: Shizhang Qiao and Richard Catlow

09⁰⁰-09³⁰ **Nanostructured materials for energy-relevant electrocatalytic processes**

Shizhang Qiao

School of Materials Science and Engineering, Tianjin University, Tianjin 300072, China; School of Chemical Engineering, The University of Adelaide, SA 5005, Australia

09³⁰-10⁰⁰ **Computer modelling as a predictive tool in materials and catalytic science**

Richard Catlow^{1,2,3}

¹Department of Chemistry, University College London, London WC1E 6BT, United Kingdom; ²School of Chemistry, Cardiff University, Cardiff CF10 3AT, United Kingdom; ³UK Catalysis Hub, Research Complex at Harwell, R92 Harwell Oxford Oxfordshire OX11 0FA, United Kingdom

10⁰⁰-10³⁰ **Crystal chemistry and properties of G-phases**

Peter Franz Rogl and Andrij Grytsiv

Institute of Materials Chemistry, University of Vienna, A-1090 Wien, Austria

Break: 10³⁰-11⁰⁰

Session II: 11⁰⁰-13⁰⁰

Chairpersons: Hamish L. Fraser and Nobuo Tanaka

11⁰⁰-11³⁰ **Goodbye hospitals and hello implantable nanosensors**

Thomas J. Webster

Chemical Engineering, Northeastern University, Boston, MA, United States

11³⁰-12⁰⁰ **Strain-engineering in advanced CMOS structures**

Dae-Hong Ko

Department of Materials Science and Engineering, Yonsei University, Seoul, Republic of Korea

- 12⁰⁰-12³⁰ **Environmental & dynamic electron microscopy of advanced materials in HV-(S)TEM**
Nobuo Tanaka and Shigeo Arai
Institute of Materials and Systems for Sustainability (IMaSS), Nagoya University,
Nagoya, 464-8603, Japan
- 12³⁰-13⁰⁰ **Integrated Differential Phase Contrast (iDPC) STEM for low Z detection and for high contrast low dose imaging applications**
Maarten Wirix
Thermo Fisher Scientific, Eindhoven, Netherlands

Break: 13⁰⁰-15⁰⁰

FIRST WRTCS ORAL SESSION

Main Conference Hall

Session I: 15⁰⁰-17⁰⁰

Chairpersons: Biljana Stojanović and Đorđe Janačković

- 15⁰⁰-15¹⁵ **Thermal stress directions and stress mechanism in Ag sintered bonding layer under thermal cycling test for Si power device structures having sintering chip-attachment**
Masaaki Aoki^{1,2}, Koki Chinone¹, Akihiro Mochizuki², Yoshio Murakami², Mutsuharu Tsunoda², Goro Yoshinari², Nobuhiko Nakano¹
¹Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa 223-8521, Japan; ²MacDermid Alpha Electronics Solutions / MacDermid Performance Solutions Japan, Hiratsuka, Kanagawa 254-0082, Japan
- 15¹⁵-15³⁰ **Thermal stress profiles and stress directions in Si chip under thermal cycling test for power device structures having Ag sintering chip-attachment**
Koki Chinone¹, Masaaki Aoki^{1,2}, Akihiro Mochizuki², Yoshio Murakami², Mutsuharu Tsunoda², Goro Yoshinari², and Nobuhiko Nakano¹
¹Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa 223-8521, Japan; ²MacDermid Alpha Electronics Solutions / MacDermid Performance Solutions Japan, Hiratsuka, Kanagawa 254-0082, Japan

- 15³⁰-15⁴⁵ **Influence of milling, annealing and sintering parameters on the formation of LLZO compound**
Dariusz Oleszak¹, Tomasz Pikula², Mirosława Pawlyta³
¹Warsaw University of Technology, Warsaw, Poland, ²Lublin University of Technology, Lublin, Poland, ³Silesian University of Technology, Gliwice, Poland
- 15⁴⁵-16⁰⁰ **Synthesis and densification of electride Mayenite - Ca₁₂Al₁₄O₃₃**
 Branko Matović
 Vinca Institute of Nuclear Sciences, University of Belgrade, Mike Petrovića Alasa 12-14, 11 351 Vinča, Belgrade, Serbia
- 16⁰⁰-16¹⁵ **Ultra-rapid microwave sintering based on controlled thermal instability and resonant absorption**
 Sergei V. Egorov, Anatoly G. Ereemeev, Vladislav V. Kholoptsev, Ivan V. Plotnikov, Kirill I. Rybakov, Andrei A. Sorokin, Yury V. Bykov
 Institute of Applied Physics, Russian Academy of Sciences 46 Ulyanov St., Nizhny Novgorod 603950 Russia
- 16¹⁵-16³⁰ **Effect of scanning strategy on mechanical properties of selective laser melted Inconel 718**
Guang-Ping Zhang¹, Hong-Yuan Wan¹, Guo-Feng Chen²
¹Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, P. R. China; ²Materials & Manufacturing Qualification Group, Corporate Technology, Siemens Ltd., China, Beijing, 100102, China
- 16³⁰-16⁴⁵ **Laser-powder bed fusion of bronze: microstructural, mechanical and electrochemical properties**
 Mustafa Naci Top¹ and H. Ozkan Gulsoy²
¹Marmara University, Inst. Graduate Studies Pure and Applied Sci., 34722, Istanbul, Turkey; ²Marmara University, Technology Faculty, Metall. And Mater. Eng., 34722, Istanbul, Turkey
- 16⁴⁵-17⁰⁰ **Scaffolding via surface-selective laser sintering of biocompatible polymer particles using water as heating sensitizer**
Nikita V. Minaev¹, Svetlana A. Minaeva¹, Semyon N. Churbanov^{1,2}, Tatiana A. Akopova³, Tatiana S. Demina^{2,3}, Peter S. Timashev^{1,2}
¹Institute of Photon Technologies FSRC “Crystallography and Photonics” RAS, Moscow, Troitsk, Russia; ²Institute of Regenerative Medicine, I. M. Sechenov First Moscow State Medical University, 119991 Moscow, Russia; ³Enikolopov Institute of Synthetic Polymeric Materials, Russian Academy of Sciences, ul. Profsoyuznaya 70, Moscow, 117393 Russia

Break: 17⁰⁰-17³⁰

SECOND WRTCS AND FIRST YUCOMAT ORAL SESSION

Main Conference Hall

Session II: 17³⁰-19³⁰

Chairpersons: Gerda Rogl and Guang-Ping Zhang

17³⁰-17⁴⁵ Investigation of the effect of GDC (Gd-doped ceria) powder morphology on the properties of the ceramics sintered using SPS

Daniel Vladimirovich Maslennikov^{1,2}, Aleksandr Anatol'evich Matvienko^{1,2}, Dina Vladimirovna Dudina^{1,2,3,4}, Maxim Alexandrovich Esikov^{3,4}, Hidemi Kato⁵

¹Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia; ²Novosibirsk State University, Novosibirsk, Russia; ³Lavrentyev Institute of Hydrodynamics SB RAS, Novosibirsk, Russia; ⁴Novosibirsk State Technical University, Novosibirsk, Russia; ⁵Institute for Materials Research, Tohoku University, Japan

17⁴⁵-18⁰⁰ The BaTiO₃ nano-scale coated morphology influence on electronic properties and ceramics fractal nature frontiers

Vojislav V. Mitić^{1,2}, Goran Lazović³, Chun-An Lu⁴, Vesna Paunović¹, Sandra Veljković¹, Hans Fecht⁵, Branislav Vlahović⁶

¹University of Nis, Faculty of Electronic Engineering, Nis, Serbia; ²Institute of Technical Sciences of SASA, Belgrade, Serbia; ³University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia; ⁴Industrial Technology Research Institute, Taiwan; ⁵Institute of Functional Nanosystems, University of Ulm, 89081 Ulm, Germany; ⁶North Carolina Central University, Durham, NC 27707 United States

18⁰⁰-18¹⁵ Sintering process optimization for Cu-Al₂O₃ powders synthesized by novel method

Marija Korać¹, Zoran Anđić², Željko Kamberović¹, Nataša Gajić³

¹Faculty of Technology and Metallurgy, University of Belgrade, Serbia; ²Innovation center of Faculty of Chemistry in Belgrade Ltd., University of Belgrade, Serbia; ³Innovation center of Faculty of Technology and Metallurgy in Belgrade Ltd., University of Belgrade, Serbia

18¹⁵-18³⁰ The effect of severe plastic deformation (SPD) via high pressure torsion (HPT) on physical and mechanical properties of thermoelectric materials

Gerda Rogl^{1,2,3}, Ernst Bauer^{2,3}, Michael J. Zehetbauer⁴, Peter Franz Rogl^{1,3}

¹Inst. of Materials Chemistry, University of Vienna, A-1090 Wien, Austria; ²Inst. of Solid State Physics, TU Wien, A-1040 Wien, Austria; ³Christian Doppler Laboratory for Thermoelectricity, Wien, Austria; ⁴Faculty of Physics, University of Vienna, A-1090 Wien, Austria

- 18³⁰-18⁴⁵ **G-quadruplex DNA oligomer for electrochemical sensing of insulin**
Izumi Kubo
Graduate School of Engineering, Soka University, Tokyo, Japan
- 18⁴⁵-19⁰⁰ **Smart composites with combined caloric and magnetoelectric effects**
Abdulkarim A. Amirov^{1,2}, Vladimir V. Rodionov¹, Viacheslav S. Nikulin¹, Evgeny Klippert¹ and Akhmed M. Aliev²
¹Laboratory of Novel Magnetic Materials & Institute of Physics Mathematics and Informational Technologies, Immanuel Kant Baltic Federal University, 236029 Kaliningrad, Russia; ²Amirkhanov Institute of Physics, Daghestan Scientific Center, Russian Academy of Sciences, 367003 Makhachkala, Russia; ³Kotelnikov Institute of Radio Engineering and Electronics, Russian Academy of Sciences, 125009 Moscow, Russia
- 19⁰⁰-19¹⁵ **Temperature dependence of graphene transport coefficients**
Stevo Jaćimovski¹, Dejan Raković²
¹ University of Criminalistic and Police Studies, Belgrade, Serbia; ² University of Belgrade, Faculty of Electrical Engineering, Belgrade, Serbia
- 19¹⁵-19³⁰ **Control of structure and thermo-reversible gelation of networks with reversible covalent Diels-Adler crosslinks**
Beata Strachota, Jiří Dybal, Libor Matějka
Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic

SECOND YUCOMAT ORAL SESSION

Thursday, September 5, 2019

Main Conference Hall

Session I: 09⁰⁰-10³⁰

Chairpersons: Dragana Jugović and Zoran Jovanović

- 09⁰⁰-09¹⁵ **The structure and electrochemical properties of fayalite Fe₂SiO₄**
Dragana Jugović¹, Miodrag Mitrić², Miloš Milović¹, Valentin N. Ivanovski², Srečo D. Škapin³, Dragan P. Uskoković¹
¹Institute of Technical Sciences of SASA, Belgrade, Serbia; ²Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia; ³Jožef Štefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia
- 09¹⁵-09³⁰ **Fabrication of graphene/Cu flexible electrode with excellent mechanical reliability and electrical performance**
Bin Zhang, Yu-Jia Yang
Key Laboratory for Anisotropy and Texture of Materials, Ministry of Education, School of Materials Science and Engineering, Northeastern University, 3-11 Wenhua Road, Shenyang 110819, PR China
- 09³⁰-09⁴⁵ **PLD growth of STO/PZT thin films on graphene oxide-buffered Si (001) surface**
Zoran Jovanović^{1,2}, Urška Gabor¹, Elena Tchernychova³, Danilo Suvorov¹, Matjaž Spreitzer¹
¹Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia; ²Laboratory of Physics, Vinča Institute of Nuclear Sciences, Belgrade, Serbia; ³National Institute of Chemistry, Ljubljana, Slovenia
- 09⁴⁵-10⁰⁰ **Deposition of nanocomposite organosilicon thin films under dusty plasma conditions**
Vilma Bursikova¹, Vojtěch Homola¹, Štěpánka Bittnerová¹, Roman Přibyl¹, Petr Tomšej¹, Monika Stupavská¹, Anna Charvatova Campbell², Petr Klapetek², Romana Mikšová³, Vratislav Perina³
¹Institute of Physical Electronics, Faculty of Science, Masaryk University, Kotlarska 2, 611 37 Brno, Czech Republic; ²Czech Metrology Institute, Okružní 31, 63800 Brno, Czech Republic; ³Institute of Nuclear Physics, Academy of Sciences of the Czech Republic, 25068 Rez near Prague, Czech Republic
- 10⁰⁰-10¹⁵ **Photovoltaic perovskites for high sensitive X-ray detection**
Veljko Đokić, Anastasiia Glushkova, Pavao Andričević, Alla Arakcheeva, Márton Kollár, Endre Horváth, and László Forró
Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

10¹⁵-10³⁰ Effect of graphite reinforcements on the tribological properties of Al₂O₃ coatings deposited by plasma spraying

Liutauras Marcinauskas¹, Mindaugas Milieška², Jacob Shiby Mathew¹, Romualdas Kėželis², Vilius Dovydaitis¹, Brigita Abakevičienė¹, Aleksandras Iljinis¹, Mitjan Kalin³

¹Kaunas University of Technology, Studentų 50 Kaunas, Lithuania; ²Lithuanian Energy Institute, Breslaujos 3 Kaunas, Lithuania; ³University of Ljubljana, Bogiščičeva 8, 1000 Ljubljana, Slovenia

Break: 10³⁰-11⁰⁰

Session II: 11⁰⁰-12⁴⁵

Chairpersons: Anatole N. Khodan and Jan Kusinski

11⁰⁰-11¹⁵ Optical and structural properties of tin oxide thin films doped with fluorine obtained by USP technique

Nora Castillo Tepox, José A. Luna López, Alvaro D. Hernández de la Luz
Centro de Investigación en Dispositivos Semiconductores, CIDS, ICUAP, Benemérita Universidad Autónoma de Puebla, 14 sur y Av. San Claudio, Cd. Universitaria, Edificios IC-5, IC-6, Puebla, Pue., 72570, México

11¹⁵-11³⁰ Photoluminescence enhancement of Dy³⁺-doped tellurite glasses through nanoparticle doping for solid-state lighting applications

Ali Erçin Ersundu, Orhan Kibrisli, Miray Çelikkilek Ersundu
Yildiz Technical University, Department of Metallurgical and Materials Engineering, Faculty of Chemical and Metallurgical Engineering, Istanbul, 34220, Turkey

11³⁰-11⁴⁵ Point defect-enhanced optical and photoelectrochemical water splitting activity of nanostructured Zn_{1-x}Fe_yO_(1-x+1.5y)

Smilja Marković¹, Vladimir Rajić², Ivana Stojković Simatović³, Ljiljana Veselinović¹, Jelena Belošević Čavor², Valentin N. Ivanovski², Mirjana Novaković², Srečo D. Škapin⁴, Stevan Stojadinović⁵, Vladislav Rac⁶, Dragan P. Uskoković¹

¹Institute of Technical Sciences of SASA, Belgrade, Serbia; ²The Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia; ³Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia; ⁴Jožef Stefan Institute, Ljubljana, Slovenia; ⁵Faculty of Physics, University of Belgrade, Belgrade, Serbia; ⁶Faculty of Agriculture, University of Belgrade, Zemun, Serbia

- 11⁴⁵-12⁰⁰ **Development of new functional materials and 3D nanocomposites for applications in THz optics**
Anatole N. Khodan¹, Kirill I. Zaytsev², Vladimir N. Kurlov³, Gennady P. Kopitsa⁴
¹Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Moscow, Russia, ²Prokhorov General Physics Institute RAS, Moscow, Russia, ³Institute of Solid State Physics RAS, Chernogolovka, Russia, ⁴Konstantinov Petersburg Nuclear Physics Institute, NRC “Kurchatov Institute”, Gatchina, Russia
- 12⁰⁰-12¹⁵ **Electron holography examination of FeSiB ribbons crystallized by using interference pulsed laser heating**
Jan Kusinski¹, Olaf Czyz¹, Agnieszka Radziszewska¹, Roman Ostrowski², Krzysztof Morawiec³, Piotr Dłużewski³, Małgorzata Kac⁴
¹AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Krakow, Poland; ²Military University of Technology, Institute of Optoelectronics, Warsaw, 2 Gen. S. Kaliskiego, 00-908 Warsaw, Poland; ³Institute of Physics Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland; ⁴Institute of Nuclear Physics Polish Academy of Sciences, ul. Radzikowskiego 152, 31-342 Krakow, Poland
- 12¹⁵-12³⁰ **Acoustically tuned quantum light emission from atom-like defects in hexagonal boron nitride**
Snežana Lazić¹, Sergio Pinilla Yanguas¹, Carlos Gibaja², Félix Zamora² and Herko P. Van der Meulen¹
¹Departamento de Física de Materiales, Instituto “Nicolás Cabrera” and Instituto de Física de Materia Condensada (IFIMAC), Universidad Autónoma de Madrid (UAM), 28049 Madrid, Spain; ²Departamento de Química Inorgánica, UAM, 28049 Madrid, Spain
- 12³⁰-12⁴⁵ **Mechanical properties of 1T-TaS₂**
Luka Ćirić, Raphael Foschia, Anastasia Glushkova, Narjes Noma, Ayat Karimi, Iva Tkalcec, Samy Adjam, Daniele Marie, Helmut Berger and Laszlo Forró
 Ecole Polytechnique Federal de Lausanne, Laboratory of Physics of Complex Matter, Lausanne, Vaud, Switzerland

THIRD YUCOMAT ORAL SESSION

Small Conference Hall

Session I: 09⁰⁰-10³⁰

Chairpersons: Đorđe Veljović and Sonja Jovanović

- 09⁰⁰-09¹⁵ **Effects of annealing on the physical properties of various metallic oxides**
Sorina Iftimie¹, Claudiu Locovei^{1,2}, Adrian Radu¹, Vlad-Andrei Antohe^{1,3}, Marcela Socol², Anca Dumitru¹, Ana-Maria Raduta¹, Lucian Ion¹, Stefan Antohe^{1,4}
¹University of Bucharest, Faculty of Physics, Magurele, 077125, Romania; ²National Institute of Materials Physics, Magurele, 077125, Romania; ³Université Catholique de Louvain (UC Louvain), Institute of Condensed Matter and Nanosciences (IMCN), Louvain-la-Neuve, B-1348, Belgium; ⁴Academy of Romanian Scientists, 030167, Bucharest, Romania
- 09¹⁵-09³⁰ **Cryo-deformation by upsetting-extrusion: effect on microstructure and mechanical properties of CoCrFeMnNi high-entropy alloy**
Anastasia Levenets, Alexander S. Kalchenko, Mikhail A. Tikhonovsky, Pavel A. Khaimovich
 National Science Center “Kharkiv Institute of Physics and Technology”, Kharkiv, Ukraine
- 09³⁰-09⁴⁵ **Microstructure and mechanical property of solid–phase joints formed by EP975 superalloy and VKNA-25 type intermetallic alloys**
Elvina Galieva¹, Andrey Drozdov², Vener Valitov¹, Elvira Arginbaeva³, Ramil Lutfullin¹
¹Institute for Metals Superplasticity Problems of Russian Academy of Sciences, 450001, Ufa, Russia; ²Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences, 119334, Moscow, Russia; ³All-Russia Research Institute of Aviation Materials (VIAM), 105005, Moscow, Russia
- 09⁴⁵-10⁰⁰ **Synthesis and catalytic properties of Co-Pt, Cu-Pd, Ni-Pt nanoalloys**
Anton Popov¹, Yury Shubin¹, Pavel Plusnin¹, Danila Kal'nyi¹, Ilya Mishakov², Yury Bauman²
¹Nikolaev Institute of Inorganic Chemistry of SB RAS, Novosibirsk, Russia; ²Boreskov Institute of Catalysis of SB RAS, Novosibirsk, Russia
- 10⁰⁰-10¹⁵ **Peculiarities of impurity effect on the oxygen adsorption on the Ti₃Al(0001) and TiAl(100) surfaces**
Svetlana E. Kulkova^{1,2}, Alexander V. Bakulin^{1,2}, Sergey S. Kulkov^{1,2}
¹Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia; ²Tomsk State University, Tomsk, Russia

- 10¹⁵-10³⁰ **Screen-printed thin smooth nanostructured BaTiO₃ films for printed electronics**
Saide Umerova, Serhii Ivanchenko, Dmitro Baranovskiy, Olha Kovalenko, Andrey Ragulya
 Frantsevich Institute for Problems of Materials Science of NASU, Kiev, Ukraine

Break: 10³⁰-11⁰⁰

Session II: 11⁰⁰-12³⁰

Chairpersons: Branko Matović and Vuk Radmilović

- 11⁰⁰-11¹⁵ **Mechanism of topochemical conversion of Bi₄Ti₃O₁₂ in SrTiO₃ nanoplates under hydrothermal conditions**
Alja Čontala^{1,2}, Nina Daneu¹, Matjaž Spreitzer¹ and Marjeta Maček Kržmanc¹
¹Jožef Stefan Institute, Advanced Materials Department, Jamova cesta 39, Ljubljana, Slovenia; ²Jožef Stefan International Postgraduate School, Jamova cesta 39, 1000 Ljubljana, Slovenia
- 11¹⁵-11³⁰ **Synthesis of anodic alumina membrane with defined pore diameters**
Iwona Dobosz, Wanda Gumowska
 AGH, University of Science and Technology, Faculty of Non - Ferrous Metals, al. Mickiewicza 30, 30-059 Krakow, Poland
- 11³⁰-11⁴⁵ **Mechanical behavior of nanocrystalline Ni-Mo layers processed by electrodeposition**
Garima Kapoor¹, László Péter², Éva Fekete², Dávid Ugi¹, György Radnóczy³, Jenő Gubicza¹
¹Department of Materials Physics, Eötvös Loránd University, Budapest, Hungary; ²Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary; ³Institute for Technical Physics and Mater. Sci., Centre for Energy Research HAS, Budapest, Hungary
- 11⁴⁵-12⁰⁰ **Prediction of the temper of hardening in the free and bounded bending of long-length, low-alloyed copper billets under high-cycle processing conditions**
Georgy I. Raab, Rashid N. Asfandiyarov, Arseniy G. Raab, Denis A. Aksenov
 Research Institute of Physics of Advanced Materials at USATU, Ufa, Russia
- 12⁰⁰-12¹⁵ **Development and characterization of carbon nanotube reinforced natural rubber composite for prosthetic foot application**
 Razaq O. Medupin^{1,2}, Oladiran K. Abubakre^{1,2}, Ambali S. AbdulKareem^{1,3}, Rasheed A. Muriana^{1,2} and James A. Adeniran⁴
¹Nanotechnology Research Group, Federal University of Technology, Minna, Nigeria; ²Mechanical Engineering Department, Federal University of Technology, Minna, Nigeria; ³Chemical Engineering Department, Federal University of Technology, Minna, Nigeria; ⁴Federal Medical Centre, Bida, Nigeria

12¹⁵-12³⁰ **Effects of cooling rate during casting on the corrosion resistance of 6xxx aluminium alloy**

Joseph B. Agboola¹, Anyoku S. Emmanuel² and Atinuke M. Oladoye²

¹Department of Materials and Metallurgical Engineering, Federal University of Technology, Minna, Nigeria; ²Department of Metallurgical and Materials Engineering, University of Lagos, Lagos, Nigeria

FOURTH YUCOMAT ORAL SESSION

Friday, September 6, 2019

Main Conference Hall

Session I: 09⁰⁰-11¹⁵

Chairpersons: Natalia Kamanina and Bojana Obradović

- 09⁰⁰-09¹⁵ **Hemodialysis composite membranes with functionalized graphene**
Iulian Antoniac¹, Aurora Antoniac¹, Andrada Serafim², Andreea Iordache^{2, 3}, Andreea Madalina Pandelescu^{2,3}, Stefan Ioan Voicu^{2,3}
¹University Politehnica of Bucharest, Faculty of Materials Science and Engineering, Bucharest, Romania; ² University Politehnica of Bucharest, Advanced Polymer Materials Group, Gheorghe Polizu 1-7, 011061 Bucharest, Romania; ³University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, Department of Analytical Chemistry and Environmental Engineering, Str. Gheorghe Polizu 1-7, Bucharest, Romania
- 09¹⁵-09³⁰ **Supercritical CO₂ utilization in preparation of poorly soluble drugs solid dispersions**
Jelena Đuriš¹, Stoja Milovanović², Đorđe Medarević¹, Vladimir Dobričić¹, Svetlana Ibrić¹
¹University of Belgrade, Faculty of Pharmacy, Vojvode Stepe 450, 11221, Belgrade, Serbia; ²University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120, Belgrade, Serbia
- 09³⁰-09⁴⁵ **New agents for nitric oxide (NO) chemotherapy of bacterial infections**
Nataliya A. Sanina
Institute of Problems of Chemical Physics Russian Academy of Sciences, Chernogolovka, Russia
- 09⁴⁵-10⁰⁰ **Controllable release of oxaprozin from hydroxyapatite nano-particles**
Vukašin Ugrinović¹, Bojan Božić², Đorđe Janačković³, Đorđe Veljović³
¹Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia; ²Institute of Physiology and Biochemistry, Faculty of Biology, Belgrade, Serbia; ³Faculty of Technology and Metallurgy, Belgrade, Serbia

10⁰⁰-10¹⁵ Polysaccharide-coated polylactide microparticles with controlled surface structure

Tatiana S. Demina^{1,2}, Liubov A. Kilyashova³, Tatiana N. Popyrina^{1,3}, Christian Grandfils⁴, Peter S. Timashev², Tatiana A. Akopova¹

¹Enikolopov Institute of Synthetic Polymer Materials RAS, Moscow, Russia; ²Institute for Regenerative Medicine, Sechenov University, Moscow, Russia; ³Moscow Aviation Institute, Moscow, Russia; ⁴CEIB, University of Liège, Liège, Belgium

10¹⁵-10³⁰ Hydroxyapatite/ β -tricalcium phosphate granules enriched with strontium induce improved bone regeneration in osteoporotic bone: comparison between 11 different bone conditions

Janis Zarins^{1,2}, Mara Pilmane², Elga Sidhoma², Ilze Salma³, Janis Locs⁴

¹Department of Hand and Plastic Surgery, Microsurgery Centre of Latvia, Brivibas Street 410, LV-1024, Riga, Latvia; ²Institute of Anatomy and Anthropology, Riga Stradins University, Kronvalda boulevard 9, LV-1010, Riga, Latvia; ³Department of Oral and Maxillofacial Surgery, Riga Stradins University, Dzirciema Street 20, LV-1007, Riga, Latvia; ⁴Rudolfs Cimdins Riga Biomaterials Innovations and Development Centre of Riga Technical University, Pulka Street 3, LV-1007, Riga, Latvia

10³⁰-10⁴⁵ Hydroxyapatite nano particles doped with Gd³⁺, Yb³⁺/Tm³⁺ and Eu³⁺ as lumino-magnetic multimodal contrast agents

Nenad L. Ignjatović¹, Lidija Mančić¹, Marina Vuković², Zoran Stojanović¹, Marko G. Nikolić³, Srečo D. Škapin⁴, Sonja Jovanović^{4,5}, Ljiljana Veselinović¹, Snežana Lazić⁶, Smilja Marković¹, Dragan P. Uskoković¹

¹Institute of Technical Sciences of the Serbian Academy of Science and Arts, Knez Mihailova 35/IV, P.O. Box 377, 11000 Belgrade, Serbia; ² University of Belgrade, Innovation center, Department of General and Inorganic Chemistry, Studentski trg 12-16, Beograd, Serbia; ³University of Belgrade, Institute of Physics, Photonic Center, Zemun, Serbia; ⁴Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia; ⁵University of Belgrade, Vinča Institute of Nuclear Sciences, PO Box 522, 11001 Belgrade, Serbia; ⁶ Universidad Autónoma de Madrid (UAM), Instituto Universitario de Ciencia de Materiales “Nicolás Cabrera” (INC) and Condensed Matter Physics Center (IFIMAC), Departamento de Física de Materiales, 28049 Madrid, Spain

10⁴⁵-11⁰⁰ **The effect of Ga-substitution on magneto-structural properties of cobalt ferrite nanoparticles**

Sonja Jovanović^{1,2}, Davide Peddis^{3,4}, Nader Yaacoub⁵, Matjaž Spreitzer¹, Marija Vukomanović¹

¹Advanced Materials Department, Jožef Stefan Institute, Jamova cesta 39, Ljubljana, Slovenia; ²Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Mike Petrovića Alasa 12-14, Belgrade, Serbia; ³nM2-Lab, Istituto di Struttura della Materia, CNR, Monterotondo Scalo (Roma) 00015, Italy; ⁴Department of Chemistry and Industrial Chemistry, University of Genova, Genova, Italy; ⁵LUNAM, Université du Maine, Institut des Molécules et Matériaux du Mans CNRS UMR-6283, F-72085 Le Mans, France

11⁰⁰-11¹⁵ **Materials properties modification via nanotechnology approach**

Natalia Kamanina

Vavilov State Optical Institute, St.- Petersburg, Russia; St.-Petersburg Electrotechnical University ("LETI"), St.- Petersburg, Russia

FIFTH YUCOMAT ORAL SESSION

Small Conference Hall

Session I: 09⁰⁰-11³⁰

Chairpersons: Smilja Marković and Veljko Đokić

09⁰⁰-09¹⁵ **Solvent-free mechanochemical reactions of chitosan: a green chemistry approach**

Tatiana A. Akopova

Enikolopov Institute of Synthetic Polymeric Materials RAS, Profsoyuznaya 70, Moscow, Russia

09¹⁵-09³⁰ **Characterization and application of molybdenum-oxides in liquid-phase hydrodeoxygenation of furfural**

Aleksa Kojčinović, Miha Grilc, Blaž Likozar

Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

09³⁰-09⁴⁵ **Zero waste recovery of mining and industrial waste**

Mateja Košir, Ana Mladenović, Alenka Mauko Pranjčić, Petra Vrhovnik, Kim Mezga
Slovenian National Building and Civil Engineering Institute, Ljubljana, Slovenia

- 09⁴⁵-10⁰⁰ **Influence of the sintering temperature on the microstructure of belite-sulfoaluminate cement clinkers**
Martina Cvetković¹, Lea Žibret¹, Andrej Ipavec², Sabina Kramar¹
¹Slovenian National Building and Civil Engineering Institute, Dimičeva ulica 12, SI-1000 Ljubljana, Slovenia; ²Salonit Anhovo d.d., Anhovo 1, SI-5210 Deskle, Slovenia
- 10⁰⁰-10¹⁵ **Dielectric loss factor of jute woven fabrics: effect of alkali treatment conditions**
Aleksandra Ivanovska¹, Dragana Cerović², Koviljka Asanović¹, Mirjana Kostić¹
¹Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade 11000, Serbia; ²Faculty of Physics, University of Belgrade, Studentski Trg 12, Belgrade 11000, Serbia
- 10¹⁵-10³⁰ **A novel type of building material derived from the by-products of steel making industry**
Irena Nikolić^{1,2}, Ivana Milašević², Nevena Cupara², Ljubica Ivanović², Dijana Đurović², Smilja Marković³, Ljiljana Veselinović³, Vuk Radmilović⁴, Velimir Radmilović⁵
¹University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro; ²Institut of Public Health of Montenegro, Podgorica, Montenegro; ³Institute of Technical Sciences of SASA, Belgrade, Serbia; ⁴Faculty of Technology and Metallurgy, Belgrade, Serbia; ⁵Serbian Academy of Sciences and Arts, Belgrade, Serbia
- 10³⁰-10⁴⁵ **Comparative studies on electrodeposition of metals from gluconate solutions**
 Ewa Rudnik
 AGH University of Science and Technology, Faculty of Non-Ferrous Metals, al. Mickiewicza 30, 30-059 Cracow, Poland
- 10⁴⁵-11⁰⁰ **Conditions of non-cryogenic brittle fracture of different starch grains under their mechanical treatment**
Anatoly Politov^{1,2}, Valeria Vasikhovskaya², Margarita Pravdina³, Chengmin Wang⁴
¹Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia, ²Novosibirsk State University, Novosibirsk, Russia, ³Kutateladze Institute of Thermophysics SB RAS, Novosibirsk, Russia, ⁴Dongguan Vladimir Biotechnology Co. Ltd, Dongguan, Guangdong, China
- 11⁰⁰-11¹⁵ **Heterogeneous enzymatic hydrolysis of non-cryogenic brittle fractured starch**
 Valeria Vasikhovskaya¹, Anatoly Politov^{1,2}
¹Novosibirsk State University, Novosibirsk, Russia, ²Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia

11¹⁵-11³⁰ **Making a curved part with LATP technology using two synchronized robots, without using a physical mandrel**

Samoil Samak¹, Vele Samak¹, Dimitar Bogdanoski¹, Zlatko Sokoloski¹, Blagoja Samakoski², Svetlana Risteska²

¹Mikrosam D.O.O, Prilep, North Macedonia; ²Institute for Advanced Composites and Robotics (IACR), Prilep, North Macedonia

POSTER SESSION I

Tuesday, September 3, 2019, 20⁰⁰-22⁰⁰

Chairpersons: Vuk V. Radmilović, Željko Radovanović

YUCOMAT SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

P.S.A.1. Physicochemical properties of cobalt ferrite nanoparticles synthesized by using linear surfactants and non-planar stereogenic-at-metal complexes

Ivan Kozenkov¹, Sonja Jovanović^{2,3}, Rafiali Rafalizade¹, Alexander Bulychov¹, Valeria Rodionova¹

¹Laboratory of novel magnetic materials, Immanuel Kant Baltic Federal University, Kaliningrad, Russia; ²Advanced materials department, Jožef Stefan Institute, Ljubljana, Slovenia; ³Laboratory of Physics, Vinca Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

P.S.A.2. Hall-Petch relation in harmonic structure designed Ni compacts

Hiroki Hino¹, Bhupndra Sharma², Mie Kawabata², Kei Ameyama²

¹Graduate School of Science and Engineering, Ritsumeikan University; ²Faculty of Science and Engineering, Ritsumeikan University, Shiga, Japan

P.S.A.3. Preferential recrystallization by thermo-mechanical processing in pure titanium with harmonic structure

Kyohei Hayashi¹, Akito Shimamura¹, Bhupendra Sharma², Mie Kawabata², Kei Ameyama²

¹Graduate School of Science and Engineering Ritsumeikan University, Kusatsu/Shiga, Japan; ²Department of Mechanical Engineering Ritsumeikan University, Kusatsu/Shiga, Japan

P.S.A.4. Microstructure and mechanical properties of harmonic structure designed Cu-9 at% Ge alloy

Kenta Hori¹, Bhupndra Sharma², Mie Kawabata², Kei Ameyama²

¹Graduate School of Science and Engineering, Ritsumeikan University, Kusatsu/Shiga, Japan; ²Faculty of Science and Engineering, Ritsumeikan University, Shiga, Japan

- P.S.A.5. **Effect of UFG structure on mechanical properties in harmonic structure designed pure-Ni**
Taiki Kambara¹, Masaya Nagata², Bhupendra Sharma³, Mie Kawabata³, Kei Ameyama³
¹Graduate School of Science and Engineering Ritsumeikan University, Kusatsu/Shiga, Japan; ²Japan Patent Office, Tokyo, Japan; ³Department of Mechanical Engineering Ritsumeikan University, Kusatsu/Shiga, Japan
- P.S.A.6. **Harmonic structure design of Co-Cr-Mo alloy and its mechanical properties**
Sho Matsumura, Bhupendra Sharma, Mie Kawabata, Kei Ameyama
 Department of Mechanical Engineering, Ritsumeikan University, Kusatsu/Shiga, Japan
- P.S.A.7. **Improvement of mechanical properties of harmonic structure SUS304L by thermo-mechanical process**
Taishu Tsujino¹, Masashi Nakatani¹, Bhupendra Sharma², Mie Kawabata², Kei Ameyama²
¹Graduate School of Science and Engineering Ritsumeikan University, Kusatsu/Shiga, Japan; ²Department of Mechanical Engineering Ritsumeikan University, Kusatsu/Shiga, Japan
- P.S.A.8. **Plasma electrolysis oxidation using a pulsed unipolar power supply to improve electrochemical behavior of 316L austenitic steel**
Victor Aurel Andrei¹, Viorel Malinovschi², Cristiana Rădulescu¹, Elisabeta Coaca³, Ioana Daniela Dulama¹
¹Valahia University of Targoviste, Institute of Multidisciplinary Research for Science and Technology, 130004 Targoviste, Romania; ²University of Pitesti, 110040 Pitesti, Romania; ³Institute for Nuclear Research, str. Campului, 1, Mioveni, Arges, Romania
- P.S.A.9. **Synthesis of titanium nitride via hybrid polymeric composites**
Anca Dumitru¹, Sorina Iftimie¹, Anita Radu², Andreea Miron², Andrei Sarbu², Cristian Panaiotu¹, Claudiu Locovei^{1,3}, Carmen Lazau⁴
¹Faculty of Physics, University of Bucharest, Bucharest-Magurele, 077125, Romania; ²National Research and Development Institute for Chemistry and Petrochemistry INCDCP-ICECHIM, Advanced Polymer Materials and Polymer Recycling, 060021 Bucharest, Romania; ³National Institute of Materials Physics, Bucharest-Magurele, 077125, Romania; ⁴National Institute for Research and Development in Electrochemistry and Condensed Matter, 300224 Timisoara, Romania

- P.S.A.10. **Synthesis, structural modelling and functional properties of amorphous transition metal polysulfides**
Ekaterina D. Grayfer¹, Sofya B. Artemkina¹, Andrey N. Enyashin², Anastassiia A. Poltarak¹, Anastasiia D. Fedorenko¹, Pavel A. Poltarak¹, Mariia N. Ivanova¹, Sung-Jin Kim³, Vladimir E. Fedorov^{1,4}
¹Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, 3, Acad. Lavrentiev Ave., Novosibirsk, 630090, Russia; ²Institute of Solid State Chemistry, Ural Branch of Russian Academy of Sciences, 91, Pervomayskaya st., Ekaterinburg, 620990, Russia; ³Ewha Womans University, Division of Nano Sciences/Department of Chemistry, Daehyun-dong, Seodaemun-gu, 11-1, Seoul 120-750, Republic of Korea; ⁴Novosibirsk State University, 2, Pirogova street, Novosibirsk, 630090, Russia
- P.S.A.11. **Application of high intensity ultrasound for obtaining magnesium hydroxide from seawater**
Jelena Jakić, Miroslav Labor, Vanja Martinac, Ana Marija Šunjić
 Faculty of Chemistry and Technology, Ruđera Boškovića 35, 21000 Split, Croatia
- P.S.A.12. **Thin films for multilayer devices by tape casting method**
Serhii Ivanchenko, Saide Umerova, Dmytro Baranovskyi, Andrey V. Ragulya
 Frantsevich Institute for Problems of Materials Science of National Academy of Sciences of Ukraine, Kiev, Ukraine; Nanotechcenter LLC, Kiev, Ukraine
- P.S.A.13. **Investigation of ZrN-ZrB₂ composition synthesis by spark plasma sintering method**
 Olexander Petukhov, Hanna Borodianska, Andrey V. Ragulya
 Frantsevich Institute for Problems of Materials Science of National Academy of Sciences of Ukraine, Kiev, Ukraine
- P.S.A.14. **Synthesis, crystal structures and magnetic properties of mono and dinuclear Cu(II) complexes with the condensation product of 2-acetylpyridine and Girard's T reagent**
Nevena Stevanović¹, Dušanka Radanović², Milica R. Milenković¹, Božidar Čobeljić¹ and Katarina Anđelković¹
¹Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia; ²Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, P.O. Box 815, 11000 Belgrade, Serbia
- P.S.A.15. **Development of sugarcane bagasse reinforced onibode clay composite for high voltage insulation**
Joseph B. Agboola¹, Suleiman B. Hassan², Afeez A. Lukman³
¹Department of Materials and Metallurgical Engineering, Federal University of Technology, Minna, Nigeria; ²National Institute of Mining and Geosciences, Jos, Nigeria; ³Department of Metallurgical and Materials Engineering, University of Lagos, Lagos, Nigeria

YUCOMAT SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

P.S.B.1. Cost effective alloys based catalysts for alkaline fuel cells application

Ljiljana Gajić-Krstajić¹, Borka Jović², Vladimir Jović², Piotr Zabinski³, Nevenka Elezović²

¹Institute of Technical Sciences of Serbian Academy of Science and Arts, Knez Mihajlova 45, 11000 Belgrade, Serbia; ²Institute for Multidisciplinary Research University of Belgrade, P.O. Box 33, 11030 Belgrade, Serbia; ³AGH University of Science and Technology, Faculty of Non-Ferrous Metals, Al. Mickiewicza 30, Krakow, Poland

P.S.B.2. Polyanionic cathode material $\text{Na}_4\text{Fe}_3(\text{PO}_4)_2\text{P}_2\text{O}_7/\text{C}$ for aqueous sodium-ion batteries

Aleksandra Gezović¹, Veselinka Grudić¹, Miloš Milović², Danica Bajuk-Bogdanović³, Milica Vujković³

¹University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro; ²Institute for Nuclear Sciences Vinča, Belgrade, Serbia; ³University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

P.S.B.3. Thermolysis prepared Co_3O_4 carbon paste electrode decorated with single wall nanotubes as voltammetric sensor for determination of antioxidant α -lipoic acid

Branka B. Petković¹, Dalibor M. Stanković², Miloš Ognjanović², Vyacheslav Viktorovich Avdin³, Magdalena Radović², Dragan D. Manojlović⁴, Sanja Vranješ Đurić²

¹University of Priština-Kosovska Mitrovica, Faculty of Sciences, Lole Ribara 29, 38220 Kosovska Mitrovica, Serbia; ²The Vinča Institute of Nuclear Sciences, Mike Petrovića Alasa 12-14, 11000, Belgrade, Serbia; ³South Ural State University, 76, Lenin prospekt, Chelyabinsk, Russia, 454080; ⁴University of Beograd, Faculty of Chemistry, Studentski trg 12-16, Beograd, Serbia

P.S.B.4. Special application possibilities of metakaolin based geopolymer foams

Adrienn Boros, Tamás Korim

Institute of Materials Engineering, University of Pannonia, Veszprém, Hungary

P.S.B.5. Ultra-fast volume-responsive temperature- and pH-sensitive poly(N-isopropylacrylamide) hydrogels

Sabina Horodecka, Khrystyna Hishchak, Beata Strachota, Adam Strachota, Miroslav Šlouf

Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, CZ-162 06 Praha 6, Czech Republic

P.S.B.6. X-ray spectra, electron structure and physical properties of the Ce₂ScSi₂ and CeScSi compounds

Ivan Shcherba¹, Victor Antonov², Henryk Noga³, Dragan Uskoković⁴, Zinovija M. Shpyrka¹, Bohdan M. Yatsyk⁵

¹Ivan Franko National University, Kyryla & Mefodiya Str. 8, 79-005 Lviv, Ukraine;

²Institute of Metal Physics, NASU, Vernadskyj Str. 36, 03-142 Kiev, Ukraine;

³Institute of Technology, Pedagogical University, Podchoranzych Str. 2, Cracow,

Poland; ⁴Institute of Technical Sciences of SASA Knez Mihailova 35/IV, Belgrade,

Serbia; ⁵Lviv National University of Veterinary Medicine and Biotechnologies, Lviv,

Ukraine

P.S.B.7. Theory and experiment - Slowing probe and conjugate pulses in potassium vapor using Four Wave Mixing

Željka Nikitović, Marija Ćurčić, Bojan Zlatković, Ivan Radojčić, Dušan Arsenović and Branislav Jelenković

Institute of Physics University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

P.S.B.8. Cup anemometer friction torque and classification according IEC standard

Miodrag Zlatanović^{1,2}, Ivan Popović²

¹Wind Electricity doo, Belgrade, Serbia; ²School of Electrical Engineering, Belgrade, Serbia

POSTER SESSION II

Wednesday, September 4, 2019, 20⁰⁰-22⁰⁰

Chairpersons: Zoran Jovanović, Đorđe Veljović

YUCOMAT SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS

P.S.B.9. Laser welding of similar materials

Agnieszka Radziszewska¹, Sławomir Kąc¹, Włodzimierz Zowczak², Olaf Czyż¹, Damian Kocłęga¹, Bogdan Antoszewski²

¹Faculty of Metals Engineering and Industrial Computer Science, AGH University of Science and Technology in Krakow, al. Mickiewicza 30, 30-059 Krakow, Poland;

²Kielce University of Technology, Faculty of Mechatronics and Machine Desing, 1000-lecia Państwa Polskiego 7, 25-314 Kielce, Poland

P.S.B.10. Corrosion resistance of high Al and MgSi Zinc alloys for batch hot dip galvanizing

Mariola Saternus, Henryk Kania

Silesian University of Technology, Gliwice, Poland

P.S.B.11. The properties of ZnAlMgSi alloys for batch hot dip galvanizing

Henryk Kania, Mariola Saternus

Silesian University of Technology, Gliwice, Poland

P.S.B.12. The effect of a single shock processing on mechanical properties Al-Li 2099 (T-83) alloy

Oleksandr Filatov¹, Sergii Bogdanov¹, Vladimir Mazanko¹, Sergii Vorona¹, Ievgen Bogdanov¹, Sergii Kotrechko¹, Oleksandra Zatsarna¹, Łukasz Kaczmarek², Marek Klich²

¹G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, Kiev, Ukraine; ²Lodz University of Technology, Faculty of Mechanical Engineering, Lodz, Poland

P.S.B.13. Influence of the impurity segregation on the adhesion properties of Al₂O₃/Ti₃Al interface

Alexander V. Bakulin^{1,2}, Artem A. Fuks², Svetlana E. Kulkova^{1,2}

¹Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia; ²Tomsk State University, Tomsk, Russia

- P.S.B.14. **Localized plastic deformation autowaves under tension of nitinol specimens**
Lidiya V. Danilova, Vadim V. Gorbatenko, Vladimir I. Danilov
 Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia
- P.S.B.15. **DMA and TMA study of glass transition in Cu-Zr based bulk metallic glasses**
Viktor Soprunyuk¹, Florian Spieckermann², Baran Sarac¹, Amir Rezvan¹, Wilfried Schranz³ and Jürgen Eckert^{1,2};
¹Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben 8700, Austria; ²Chair of Materials Physics, University of Leoben, Leoben 8700, Austria; ³University of Vienna, Faculty of Physics, Physics of Functional Materials, Boltzmanngasse 5, A-1090 Wien, Austria
- P.S.B.16. **High-temperature phase relations in the Bi₂O₃-Mn₂O₃-M₂O₃ (M=Fe, Ga, Al) pseudo-ternary systems**
Srečo Davor Škapin¹, Amalija Golobič², Danilo Suvorov¹, Matjaž Spreitzer¹
¹Advanced Materials department, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia; ²Faculty of Chemistry and Chemical Technology, Večna pot 113, 1000 Ljubljana, Slovenia
- P.S.B.17. **Low-temperature superplasticity of Ek61 and Ep975 superalloys with ultrafine-grained structure**
Vener Valitov, Elvina Galieva, Aerika Bikmukhametova
 Institute for Metals Superplasticity Problems of Russian Academy of Sciences, Ufa, Russia
- P.S.B.18. **Mechanical and microstructural properties of TRIP-matrix composites studied by neutron scattering methods**
Gizo Bokuchava¹, Yulia Gorshkova¹, Igor Papushkin¹, Sergey Guk²
¹Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia; ²Institute for Metal Forming, TU Bergakademie Freiberg, Freiberg, Germany

YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS**P.S.C.1. Microstructure of Half-Heusler thermoelectric alloys after severe plastic deformation**Jiří Buršík¹, Gerda Rogl², Peter Franz Rogl²¹Institute of Physics of Materials of the Czech Academy of Sciences, Žitkova 22, CZ-61662 Brno, Czech Republic; ²Institute of Materials Chemistry, University of Vienna, Währingerstrasse 42, A-1090 Wien, Austria**P.S.C.2. Multiple twinning and stacking faults in silver dendrites**Vuk V. Radmilović¹, Josh Kacher², Evica R. Ivanović³, Andrew M. Minor⁴ and Velimir R. Radmilović^{1,5}¹Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, P.O.B. 3503, 11120 Belgrade, Serbia; ²Department of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States; ³Faculty of Agriculture, University of Belgrade, Nemanjina 6, Zemun, 11000 Belgrade, Serbia; ⁴Department of Materials Science and Engineering, University of California, Berkeley, and National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States; ⁵Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000, Belgrade, Serbia**P.S.C.3. HPHT synthesis of nano-sized diamonds doped with Si or ¹³C for biological and medical applications**Viatcheslav Agafonov¹, Valery Davydov², Ludmila Kulikova², Rustem Uzbekov³, Taras Plakhotnik⁴¹GREMAN, University of Tours, Tours, France; ²L.F. Vereshchagin Institute for High Pressure Physics, RAN, Troitsk, Moscow, Russia; ³Laboratory of Cell biology and Electron microscopy, University of Tours, Tours, France; ⁴School of Mathematics and Physics, the University of Queensland, Queensland, Australia**P.S.C.4. Oxygen storage capacity versus catalytic activity of ceria–zirconia solid solutions in CO and HCl oxidation**Igor Đerd¹, Yu Sun^{2,3}, Chenwei Li^{2,3}, Omeir Khalid², Pascal Cop², Joachim Sann², Tim Weber², Sebastian Werner², Kevin Turke², Yanglong Guo³, Bernd M. Smarsly² and Herbert Over²¹Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, 31000 Osijek, Croatia; ²Physikalisch-Chemisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 17, 35392 Gießen, Germany; ³Key Laboratory for Advanced Materials, Research Institute of Industrial Catalysis, School of Chemistry and Molecular Engineering, East China University of Science and Technology, Shanghai 200237, PR China

- P.S.C.5. **Structure, morphology and photocatalytic properties of $\text{Co}_x\text{Mg}_{1-x}\text{Fe}_2\text{O}_4$ ($0 < x < 1$) spinel ferrites obtained by sol-gel synthesis**
 Zorka Z. Vasiljević¹, Milena P. Dojčinović², Vera P. Pavlović³, Jelena Vujančević¹, Nenad B. Tadić³, Maria Vesna Nikolić²
¹Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia, ²Institute for Multidisciplinary Research, University of Belgrade, Serbia, ³Faculty of Mechanical Engineering, University of Belgrade, Serbia, ⁴Faculty of Physics, University of Belgrade, Serbia
- P.S.C.6. **High-performance supercapacitors based on core-shell structured carbon fibers@spinel oxide composites**
 Daniel M. Mijailović¹, Vuk V. Radmilović², Uroš Č. Lačnjavec³, Dušica B. Stojanović², Vladimir D. Jović¹, Velimir R. Radmilović^{2,3}, Petar S. Uskoković²
¹University of Belgrade, Innovation Center, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120, Belgrade, Serbia; ²University of Belgrade, Institute for Multidisciplinary Research, Kneza Višeslava 1, 11030 Belgrade, Serbia; ³University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120, Belgrade, Serbia; ⁴Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia
- P.S.C.7. **Citrate assisted solvothermal synthesis of $\beta\text{-NaYF}_4$: Yb, Er up-converting nanoparticles**
 Ivana Dinić¹, Marina Vuković¹, Predrag Vulić², Marko Nikolić³, Olivera Milošević⁴ and Lidija Mančić⁴
¹Innovation Center of the Faculty of Chemistry, University of Belgrade, Serbia; ²Faculty of Mining and Geology, University of Belgrade, Serbia; ³Photonic Center, Institute of Physics Belgrade, University of Belgrade, Serbia; ⁴Institute of Technical Sciences of SASA, Belgrade, Serbia
- P.S.C.8. **Effect of rare earth elements (Eu^{3+} , Sm^{3+} , $\text{Yb}^{3+}/\text{Er}^{3+}$) doping on luminescence properties of Y_2MoO_6**
 Nadežda Stanković¹, Nina Daneu², Marko Nikolić³, Branko Matović¹
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- P.S.C.9. **The effect of pH on visible-light photocatalytic properties of pseudobrookite nanoparticles**
 Zorka Z. Vasiljević¹, Milena P. Dojčinović², Jelena Vujančević¹, Nenad B. Tadić³, Maria Vesna Nikolić²
¹Institute of Technical Sciences, Serbian Academy of Science and Arts, Belgrade, Serbia; ²Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia; ³Faculty of Physics, University of Belgrade, Belgrade, Serbia

P.S.C.10. Ion-irradiation of ZrNb nanoscale multilayers

Miroslav Karlík^{1,2}, Nabil Daghbouj³, Jan Lörinčík⁴, Tomáš Polcar³, Mauro Callisti⁵, Vladimír Havránek⁶

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P.S.C.11. Orientation dependence of microstructure formation in Cu-8% at. Al single crystals

Dorota Moszczyńska¹, Bogusława Adamczyk-Cieślak¹, Milena Koralnik¹, Tomasz Tokarski², Jarosław Mizera¹

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P.S.C.12. Utilizing ion beam irradiation for structural modification of 12-tungstophosphoric acid

Željko Mravik^{1,2}, Danica Bajuk-Bogdanović³, Ana Mraković⁴, Ivan Trajić¹, Ljubiša Vukosavljević¹, Davor Peruško⁵, Zoran Jovanović^{1,2}

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P.S.C.13. Rapid reaction of Mo₂N nanowires with Pb²⁺ ions in water and its use for production of PbMoO₄ nanoparticles

Aleš Mrzel¹, Damjan Vengust¹, Matejka Podlogar^{1,2}, Mojca Vilfan¹

¹J. Stefan Institute, Jamova 39, 1000, Ljubljana, Slovenia; ²National Institute of Chemistry, Hajdrihova 19, 1000, Ljubljana, Slovenia

P.S.C.14. **Consequences of confinement conditions on absorption in molecular nanofilms**

Ana J. Šetrajčić–Tomić¹, Matilda Vojnović¹, Igor J. Šetrajčić², Siniša M. Vučenović³,
Jovan P. Šetrajčić^{4,5}

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POSTER SESSION III

Thursday, September 5, 2019, 20⁰⁰-22⁰⁰

Chairpersons: Ivana Dinić and Veljko Đokić

YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS

P.S.C.15. Structural investigations of alloyed Al with TiCN nanopowder under load and tensile

Stefan Valkov¹, Rumiana Lazarova², Julia Goschkova³, Gizo Bokuchava³, Peter Petrov¹

¹E. Djakov Institute of electronics, Bulgarian Academy of Sciences, 72 Tzarigradsko chaussee, 1784 Sofia, Bulgaria; ²Institute of Metal Science, Equipment and Technologies with Hydro and Aerodynamics center, Bulgarian Academy of Sciences, 67 Shipchenski Prohod blvd., 1574 Sofia, Bulgaria; ³Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, 6 Joliot-Curie Str., 141980 Dubna, Russia

P.S.C.16. Cubic silver nanoparticles fixed on TiO₂ nanotubes as a simple and efficient substrates for surface enhanced Raman scattering

Robert Ambroziak¹, Marcin Hołdyński², Tomasz Płociński³, Marcin Pisarek², Andrzej Kudelski¹

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P.S.C.17. Formation of borides, silicides and boride-silicide powder composite materials by mechanical alloying

Marina Vasylykivska, Izabella Timofeeva

Frantsevich Institute for Problems of Materials Science of National Academy of Sciences of Ukraine, Kiev, Ukraine

P.S.C.18. Preparation of polylactide-kaolinite nanocomposite

András Kovács¹, Éva Makó¹, Norbert Miskolczi²

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²Institute of Chemical and Process Engineering, University of Pannonia, Veszprém, Hungary

YUCOMAT SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

P.S.D.1. Identification and evaluation of changes and migration mechanisms of petroleum pollutant in the environment using the alkane fraction biological markers (river Vrbas, Bosnia and Herzegovina)

Ivan Samelak¹, Milica Balaban¹, Mališa Antić², Tatjana Šolević-Knudsen³ and Branimir Jovančičević⁴

¹Faculty of Natural Sciences and Mathematics, University of Banja Luka, Mladena Stojanovića 2, 78000 Banja Luka, Bosnia and Herzegovina; ²University in Belgrade, Faculty of Agriculture, Nemanjina 6, 11080, Belgrade, Serbia; ³Center of Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11001 Belgrade, Serbia; ⁴University of Belgrade, Faculty of Chemistry, Studentski trg 12-16. 11001 Belgrade, Serbia

P.S.D.2. Potential application of activated carbonaceous materials for removing residual contaminants from complex biochemical and pharmacological mixtures

Branka Kaluđerović, Đuro Čokeša, Jelena Hranisavljević, Vesna Mandušić
INN Vinča, University of Belgrade, INN Vinča, P.O.Box 522, 11001 Belgrade, Serbia

P.S.D.3. The influence of modification and the particle size of the montmorillonite on the hydrolytic stability of urea-formaldehyde composite

Suzana Samaržija-Jovanović¹, Branka Petković¹, Tijana Jovanović², Vojislav Jovanović¹, Gordana Marković³, Milena Marinović-Cincović⁴, Jaroslava Budinski-Simendić⁵

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P.S.D.4. Group chase and escape in the presence of obstacles

Julija R. Šćepanović, Aleksandar Karač, Zorica M. Jakšić, Ljuba Budinski-Petković, Slobodan B. Vrhovac

Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia

P.S.D.5. Regulation of lipid production of *Torulaspora globosa* yeast, cultivated in the medium with ethanol as a carbon source

Nadezda N. Stepanova¹, Grigorii I. Morgunov², and Svetlana V. Kamzolova¹

¹G.K. Skryabin Institute of Biochemistry and Physiology of Microorganisms, Federal Research Center "Pushchino Center for Biological Research of the Russian Academy of Sciences", Pushchino, Moscow region, 142290 Russia; ²Peoples' Friendship University of Russia (RUDN University), Moscow, 117198 Russia

YUCOMAT SYMPOSIUM E: BIOMATERIALS

P.S.E.1. **Development of a 3D system for cancer cell studies**

Jasmina Stojkovska^{1,2}, Milena Milivojević³, Milena Stevanović^{3,4,5}, Bojana Obradović¹

¹Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia;

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⁵Serbian Academy of Sciences and Arts, Belgrade, Serbia

P.S.E.2. **From wood to bone: how to convert wood structures into biomimetic hydroxyapatite scaffolds**

Miklós Jakab, Margit Enisz-Bódogh

University of Pannonia, Institute of Materials Engineering, Veszprém, Hungary

P.S.E.3. **Functionalization and biomimetics of insect photonic structures**

Danica Pavlović¹, Dejan Pantelić¹, Branislav Salatić¹, Dušan Grujić¹, Svetlana Savić Šević¹, Ljubiša Tomić², Goran Dikić³, Branislav Jelenković¹

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Vojvode Stepe 283, 11010 Belgrade, Serbia

P.S.E.4. **Evaluation of colour modifications and surface morphology of dental composites**

Marioara Moldovan¹, Doina Prodan¹, Codruta Sarosi¹, George Popescu², Amalia-Ionela Mazilu (Moldovan)^{2*}, Violeta Popescu²

¹Babes Bolyai University, “Raluca Ripan” Chemistry Research Institute, Department of Polymer Composites, Cluj-Napoca, Romania; ²Physics and Chemistry Department, Technical University of Cluj-Napoca, Cluj-Napoca, Romania

P.S.E.5. **The morphology studies of different nanohybrid dental composites**

Codruta Sarosi¹, Ioan Petean², Doina Prodan¹, Cristina Prejmorean¹, Marioara Moldovan¹

¹Babes Bolyai University, Institute of Chemistry Raluca Ripan, Cluj-Napoca, Romania; ²Babes Bolyai University, Faculty of Chemistry and Chemical Engineering, Cluj-Napoca, Romania

P.S.E.6. The identification of branched-chain amino acids and the testing of the antibacterial effect of whey and soy protein powders

Violeta Popescu¹, Marioara Moldovan², Codruța Sarosi², Mihaela Vlassa², George Liviu Popescu¹, Diana Elena David¹, Ileana Cojocaru³, Doina Prodan²

¹Physics and Chemistry Department, Technical University of Cluj-Napoca, Cluj-Napoca, Romania; ²Babeș Bolyai University, “Raluca Ripan” Chemistry Research Institute, Department of Polymer Composites, Cluj-Napoca, Romania; ³University of Craiova, Craiova, Romania

P.S.E.7. Comparison of the carbon content in various biomasses based on calorimetric tests

Hadi Waisi^{1,2}, Vladimir Dodevski³, Bojan Janković¹, Marija Janković⁴, Nikola Živković⁵, Blažo Lalević⁶, Miloš Marinković⁷

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P.S.E.8. Hybrid bio-nanoentities with potential applications in biomedical field

Yulia Gorshkova¹, Marcela Elisabeta Barbinta-Patrascu², Gizo Bokuchava¹, Nicoleta Badea³, Camelia Ungureanu³, Andrada Lazea-Stoyanova⁴, Angela Vlad⁴, Vitaly Turchenko¹, Alexander Zhigunov⁵, Ewa Juszynska-Galazka⁶

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SYMPOSIUM F: WRTCS

- P.S.F.1. **Sintering heating and cooling rates as a method of modifying electrical properties of BiFeO₃ ceramics**
Nikola Ilić¹, Jelena Bobić¹, Mirjana Vijatović Petrović¹, Adis Džunuzović¹, Biljana Stojanović²
¹Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia;
²Academy of Engineering Sciences of Serbia, Belgrade, Serbia
- P.S.F.2. **Nickel ferrite/zinc ferrite nanopowder with core/shell structure: magnetic properties and sinterability**
 Ivan Stijepović, Marija Milanović, Andrea Nesterović, Jelena Vukmirović, Vladimir Srdić
 University of Novi Sad, Faculty of Technology, Department of Materials Engineering, Novi Sad, Serbia
- P.S.F.3. **Sintering of scaffolds based on doped hydroxyapatite powders**
Željko Radovanović¹, Đorđe Veljović², Rada Petrović², Đorđe Janačković²
¹University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia; ²University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
- P.S.F.4. **Two-step sintered monophasic HAp dental inserts as materials for dentin replacement**
 Giuma Ayoub¹, Maja Ležaja Zebić², Vesna Miletić², Rada Petrović¹, Đorđe Veljović¹, Đorđe Janačković¹
¹University of Belgrade, Faculty of Technology and Metallurgy, Department of Inorganic Chemical Technology, Karnegijeva 4, 11120 Belgrade, Serbia; ²University of Belgrade, School of Dental Medicine, DentalNet Research Group, Rankeova 4, Belgrade, Serbia
- P.S.F.5. **Surface-selective laser sintering of ultrafine polymer powders. A new approach to high resolution three-dimensional printing**
Svetlana A. Minaeva¹, Maria A. Syachina¹, Anton V. Mironov¹, Nikita V. Minaev¹, Eduards Krumins², Steven M. Howdle², Vladimir K. Popov¹
¹FSRC “Crystallography and Photonics” RAS, Troitsk, Moscow, Russia; ²School of Chemistry, University of Nottingham University Park, Nottingham, United Kingdom
- P.S.F.6. **Influence of 3D-printing additive to freeze casting structure**
 Yueh-Ying Chou¹, Po-Yu Chen¹, Vojislav V. Mitic^{2,3}, Goran Lazović⁴
¹National Tsing Hua University, Taiwan; ²Institute of Technical Sciences of SASA, Belgrade, Serbia; ³Faculty of Electronic Engineering, University of Nis, Serbia;
⁴Faculty of Mechanical Engineering University of Belgrade, Serbia

P.S.F.7. **Resintering effect on high gamma phase content cemented carbide**

Marco Mendez, Luis Garcia

Hyperion Materials & Technologies, Ind. Roca - C/ Verneda s/n, Martorelles,
Barcelona 08107, Spain

Abstracts

Oral Presentation

MRS-Serbia 2019 Award

Epitaxial integration of oxides with silicon

Danilo Suvorov, Daniel Diaz, Tjaša Parkelj, Urška Gabor, Matjaž Spreitzer

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Epitaxial integration of transition metal oxides with semiconductors offers various phenomena for novel device applications, specifically bringing ferroelectric, ferromagnetic, electro-optic, photocatalytic, multiferroic, piezoelectric and other properties to the well-established silicon platform. A convenient way of integrating functional oxides with Si(001) substrate is through a SrTiO₃ (STO) intermediate layer, which can be fabricated on Si(001) in epitaxial form and with high crystallinity using mainly Molecular Beam Epitaxy (MBE) and Atomic-Layer Deposition (ALD) methods. However, slow deposition processes and difficult stoichiometry control make these methods inappropriate from an industrial point of view. Alternative way of this two sets of material in a unique way is synthesis with Pulse Laser Deposition (PLD) which is the subject of this talk.

The epitaxial growth of functional oxides on silicon substrates with PLD requires atomically defined surfaces, which are most effectively prepared using SrO- or Sr-induced deoxidation and passivation. As-prepared surfaces enable overgrowth with various oxides for novel device applications. In our work pulsed laser deposition (PLD) was used to integrate oxides with silicon. We showed the ability to prepare highly-ordered sub-monolayer SrO- and Sr-based surface structures, including two-domain (2×3)+(3×2) pattern at 1/6 ML Sr coverage as determined by the reflection high-energy electron diffraction (RHEED) technique. On the passivated silicon surface epitaxial layers of STO was grown by the method of kinetically controlled sequential deposition, with out-of plane relationship of STO(001)∥Si(001) and in-plane relationship of STO[110]∥Si[100]. Detailed study of initial deposition parameters in terms of background gas pressure, deposition temperature, fluence, and oxidation proved to be extremely important in achieving epitaxial relation of STO with the underlying substrate. On as-prepared pseudo-substrate Pb[Mg_{1/3}Nb_{2/3}]O₃-PbTiO₃ (PMN-PT) films were grown for applications in microelectromechanical systems, due to its high values of longitudinal piezoelectric coefficients and electromechanical coupling. In this presentation growth peculiarities of PMN-PT thin films, including the effect of lead surplus and bottom electrode will also be outlined.

Y.PL.S.I.1.

Stable perovskite solar cells by compositional and interface engineering

Sanghyun Paek, Hiroyuki Kanda, Yi Zhang, Hobeom Kim, Yonghui Lee, Kyung Taek Cho, Mousa Abuhelaia, Aron Joel Huckaba, Cristina Roldan Carmona and Mohammad Khaja Nazeeruddin

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Perovskite solar cells (PSC) are a new paradigm in renewable energy because of their high efficiency reaching over 24% in less than 10 years [1,2]. The high efficiency of perovskite solar cells is due to their excellent optoelectronic properties, which were optimized by various cations and anions with different ratios. Another advantage of perovskite solar cell is their simple fabrication through solution-processing methods, either in n-i-p or p-i-n configurations [3,4] The perovskite absorbing layer is consisting of methylammonium lead (II) iodide (MAPbI₃) is intrinsically unstable at elevated temperature due to methylammonium cation release. In this talk, we present 23% efficiency perovskite solar cells with stability using compositional engineered cations and anions, and layer by layer deposition of 3-Dimensional and 2-Dimensional perovskites, and the novel charge transporting materials [5].

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Y.PL.S.I.2.

Graphene and related materials, from production to applications

Andrea C. Ferrari

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Disruptive technologies are usually characterised by universal, versatile applications, which change many aspects of our life simultaneously, penetrating every corner of our existence. In order to become disruptive, a new technology needs to offer not incremental, but dramatic, orders of magnitude improvements. Moreover, the more universal the technology, the better chances it has for broad base success. Significant progress has been made in taking graphene and related materials from a state of raw potential to a point where they can revolutionize multiple industries.

Graphene is an ideal material for optoelectronic applications. Its photonic properties give several advantages and complementarities over Si photonics. I will show that graphene-based integrated photonics could enable ultrahigh spatial bandwidth density, low power consumption for next generation datacom and telecom applications. Heterostructures based on layers of atomic crystals have a number of properties often unique and very different from those of their individual constituents and of their three dimensional counterparts. I will show how these can be exploited in novel light emitting devices, such as single photon emitters, and tuneable light emitting diodes.

Y.PL.S.I.3.

Next-generation large-area graphene for electronic devices

Simon Thomas¹, Ivor Guiney¹ and Colin Humphreys²

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In 2015, Bosch issued a press release claiming that their Hall effect magnetic sensor made from an exfoliated flake of graphene was the most sensitive in the world, but they added that graphene-based sensor applications will require 5-10 years before they can compete with established technologies because of the current lack of large-scale wafer-based and transfer-free synthesis techniques.

Large-area (up to 4-inch diameter so far) sheets of graphene produced by chemical vapour deposition (CVD) are available, but the CVD process uses a metal substrate, usually copper, as a catalyst to decompose the growth gases used. This results in copper atoms being incorporated in the graphene. The graphene then needs to be removed from the copper substrate using, for example, iron chloride, resulting in further contamination with iron as well as copper. Such large-area CVD graphene has been attempted to be used in electronic device manufacturing, however the contamination has proven to be a completely limiting factor.

We have produced large-area graphene directly on a substrate and it is therefore free of metallic contamination. In response to the press release of Bosch, quoted above, we have produced a graphene Hall sensor for measuring magnetic fields. It is the most sensitive Hall sensor in the world and is manufacturable. It promises to revolutionise sensors, photonics and electronics.

Y.PL.S.I.4.

Functionality and versatility of metal oxides

Elvira Fortunato

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In the last 50 years we observed a drastic change in our daily life since society was never before so efficient and interconnected. This provides a collaborative environment that is essential for economic growth and progress like: Silicon Valley for microelectronic technology and Boston for biotechnology. This breakthrough development has been in part dictated by an empirical technologically and economically driven rule known as “Moore’s law”. Indeed today a microprocessor has more than 7 billion integrated transistors in an area of 350 mm². This unbelievable integration capability with higher processing speeds, memory capacity and functionality gives rise to what we call today: ubiquitous electronics. Despite the importance of Si technology there are applications where it is impossible, either technically or economically use it. Displays are the most notorious example, more if we want them to be flexible and conformable. With the intensification of cloud computing, the importance on the speed of the microprocessors is no longer so significant. The main unit of analysis is no longer the processor, but the rack of servers or the data centre and the interface/display (the human interface). Moore’s law will come to an end in the near future. Taking this into account, the global semiconductor industry is seeking a new trend called “More-than-Moore”, where added values to devices are provided by incorporating functionalities that do not necessarily scale according to Moore’s Law, where the driving force is not the miniaturization but the diversification by developing products with high added value. Over the last decades, human-device interactions have changed from text inputs to graphical user interfaces. Then, we really need to see how we can serve the multifaceted human interface! Another reality is the Internet of Things (IoT), which will transform our everyday life, from managing airports’ passenger flow to heating buildings and caring for the elderly. The IoT is a revolution that promises to change people’s lives, from inside the home to right across society. The reason why it will happen is because of the boom in low-cost computing, from which new platforms are needed. We at CENIMAT|i3N will contribute for a new era of interactivity, where, by exploring devices with multifunction’s, interfaces can “see”, “hear”, “feel,” and “understand,” besides being self-powered, transforming our experiences with their contents of all form-factors to be more engaging and immersive. These advances coupled with remarkable innovations in sensing and display/interface technologies, will transform computing and communication systems. On the other way system-on-panel (SoP) concept has been proposed to enable various functional devices, such as driver, sensor, memory, energy storage devices and controller devices, to be integrated on a single panel for achieving high-performance, low-cost and more compact display and electronic products. To this we need the right technologies, eco and sustainable materials whose performances can be fully controlled and adjusted. But until now this concept was not successfully implemented since there was not available a unique technology simultaneously compatible with the low cost and the SoP needs. Recently transparent amorphous oxide semiconductors (TAOSs) have been attracting substantial attention as candidate materials for the use of thin film transistors (TFTs) for

the next generation of flat panel displays (FPDs) technology due to their high carrier mobility, transparent to visible light, easy fabrication, and can be deposited at room temperature. In particular, due to their high electron mobility and uniformity all devices can be integrated on a panel, using the SoP technology.

Y.PL.S.I.5.

Boron nitride nanotube/nanosheet for energy applications

Yoshio Bando^{1,2,3}

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The highly efficient thermal management is very important for quick heat release in the face of increasing power consumption of electronic devices. BN is highly insulating and wide-bandgap in properties and more stable than graphite in thermology and chemistry. However, their insufficient production rather limited the studies and the full realization of potentials. We have recently developed effective methods for the high-yield syntheses of BN nanotubes and nanosheets. We have synthesized gram-level high-quality BN nanotubes through the carbon free-chemical vapour deposition and gram-level nanosheets by the chemical blowing method, which make them possible to initiate the studies of polymetric composites. Our BN nanotubes and nanosheets have been filled into polymer matrix to make thermal conductive composites, which were created with 20-times increase of original thermal conductivity. They are useful for heating-release insulating packaging of down-sizing faster cooler electronics. Our synthesis methods are thus extended for producing new graphene materials, e.g. 3D strutted-graphene (SG) via chemical blowing. The SG consists of continuous graphitic membranes which are homogenously connected and spatially supported by the networks of micrometer-width graphitic struts. The high electrical conductivity, specific surface area, mechanical strength and elasticity are thus simultaneously achieved. In addition, we indeed demonstrate the striking effects of tensile, compressive and bending deformation on the electrical response of BN nanotubes and nanosheets under manipulation and electrical probing in HRTEM using STM/AFM-TEM special holders. The author would like to acknowledge to Professor D. Golberg and others in NIMS.

W.PL.S.I.1.

Challenges and further developments in modeling of sintering

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The existing challenges in modeling of sintering should be considered as incentives for further scientific endeavors, as opposed to serving as an impediment to the allowance for progress. Six possible directions of further developments in modeling of sintering are pointed out, including multi-scale modeling of sintering, development of on-line sintering damage criteria, modeling of nano-powder sintering, modeling of sintering with phase transformations or chemical reactions, modeling of field-assisted sintering, and the development of in- and post-3D printing sintering models.

W.PL.S.I.2.

Micromechanics of sintering in particle scale

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Frenkel and Kuczynski laid the foundation for understanding the sintering phenomena in particle scale, emphasizing the center-to-center approach and the neck growth in the initial stage. In the late 1980s the development of continuum mechanics led to a paradigm shift; the macroscopic strain rate is proportional to the driving force called sintering stress, and is inversely proportional to bulk viscosity. Both sintering stress and bulk viscosity are physical quantities that can be measured experimentally. From this mechanical point of view, the relative velocity between two spherical particles is described as a response to the sintering force acting on a circular contact, and is inversely proportional to the square of contact area, when the sintering occurs by coupled grain boundary diffusion and surface diffusion. It is well known that the sintering depends not only on temperature, applied stress, particle/pore size, relative density, but also on complex microstructure. Therefore, it is a challenge for the modern sintering theory to understand how the macroscopic sintering stress and bulk viscosity arise from microstructural evolution in the course of sintering. The question remains unanswered: is the concept of sintering force can be extended to the later stage where complex topological transformations of microstructure occur? For example, pinch-off of pore channel, formation and disappearance of closed pore, grain boundary sliding, particle rearrangements, coarsening and grain growth. We give here some answers by using simple but accurate geometrical models. This knowledge will help to develop realistic simulation method, and can be used to check the validity of simulations such as discrete element method (DEM), kinetic Monte Carlo simulation + DEM, and phase field model + DEM, all of which incorporate the micromechanics in particle scale.

W.PL.S.I.3.

Coupled experimental and numerical investigation of evolution of anisotropic microstructures during stress-assisted and constrained sintering

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In many cases, a porous body is subjected to non-hydrostatic stresses during sintering. Two practically important cases are sintering under external uniaxial stress (sinter-forging) and constrained sintering of ceramic coatings and films. In this talk, the densification and evolution of the microstructure, during sinter-forging and constrained sintering, will be discussed. For these cases, although the stress state is different, there is an equivalence in the strain state.

Experimentally and using multi-scale, we show that the pore shape evolution during stress assisted sintering is dependent on the size of the pore. We define two types of pores – intrinsic small inter-particle pores, and extrinsic significantly larger than the intrinsic pores. We present experimental results on the development of pore shape anisotropy during sintering under nonhydrostatic stresses of ceramics containing both type of pores. The effect of stress on the microstructure is investigated. As expected during sintering under non-hydrostatic stress, the pore shape becomes anisotropic and the pores orient preferentially. However, the orientation of the pores, depends on both the size of the pores (intrinsic or extrinsic) and the anisotropic nature of the strain. Multiscale numerical simulations provide insights into the origin of this behavior. Based on these results, we also provide a fundamental definition of the transition pore size – pore size at which the behavior changes from intrinsic to extrinsic.

W.PL.S.I.4.

Fundamentals of solid state sintering in multicomponent high entropy alloys

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Solid state sintering is driven by the vacancy gradients created by surface curvatures of the powder particles during sintering or of the pores at the final state of sintering. Contact formation and densification are theoretically calculated for model systems and give quite good description of the changes that can be observed in sintering experiments. Normally the model theories assume elemental systems with one sort of atoms to describe the diffusion processes that lead to contact growth and shrinkage of the system. Surprisingly there is no literature about multicomponent system, obviously because automatically these systems are assumed to behave completely similar to elemental systems with some effective diffusion coefficient. However, already in early publications about sintering fundamentals the possibility of segregation during sintering was discussed, if the atoms in the alloy would have large differences in their diffusion coefficients. Motivated by the activities in High Entropy Alloys that normally consist out of at least 5 elements in nearly equiatomic proportions the authors analyzed the problem of sintering in multicomponent systems. The theoretical analysis shows, that at standard conditions no segregation happens and very small gradients of the elemental concentrations are built up during diffusion. These gradients adjust the mobility of all elements to the same value ensuring that neck regions and pores are filled with a homogeneous solid solution of the initial composition. It will be shown, that the effective diffusion coefficient can be calculated by a combination of the partial diffusion coefficients of the elements. Since the concentration gradients are defined by the gradient of vacancy concentration in extreme conditions of nanometer particles more pronounced effects can be expected.

W.PL.S.I.5.

What we should consider for full densification when sintering

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Densification of a powder compact, the primary goal of sintering, is affected by various processing parameters, including the particle/pore size and distribution, and the thermal cycle (sintering temperature and heating rate). The effects of these parameters have been closely and widely analyzed for systems without grain growth in most cases. Sintering theories so developed can predict the densification kinetics with respect to certain processing parameters, in particular the particle size and sintering temperature. For full densification of the powder compact, however, it is essential to prevent the entrapment of isolated pores within growing grains and to retain them at the grain boundaries. Theories of microstructural evolution in porous systems have been developed in terms of the relative kinetics of densification and normal grain growth. To achieve full densification, grain growth, abnormal grain growth (AGG) in particular, must be suppressed. When AGG takes place, many isolated pores can be entrapped within growing grains, a process which limits the densification.

This presentation will discuss general directions for the full densification of powder compacts. First, we will briefly review the effects of the particle size and powder packing on densification. The effect of the thermal cycle will also be reviewed. Based on the recently established mixed mechanism principle of microstructural evolution, strategies for suppressing AGG will be presented.

W.PL.S.I.6.

Increase of fracture toughness of transparent ceramics by functional, low thermal-expansion coatings

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A simple but effective concept has been developed for toughening transparent ceramics. For the first time, unprecedented surface compression of a polycrystalline transparent ceramic was demonstrated by applying functional, low thermal-expansion coatings. For proof of concept, a thin, transparent yttria coating was deposited on a transparent yttria-stabilized zirconia substrate by physical vapor deposition. Details of processing substrate and coating are summarized. After cooling down from processing temperature, lower coefficient of thermal expansion (CTE) of yttria generated residual compressive stresses on the sample surface, which in turn, increased the fracture toughness. Toughness could be further improved by thermal post-treatment due to cation counter-diffusion at the substrate-coating interface. In sum, compressive stresses of up to 750 MPa - same order of magnitude as for ion-exchange strengthened glasses – resulted in fracture toughness increase by a factor 2 – 3 depending on the processing conditions. As side effect, transmittance can be increased when selecting a coating material with a lower refractive index than substrate due to reduced reflection. Our transmittance measurements revealed this correlation. It is expected that transmittance increase can be even tailored to specific wavelengths by adjusting the coating thickness. The novel technique does not require post-polishing and can be applied as an after-treatment to finished products. If choosing the right material combinations, the concept can be transferred to other transparent polycrystalline ceramics as well.

Y.PL.S.II.1.

Model based characterisation of magnetic moments and charge densities in the transmission electron microscope

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Off-axis electron holography is a powerful technique, which can be used to record the phase shift of an electron wave that has passed through an electron-transparent specimen in a transmission electron microscope. The phase shift is sensitive to local variations in electromagnetic potential, which are in turn dependent on nanoscale properties of a specimen of interest, such as magnetization or charge density.

We have developed a model-based iterative reconstruction technique, which can be used to retrieve the projected in-plane magnetization distribution from the magnetic contribution to a recorded phase image, or alternatively the three-dimensional magnetization distribution from a set of at least two tilt series of magnetic phase images [1]. The technique is based on the optimized implementation of a forward model, which maps a given magnetization distribution onto one or more phase images. The ill-posed problem is tackled by first replacing the original problem by a least squares minimization, which is augmented by regularization techniques to find a unique solution for the reconstructed magnetization distribution. We are also using the same model-based approach for reconstructing the projected or three-dimensional charge density distributions inside specimens from phase images. Just as for reconstructing magnetic moments, this approach allows the incorporation of *a priori* information, such as the shape of the object (*i.e.*, the region in which charge can be located), as well as the use of a confidence mask to exclude regions containing artefacts from the analysis. Examples will be presented from the characterisation of magnetic moments in nanoscale grains and charge density distributions in electrically biased needle-shaped specimens [2].

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Y.PL.S.II.2.

Using STEM-EELS to optimize gold nanoparticles for early cancer detectionRobert Sinclair, Yitian Zeng and Steven MadsenDepartment of Materials Science and Engineering, Stanford University, Stanford, CA 94305,
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There are various ways in which nanotechnology can assist in early cancer detection, oftentimes utilizing sensitive physical properties of nanomaterials to detect them attached to tumors or circulating cancer cells [1]. The group with whom we collaborate has successfully employed gold nanoparticles contained within a silica shell as a triple modality detection agent [2]. One of the properties utilized is surface-enhanced Raman spectroscopy (SERS) whereby the gold nanoparticles significantly enhance the Raman signal from an organic dye when exposed to an illuminating laser beam, which has been incorporated into a working endoscopic system [3]. While this works well, to our knowledge there has never been any systematic study as to the influence of nanomaterial structure parameters such as size, shape, separation, coating etc. on the strength of the Raman signal, and hence its utility in detecting small tumors. It is recognized that surface plasmons in noble metal nanoparticles directly contribute to the Raman signal [4], and that the surface plasmon energy is in turn determined by the nanomaterial parameters mentioned above [5]. In this paper, we describe an approach to study the effect of these parameters in order to establish the optimum conditions to generate the highest possible Raman signal.

An array of gold nanoparticles of various size, shape and separation is fabricated from a vapor-deposited gold thin film utilizing standard electron lithographic processes. When a Raman dye is spread over the array, Raman imaging shows the variations of signal and hence the parameters giving rise to maximum signal. Nanoparticle size seems to be a critical feature. The plasmon resonances and energies are then determined across the array using electron energy loss spectroscopy (EELS) in a scanning TEM (STEM) [6] and the individual spectra are then correlated with the Raman signal from the exact same nanoparticle structures. By this procedure we can establish the critical parameters which yield the highest Raman signal, which leads to the systematic design of the most effective SERS nanoparticles.

Acknowledgements

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Y.PL.S.II.3.

Engineering of novel pharmaceutical drug delivery systems for combination therapy of multidrug resistant cancer

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Multidrug resistance (MDR) significantly decreases the therapeutic efficiency of anti-cancer drugs. Downregulation of MDR-related proteins with siRNA is a promising way to reverse the MDR. The delivery of small molecule drugs simultaneously with siRNA can enhance the efficiency of chemotherapy by dual action in MDR cells. Different nanocarrier systems have been developed for the combination treatment and drug co-delivery for MDR tumors.

Continuing our studies, we conjugated the dendrimer, generation 4 polyamido amine (G4 PAMAM), with a polyethylene glycol (PEG)-phospholipid copolymer. The amphiphilic conjugates obtained spontaneously self-assemble into a micellar nanopreparation, which can be co-loaded with siRNA onto PAMAM moieties and poorly water soluble drugs into the lipid core. This system was co-loaded with doxorubicin (DOX) and Pgp siRNA and tested for cytotoxicity against human MDR cells. The combination nanopreparation effectively downregulated P-gp in MDR cells and reversed the resistance towards DOX.

Modification of nanoparticle surfaces with PEG has been considered the gold standard. However, PEGylation presents serious challenges including lack of functionality, hindered cellular interaction, allergic reactions, and stimulation of IgM production accelerating nanoparticles blood clearance. We developed novel liposomal formulations surface-modified with a low molecular weight, branched polyethyleneimine (bPEI)-lipid conjugate for use as an alternative to PEG. The formulations had very good stability, and protein adsorption onto the liposomal surface did not interfere with the cellular interaction. bPEI-modified liposomes (PEIPOS) showed enhanced association with different cell lines by up to 75 times compared to plain or PEGylated liposomes and were without carrier toxicity. They also penetrated the deeper layers of 3D spheroids. Encapsulating paclitaxel (PTX) into PEIPOS did not change its main mechanism of action. PEIPOS complexed and intracellularly delivered siRNAs and downregulated resistance-associated proteins. Finally, tumor growth inhibition was observed in a mouse ovarian xenograft tumor model, without signs of toxicity, in animals treated with the siRNA/PTX co-loaded formulation.

These simple-in-design novel formulations constitute viable and promising additions to the family of combination preparation to treat MDR cancers.

Y.PL.S.II.4.

Synthesis and applications of megamolecules

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This talk will describe an approach for synthesizing molecules that have sizes greater than 100 nm and yet are structurally perfectly defined. The approach relies on the selective and covalent reaction of an enzyme domain with an irreversible linker. Fusion proteins containing two or more of the enzyme domains are treated with linkers terminated in two or more of the irreversible inhibitors, leading to the rapid reaction of the partners and efficient assembly of the megamolecule. Several enzyme-inhibitor pairs have been developed, and used to prepare megamolecules that are linear, cyclic, branched, and that have molecular weights greater than 500,000 Dalton, and sizes greater than 100 nm (Figure 1). The talk will describe the use of this approach to create synthetic antibodies for therapeutic applications, and outline routes to a broad array of functional molecules.

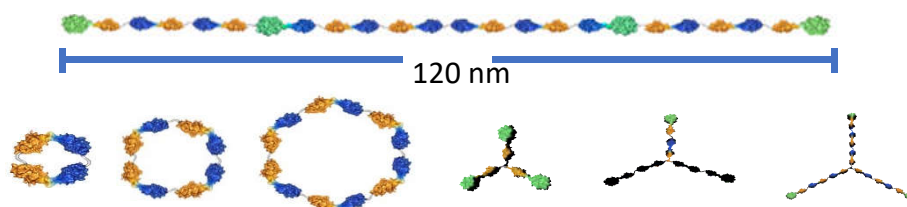


Figure 1. Megamolecules are prepared by reacting fusion proteins with molecular linkers that assemble by way of reactions of irreversible inhibitors with specific enzyme domains. Examples of megamolecules that can be assembled include linear structures (top), cyclic structures (left) and branched structures (right).

The megamolecules offer new approaches for preparing scaffolds that can spatially organize protein domains. This talk will describe the assembly of synthetic antibodies that position two (or more) Fab domains with control over the distance and orientation of the domains, as well as bispecific antibodies that present two distinct Fab domains. The talk will include a discussion of applications of this method to prepare nanoscale membranes having biological functions.

Y.PL.S.II.5.

Combustion spray synthesis of nanostructured materials: from carbon black to breath sensors

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The lecture will start with a fascinating overview of combustion aerosol technology from ancient China and the bible printing of Gutenberg to the current manufacture of commodities. Recent advances in particle formation and growth through discrete element modeling and molecular dynamics allow now optimal process design, away from the Edisonian approaches of the past. In specific, the rapid attainment of asymptotic agglomerate structure and self-preserving size distribution by coagulation greatly facilitate scalable process design for material synthesis [1].

This leads to scalable synthesis of sophisticated nanoparticles with controlled morphology size and composition by *flame spray pyrolysis* putting new high value products (like nanosilver and carbon-coated Co nanoparticles) in the market already while several promising ones are emerging such as *single atom* catalysts and chemoresistive gas sensors for breath analysis. As time permits, the latter are highlighted for highly selective monitoring of acetone, NH₃, isoprene and even formaldehyde. These are tracers of body fat burning, end stage renal disease, cholesterol and indoor air pollution, respectively, while sensor arrays are assembled to sniff-out earthquake victims [2].

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Y.PL.S.II.6.

Making the hospital a safer place by the sonochemical coating of all its textiles and medical devices with antibacterial nanoparticles

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Sonochemistry is an excellent technique to coat nanomaterials on various substrates, imparting new properties to the substrates. After a short demonstration of coating NPs on ceramics and stainless steel, I'll present the coating of textiles such as polyester, cotton, and nylon. In all cases a homogeneous coating of NPs was achieved. Lately, the FDA shows less enthusiasm towards nano Ag, as a result, we have moved to NPs of ZnO, and CuO as antibacterial agents. They were coated on the above-mentioned fabrics and showed excellent antibacterial properties. The coated textiles were examined for the changes in the mechanical strength of the fabric. A special attention was dedicated to the question whether the NPs are leaching off the fabric when washed repeatedly. The coated ZnO NPs on cotton underwent 65 washing cycles at 75 °C in water in a Hospital washing machine, no NPs were found in the washing solution and the antibacterial behavior was maintained. Recently, an experiment was conducted at PIGOROV Hospital in Sofia, Bulgaria in which one operation room was equipped with antibacterial textiles, namely, bed sheets, pajamas, pillow cover, and bed cover. 22 Patients in this operation room were probed for bacterial infections. Their infection level was compared with 17 control patient that were using regular textiles. The results are demonstrating that a lower infection level is observed for those patients exposed to the antibacterial textiles. The following medical devices were coated with metal oxide Nanoparticles and showed very good biocidal properties and inhibition of biofilm formation 1) Urinal Catheters 2) Contact lens 3) Cochlear electrodes, 4) metallic implants, and 5) silicon implants. In my lecture examples of 1) and 2) will be demonstrated. Coating of Catheters with the above-mentioned NPs were performed and the coated catheters were inserted in rabbits. Results showed that the urine of the rabbits was not contaminated with bacteria.

Y.PL.S.II.7.

Earthicle and its discontents

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Despite the advances in molecularly targeted therapies, delivery across the blood-brain barrier (BBB) and the targeting of brain tumors remains a challenge. To tackle these challenges, we made a variation on the previously proposed concept of the earthicle [1, 2] and fabricated an aqueous, surfactant-free ferrofluid containing superparamagnetic iron oxide nanoparticles coated with silicate mesolayers and carbon shells, having 13 nm in size on average [3]. The nanoparticulate ferrofluids preferentially bind to brain cancer cells and, hence, exhibit a greater toxicity in these cells compared to the primary cells. In 3D tumor spheroids, nanoparticles greatly reduce the metastatic migration of cancer cells, while the tumor viability gets reduced compared to the control group by applying magnetic hyperthermia to nanoparticle-treated spheroids. In a MDCK-MDR1 blood-brain barrier model, the nanoparticles cause mislocalization of claudin-1 at the tight junctions, underexpression of ZO-1 and no effect on occludin-1 and transepithelial resistance. In spite of preserving the integrity of the blood-brain barrier, the nanoparticles traverse it transcellularly and get localized to the optic lobes of the third instar larval brains of *Drosophila melanogaster*. Examination of LAMP1 demonstrated that nanoparticles escape the lysosome during their noninvasive passage across the blood-brain barrier, causing no adverse systemic effects to the animals. All in all, both *in vitro* and *in vivo* models of the blood-brain barrier evidence the ability of these composite nanoparticles to cross the blood-brain barrier and localize to the brain tissue. In conclusion, these composite nanoparticles show great promise as an anticancer biomaterial for the treatment of different types of cancer and may serve as an alternative or addendum to traditional chemotherapies. Their other applications, including magnetic hyperthermia [4] and targeted magnetic separation of cancer cells and other biological entities [5] are currently under investigation.

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Y.PL.S.III.1.

Heterostructured materials: a new paradigm for superior mechanical properties

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Strong and tough materials are desired for light-weight applications such as electric cars. Recently, heterostructures are found to produce unprecedented strength and ductility that are considered impossible from our textbook knowledge and materials history. Heterostructured (HS) materials consist of domains with dramatic strength differences, which causes hetero-deformation, which induces back stress in the soft domain and forward stress in the hard domain. This collectively produces hetero-deformation induced (HDI) hardening, and HDI stress, making the materials strong and tough. Importantly, HS materials can be produced by current industrial facilities at large scale and low cost. There are many scientific issues with such materials that challenge the communities of experimental materials science and computational material mechanics. Heterostructured materials is quickly becoming a hot research field in the post-nanomaterials era. In this talk I'll present the current advances as well as future challenges and issues in this emerging field.

Y.PL.S.III.2.

Optimizing the properties of titanium alloys processed using additive manufacturing

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There are a number of defects associated with the additive manufacturing (AM) of titanium alloys. These include the formation of coarse columnar microstructures, generally parallel to the growth/deposition direction in builds produced by blown powder, the presence of porosity, and residual stresses. This talk focuses on the first of these, coarse microstructures. Emphasis has been on the use of alloying to effect an equiaxed microstructure through modification of the solidification mechanism, by inducing a columnar to equiaxed transition (CET). The experiments have employed a combinatorial approach developed in our laboratory, where a LENSTM (blown powder) AM device with two powder hoppers has been used to produce variations in the minor alloying elements of interest, such that modifications to microstructure can be directly related to changes in composition. The microstructures produced as a result of the additive manufacturing process have been characterized. In the main, the use of selective alloying has been successful in terms of effecting a CET, such that refined equiaxed grains are produced. A variety of microstructures may be produced during subsequent heat-treatment, and the underlying mechanism of formation of these has been studied. The mechanical properties of new Ti alloys, with alloying additions that result in CETs, have been assessed and their values have been compared with those predicted by a machine learning approach. These comparisons will be discussed.

Y.PL.S.III.3.

Hybridization of solid carbohydrates or hydrocarbon with metal oxides under mechanical stressing toward sustainable materials

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Mechanochemical treatment of solid carbohydrates or hydrocarbon, such as cellulose or paraffin wax with metal oxide nanoparticles brings about numerous functional nanocomposites. They are combined with sustainable materials via affordable chemical processes. Starting from physicochemical basics of mechanochemical reactions at the boundaries between carbohydrates or hydrocarbon and metal oxides, case studies are given on the changes in the microstructural properties of cellulosic compounds (SSC) with TiO₂ or its hydrates by milling SSC with aqueous precursors of TiO₂ or TiO₂ nanoparticles. Discussion will be concentrated on the non-covalent chemical interaction between SSC and TiO₂ with and without the aid of surrounding polarized water molecules. Simultaneous micronization of SSC structural units and changes in the properties of composites upon subsequent heating are also discussed, in conjunction with the drying condition of the wet complex mass. Despite its basic science oriented experimental works, the authors also try to discuss some unique photo response of titania in the nanocomposite. When time permits, mechanochemical reduction of a stable oxide, V₂O₅, with paraffin wax to VO₂ is referred. Stabilization of thermodynamically less stable VO₂ by oxygen vacancies introduced during co-milling with paraffin wax will also be explained, together with a possibility of applying to latent heat energy storage devices.

W.PL.S.II.1.

Electroceramics without sintering

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In recent years the progress in Room Temperature Fabrication (RTF) method of electroceramics has been fast. This includes ferrites and dielectrics which electrical properties can be adjusted showing feasibility to high frequency applications. Since no sintering is required, 2D and 3D printed structures have been also introduced. Very recently RTF have been utilized also for so called “upside-down” composites with ferroelectric and piezoelectric performance, as well as to ultra low permittivity dielectric feasible for advanced antenna systems for 5G networks. This presentation surveys all compositions realized so far with the RTF discussing their electrical properties, advantages and disadvantages, and demonstrated devices.

W.PL.S.II.2.

The mechanisms behind solute-drag and solute-acceleration during microstructural evolution of alumina

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Alumina is one of the most used ceramic materials, and as such understanding its sintering and densification processes is important. It is known that the microstructural evolution is strongly affected by dopants, such as MgO which promotes sintering and limits grain growth. Key impurities, such as CaO and SiO₂, are known to cause exaggerated grain growth. Over the years various models have been proposed to explain the influence of defects, but experimental limitations, such as knowledge of high temperature solubility limits, has prevented corroborated evidence of impurity adsorption affecting grain boundary mobility, compared to liquid-phase enhanced grain boundary mobility.

This presentation will focus on the influence of CaO and/or MgO on the evolving microstructure of alumina for a range of concentrations below the solubility limit. The amount of dopant in the alumina was fully quantified by conducting wavelength dispersive spectroscopy, and the change in grain boundary mobility as a function of *measured* dopant concentration was characterized using scanning electron microscopy via grain size measurements. Annealing experiments were conducted in a graphite furnace under flowing He, and the mobilities were compared to samples annealed in air.

Unlike segregating dopants which reduce grain boundary mobility by solute-drag (such as MgO), CaO *increases* the rate of grain growth, and a trend of increased mobility with increasing dopant level will be demonstrated. The increased mobility due to Ca segregation is believed to be due to an increase in vacancy concentration in the immediate vicinity of the grain boundaries. Co-doping with Mg and Ca leads to a higher Mg solubility limit, and thus more Mg at the grain boundaries in balance with the Mg in solution, and a reduced grain boundary mobility. Presumably grain boundary motion in alumina is via the motion of disconnections, which has been experimentally demonstrated for SrTiO₃. How dopants, including carbon, interact with disconnections will be discussed.

W.PL.S.II.3.

Understanding of sintering in Ukraine: overview of results

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The International Institute for Science of Sintering has fulfilled its historic mission of bringing together the knowledge of scientists from the West and the East in sintering discipline. One of the greatest contributions to the development of the theory and practice of sintering on the Eastern side was made by representatives of scientific institutes and universities located on the territory of today's Ukraine. In the 1950s and 1960s, the works of the Kharkov University and the Institute of Materials Science Problems named after Frantsevich were the most significant ones. Fundamental research in the field of condensed matter physics, diffusion, and mass transfer in non-equilibrium disperse systems were performed by B.Ya. Pines, I.M. Lifshitz, V.V. Slezov and Ya.E. Geguzin. R.A. Andrievsky was the first who determined the driving forces for sintering using porous specimen and the zero-creep method. Experimental results on sintering of dissimilar powder materials have been proposed by G.V. Samsonov and P.S. Kyslyi. The basis of continual theory of sintering has been proposed by V.V. Skorokhod. Today, this continual approach to the sintering problem as well as multiscale modeling is well developed by O.A. Olevisky, M.B. Stern. The sintering of nanostructured materials and related problems is contributed by A.V. Ragulya. The paper will present the most significant milestones in the development of the science of sintering.

W.O.S.

Field assisted reaction sintering of ceramic materials

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Chemical reaction may be activated by electric pulses of various frequencies. Low frequency spark plasma sintering or high frequency microwave sintering both represent unique instruments for manipulation with microstructure of ceramics and manufacturing of novel materials including ceramic matrix nanocomposites. There had been well established that the direct pulsed electric current is able to create special conditions for the accelerated heat and mass transfer, mixing of atoms during chemical reactions and phase formation. All these manipulations with particulate system allow control the grain size, phase composition, density and combination of properties in ceramic materials. Examples of reaction SPS and MWS will elucidate recent experimental results attractive for numerous applications. The grain size control under reaction SPS occurs through the acceleration of the nucleation and inhibition of nuclei growth and strongly depends on number of phases. Several details of reaction SPS and MWS will be presented to discuss new mechanisms of densification previously not considered. Some sintering modes allow the grain growth to be completely impeded, or vice versa, abnormally accelerated.

Y.PL.S.IV.1.

Nanostructured materials for energy-relevant electrocatalytic processes

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Replacement of precious metal catalysts by commercially available alternatives is of great importance among both fundamental and practical catalysis research. Nanostructured carbon-based and transition metal materials have demonstrated promising catalytic properties in a wide range of energy generation/storage applications. Specifically engineering carbon with guest metals/metal-free atoms can improve its catalytic activity for electrochemical oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), thus can be considered as potential substitutes for the expensive Pt/C or IrO₂ catalysts in metal-air batteries and water splitting process. In this presentation, I will talk about the synthesis of nonprecious metal and metal free elements-doped graphene, and their application on electrocatalysis [1-8]. The excellent OER and HER performance (high catalytic activity and efficiency) and reliable stability indicate that new materials are promising highly efficient electrocatalysts for clean energy conversion. I will also present some research results of CO₂ electrocatalytic reduction conducted in my research group [9,10].

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Y.PL.S.IV.2.

Computer modelling as a predictive tool in materials and catalytic science

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We will describe how the concerted use of modelling techniques especially in conjunction with synchrotron and neutron based experimental methods can yield unique information on structures, dynamics and mechanism in a range of catalytic and energy materials. Our discussion will concentrate on the following systems:

- (i) The structures and reactivities of oxide supported nano-particulate catalysts, including insights in the re-structuring of nano-particles during catalytic reactions, where we will highlight recent computational-experimental studies.
- (ii) The dynamics and reactivities of sorbed hydrocarbons in microporous catalysts.
- (iii) The activation of hydrocarbons and carbon dioxide on oxide surfaces, where we shall emphasise the information on key mechanistic aspects revealed by recent QM/MM modelling studies.
- (iv) The electronic structure and band alignment of titania polymorphs.

We will also consider other areas of materials and catalytic science where the synergistic use of modelling with synchrotron based and other experimental techniques could be fruitfully applied.

Y.PL.S.IV.3.

Crystal chemistry and properties of G-phases

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Socalled G-phases ($\text{Th}_6\text{Mn}_{23}$ -type and ordered derivatives with $\text{Mg}_6\text{Cu}_{16}\text{Si}_7$ -type, all space group $Fm-3m$) constitute a large class of intermetallic compounds comprising aluminides, gallides, silicides, germanides and stannides.

Our systematic investigation (phase relations, X-ray single crystal structure analysis, neutron powder diffraction) of titanium based transition metal (TM) aluminide solid solutions $\text{Ti}_6\{\text{TM},\text{Al}\}_{\sim 23}$ however, revealed a filled variant of the $\text{Th}_6\text{Mn}_{23}$ type (space group $Fm-3m$) for the Al-rich single-phase region, whereas a novel structure variant with space group $F-43m$ was established for the Ti-rich side of the G-phase region. The direct group-subgroup relation between space groups $Fm-3m$ and $F-43m$ may favour a second order phase transition.

In contrast to the various structure variants observed for titanium aluminium-based G-phases $\text{Ti}_6(\{\text{Fe},\text{Co},\text{Ni},\text{Ru},\text{Rh},\text{Pd},\text{Os},\text{Ir},\text{Pt}\}_{1-x}\text{Al}_x)_{23+1}$ and $\text{Ti}_6\text{Ni}_{16+x}\text{Si}_7$, the G-phase $\text{Mn}_6\text{Ni}_{16}\text{Si}_7$ was confirmed to crystallize as a simple ordered variant of the $\text{Th}_6\text{Mn}_{23}$ structure type.

It should be noted that the ternary intermetallic G-phase silicide precipitates preferentially at grain boundaries and dislocations in both ferrite and austenite of duplex stainless steels and recently gained significant interest for ultra-high strength steels.

In view of applications, the presentation will provide a comprehensive overview on the structural chemistry of G-phases, particularly focusing on aluminides and silicides covering also stannides.

Y.PL.S.IV.4.

Goodbye hospitals and hello implantable nanosensors

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There is an acute shortage of organs due to disease, trauma, congenital defect, and most importantly, age related maladies. While tissue engineering (and nanotechnology) has made great strides towards improving tissue growth, infection control has been largely forgotten. Critically, as a consequence, the Centers for Disease Control have predicted more deaths from antibiotic-resistant bacteria than all cancers combined by 2050. moreover, there has been a lack of translation to real commercial products. This talk will summarize how nanotechnology can be used to increase tissue growth and decrease implant infection without using antibiotics but using sensors (while getting regulatory approval). Our group has shown that nanofeatures, nano-modifications, nanoparticles, and most importantly, nanosensors can reduce bacterial growth without using antibiotics. This talk will summarize techniques and efforts to create nanosensors for a wide range of medical and tissue engineering applications, particularly those that have received FDA approval and are currently being implanted in humans.

Y.PL.S.IV.5.

Strain-engineering in advanced CMOS structures

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As the conventional method of scaling-down the device size of MOSFETs had faced limitations in performance improvement, alternative route of strain engineering has been gaining much attention. SiGe stressors epitaxially grown in source and drain effectively introduced compressive stress in the Si channels not only for the planar type but also for the 3-D FinFETs in P-type MOSFETs. In comparison, for N-type MOSFETs, Si[C][P] stressors have been developed for the generation of tensile stress in the MOSFET channels. We investigated the strain distribution in nanoscaled MOSFET structures with SiGe and Si[C][P] in the source and drain regions for the planar-type MOSFETs and 3-D FinFET structures as well. After the formation of stressors in the S/D regions with SiGe or Si[C][P] by selective epitaxial deposition, we characterized the induced strain using both nano beam electron diffraction (NBD) and reciprocal space mapping (RSM), and compared them with the simulation results. The strain distributions depend on the various factors of stressor compositions, device dimensions and structures, and also post processes such as oxidation or silicidation. In this report, we will discuss the several examples of the strain evolutions in the nano-scaled MOSFET structures including 3-D FinFETs.

Y.PL.S.IV.6.

Environmental & dynamic electron microscopy of advanced materials in HV-(S)TEM

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Environmental transmission electron microscopy (E-TEM) attracts recently a strong interest of materials researchers, particularly, those of fuel cells and lithium batteries, because the actual chemical reaction processes in gases and liquids need to be clarified in real space and in atomic level. E-TEM observations of thicker samples of a few micron in a gas environment, particularly in hydrogen and oxygen gases, become very important for cutting-edge materials in practical use. 3D observation of samples is also necessary for clarifying morphologies of various active materials such as practical catalysts.

We have developed 1MV TEM/STEM equipped with an open-type environmental cell which enables observations in 100 Torr atmosphere of hydrogen, oxygen, nitrogen and carbon monoxide, named "Reaction Science HVEM" (RSHVEM)[1]. The transmission of high-energy electrons has realized point-to-point resolution less than 0.2 nm even in gas-environment such as 100 Torr. High-speed beam blanking system reduces irradiation effects of incident electrons, and potentially realizes so-called "in place observation" without effects of beams [1].

In this talk, I would like to present some application data obtained by the E-HV(S)TEM such as (1) in-situ observation of porous gold (Au) catalyst, whose inner surface with zigzag atom arrangement enhances the catalytic oxidation in carbon-mono oxide (CO) gas of 30 Pa [2], (2) observation of diesel soot oxidized in air, and (3) in-situ observation of mechanical test related to "hydrogen brittleness" on a copper(Cu)/silicon(Si) interface and as well as Ni₃Al structural materials in mixed gas of hydrogen and nitrogen [3][4]. Observation of Li-related battery materials is also available using a non-exposure transfer holder [5].

Acknowledgements are due to Prof. Muto and Drs. Fujita, Ogura and Takahashi for their kind collaboration of the present study.

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Y.PL.S.IV.7.

Integrated Differential Phase Contrast (iDPC) STEM for low Z detection and for high contrast low dose imaging applications

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One of the main challenges in conventional STEM techniques is the difficulty to fully image and interpret a lattice consisting of both high and low Z elements. While only high Z elements can be imaged in HAADF-STEM, (A)BF-STEM can display low Z elements, though atomic positions in the images are difficult to interpret as there is no clear contrast variation between different atoms [1].

Novel integrated differential phase contrast (iDPC) STEM imaging is instrumental in showing both low Z and high Z elements with clear contrast variation [2]. iDPC STEM is based on center of mass (COM) based imaging [3], and its strength in simultaneous high and low Z detection has been shown experimentally in GaN [2, 4] and V-TiH [5] domains. Moreover, iDPC STEM images have also been shown to exhibit improved contrast in beam sensitive materials, exemplified with graphene [2].

In materials science, we are seeing an increasing particular interest in structures that are comprised of low Z elements and beam sensitive materials (i.e. 2D materials, zeolites, MOFs, etc.) requiring low dose imaging techniques. With an enhanced contrast as well as wide Z-range detection capability, iDPC STEM should be considered as the key sub-angstrom imaging method in these research areas.

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W.O.S.I.1.

Thermal stress directions and stress mechanism in Ag sintered bonding layer under thermal cycling test for Si power device structures having sintering chip-attachment

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Ag sintered bonding layer has a high thermal conductivity of about 250 W/mK and the thickness of about 30 μm . Ag sintering chip-attachment can increase the maximum allowable power dissipation under fixed $T_{j\text{max}}$. The present subject is to certify the reliability of Ag sintered layer, particularly for EV and high power applications. This paper presents the thermal stress results under thermal cycling test (TCT) by 3D multi-physics solver for direct Ag sintering chip-attachment on Cu plate. We performed simulations at the fixed ambient temperature (T_a), focusing on the stress directions and mechanism in Ag sintered layer. Target structure has a 10 mm square chip with the thickness of 150 μm , Ag sintered bonding layer, and a 20 mm square Cu plate. We measured material parameters such as Young's modulus of sintered samples which were sintered at 250 degrees Celsius under 10 MPa in atmosphere, and used these values for our simulations.

Results ($T_a = -40$ degrees Celsius) show that at the center in both upper and lower sides of Ag sintered layer von Mises stress values are almost equal to shear stress values. It was found that this stress is the tensile stress which is caused by the mismatch between thermal expansions of Ag sintered layer and Si. The upper side stress is slightly larger than the lower side stress. The shear stress at upper side of 30 μm sintered layer was 73.6 MPa at the Cu thickness of 1 mm, and gradually decreases as the Cu thickness increases. The maximum von Mises stress point is at the corner in lower side of sintered layer. At the corner in both upper and lower sides of Ag sintered layer von Mises stress values are mainly the normal stress. We found that this normal stress is the compressive stress. According to stress profile results at the diagonal cross section, this compressive normal stress is thought to be mainly caused by Si chip warpage. The normal stress at lower side corner of 30 μm sintered layer was 509 MPa at the Cu thickness of 1 mm, and decreases as the sintered layer thickness increases from 30 to 150 μm . In conclusion the results in this paper are very useful for qualifying Ag sintered bonding layers.

W.O.S.I.2.

Thermal stress profiles and stress directions in Si chip under thermal cycling test for power device structures having Ag sintering chip-attachment

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Power semiconductor devices and modules need highly efficient heat dissipation system having a chip bonding layer with high thermal conductance and reliability. Ag sintered bonding layer has a high thermal conductivity of about 250 W/mK and the thickness of about 30 μm . Because of this excellent property Ag sintering chip-attachment can increase the maximum allowable power dissipation under fixed $T_{j\text{max}}$. The present subject is to certify the reliabilities of power device chips with Ag sintered bonding layers.

This paper presents the thermal stress results under thermal cycling test (TCT) by 3D multi-physics solver for Si power device chip systems using direct Ag sintering chip-attachment on Cu plate. We particularly focus on the thermal stress profiles and directions in Si chips. Target heat dissipation structure has a 10 mm square chip, Ag sintered bonding layer, and a 20 mm square Cu plate (heat spreader). We performed simulations at the fixed ambient temperature (T_a), assuming the elastic stress-strain relationships.

Results ($T_a = -40$ degrees Celsius) show that at the center in both upper and lower sides of Si chip with the thickness of 150 μm von Mises stress values are almost equal to shear stress values. We found that this stress is the compressive stress which is caused by the mismatch between thermal expansions of Si and Ag sintered layer. The lower side stress is slightly larger than the upper side stress. This compressive shear stress of Si chip having 30 μm sintered layer was 466 MPa in lower side at the Cu thickness of 1 mm, and gradually increases as the Cu thickness increases. The maximum von Mises stress point is at the corner in lower side of chip. This maximum stress value consists of both normal and shear stress values, which are both compressive values. These von Mises, normal and shear stresses were 673, 328 and 349 MPa at the Cu thickness of 1 mm, and gradually decreases as the sintered layer thickness increases from 30 to 150 μm . In conclusion we have revealed the thermal stress profiles and mechanism in power device chips with sintered bonding layers.

W.O.S.I.3.

Influence of milling, annealing and sintering parameters on the formation of LLZO compoundDariusz Oleszak¹, Tomasz Pikula², Mirosława Pawlyta³¹Warsaw University of Technology, Warsaw, Poland, ²Lublin University of Technology, Lublin, Poland, ³Silesian University of Technology, Gliwice, Poland

This work describes the influence of milling, annealing and sintering parameters on the formation of single phase cubic $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) compound. The mixtures of lithium carbonate, lanthanum hydroxide and zirconium oxide powders were subjected to mechanical alloying, followed by isothermal annealing. Next, the powders were subjected to compaction by spark plasma sintering method. XRD, including Rietveld analysis, SEM and TEM experimental techniques allowed full characterization of the final milled and heat treated powders as well as sinters.

W.O.S.I.4.

Synthesis and densification of electride Mayenite - $\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$

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The binary compounds of the calcia–alumina ($\text{CaO}-\text{Al}_2\text{O}_3$) system are significant in a wide range of applications in metallurgical slags, ceramic materials, and cement technology. However, intermediary phase mayenite ($\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$) become one of the more interesting advanced ceramic material. It stimulated research because of its oxygen mobility, ionic conductivity, high anti-carbon and anti-sulfur characteristics and catalytic properties. In this work Mayenite has been prepared using various methods: ceramic route, by solid state reaction between CaCO_3 and $\gamma\text{-Al}_2\text{O}_3$, by modified glycine/nitrate procedure, crystallization from the melt as well as by combustion synthesis. Densification was done by pressureless sintering, hot pressing (HT) and by Spark Plasma Sintering (SPS). Sintering behavior is studied by dilatometer. A relative density of 94% is obtained at 1300 °C using pressureless sintering, on the other side, full density is obtained by the HT and SPS densification methods. The obtained powders were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Raman spectroscopy at room temperature, Electron paramagnetic resonance (EPR) at – 196 °C. Micro-indentation as well as nano-indentation were performed to studied a mechanical property of sintered samples.

W.O.S.I.5.

Ultra-rapid microwave sintering based on controlled thermal instability and resonant absorption

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Over the last few years we have demonstrated ultra-rapid microwave sintering of oxide ceramic materials, including Al_2O_3 , ZrO_2 , Y_2O_3 , MgAl_2O_4 , etc. The enhanced densification was shown to be associated with the development of thermal instability under volumetric microwave heating. The density of the volumetrically deposited power at the onset of thermal instability was $10\ldots 100 \text{ W/cm}^3$, which is the same order of magnitude as the power density required for the dc field-assisted flash sintering processes. The proposed mechanism of ultra-rapid densification involves grain boundary softening / melting and enhanced mass transport through the transient liquid phase.

Most experiments were carried out using a 24 GHz / 6 kW gyrotron system for microwave processing of materials. The purposeful use of the thermal instability for ultra-rapid sintering is contingent upon the fast and precise control over the microwave power. Optical methods of process control have been implemented to monitor shrinkage and temperature distributions in the ceramic samples undergoing sintering.

First experiments on ultra-rapid localized densification have been accomplished using a focused wave beam of a 263 GHz / 1 kW gyrotron. By scanning the beam over the surface of a hydroxyapatite powder layer at a velocity on the order of 1 mm/s, the formation of extended densified structures has been demonstrated. This suggests that the ultra-rapid microwave sintering technique is promising for the development of additive manufacturing applications.

Ultra-rapid microwave sintering of powder metals has been investigated by numerical simulation. Efficient microwave absorption in metal powder compacts leading to very rapid heating and densification has been demonstrated to be possible due to resonance effects.

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W.O.S.I.6.

Effect of scanning strategy on mechanical properties of selective laser melted Inconel 718

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Selective laser melting (SLM), is one of the promising additive manufacturing (AM) technologies, which is capable of fabricating near-net shape metallic components with geometrically complex structures. Although most previous researchers focused on controlling the solidification microstructure and crystalline orientation by tailoring the scanning strategy, few studies are available on the effect of the scanning strategy on mechanical properties, especially fatigue properties. In this talk, we will present an investigation on the effect of scanning strategy, i.e. bidirectional scanning without (SS-X) and with a 90°-rotation (SS-XY) for every layer, on mechanical properties of SLM-fabricated Inconel 718. We will show that tensile strength and fatigue strength of SS-X specimens are superior to that of the SS-XY ones. Such excellent mechanical properties of the SS-X specimens at room temperature were found to mainly result from the processing-induced fine grain structures compared with void size, crystalline orientation or dendrite structure.

W.O.S.I.7.

Laser-powder bed fusion of bronze: microstructural, mechanical and electrochemical properties

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Laser-powder bed fusion (L-PBF), a metal 3D printing process, offers the potential for printing customized and functionalized engineering parts. This method, which allows the production of parts by melting the layer by layer metal powders, has been very popular recently. Many metallic parts can be produced by this technique, but the production of bronze (Cu-10Sn) parts by this technique is not common. Especially, the influence of processing conditions (energy density) and scanning strategies on the density and mechanical properties of bronze parts using the L-PBF process has not received much attention in the open literature.

In this paper, microstructural details, mechanical and electrochemical properties of L-PBF bronze alloy parts were studied. The density, ultimate tensile strength, elongation, hardness and electrochemical properties of the bronze L-PBF parts were sensitive to process parameters. The density, mechanical properties and electrochemical properties of L-PBF bronze samples were examined and tried to be explained. In the preparation of standard samples, the particle size of bronze powder was chosen as 10-35 μm . Powders were produced in different parameter ranges (laser power, powder layer thickness, scanning speed and direction) using SLM technique and subjected to heat treatment after production. All findings were discussed in the light of the literature.

W.O.S.I.8.

Scaffolding via surface-selective laser sintering of biocompatible polymer particles using water as heating sensitizer

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Surface-selective laser sintering were used for formation of scaffolds from the original biocompatible and bioresorbable materials. Experimental samples of scaffolds were formed on the original setup, which used the radiation of a continuous laser with a wavelength of 1.9 μm , which is practically not absorbed by polymer particles. Water was used as a surface photosensitizer for heating, which was applied as a fine mist on the surface of a polymer powder. This approach allows the powder particles to be fused together by means of a molten surface layer, without melting the bulk of the particles. For various types of powder materials based on aliphatic polyesters, the modes of surface-selective laser sintering were determined. Using a system of layer-by-layer formation of powder layers, several series of centimeter-sized three-dimensional scaffolds were formed according to a given three-dimensional model, forming test structures that were submitted to biocompatibility tests. Formed scaffolds showed promising biocompatibility results.

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W.Y.O.S.I.

Investigation of the effect of GDC (Gd-doped ceria) powder morphology on the properties of the ceramics sintered using SPS

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Nowadays Gd-doped ceria (abbr. GDC or CGO) is a material widely used as a solid electrolyte in electrochemical devices such as solid oxide fuel cells (SOFC). The reason for its popularity is high oxygen conductivity at intermediate temperatures 500-600 °C that is favorable for using it in SOFC. One of the problems in manufacturing materials from such ceramics is poor sinterability. In order to improve this, it is possible to add sintering aids to the powder; however, they can affect the important properties of the ceramics, such as ionic conductivity. Another way to decrease the sintering temperature of the powder is to change its morphology or use non-conventional methods for sintering, for example, spark plasma sintering (SPS). In this work, powders of GDC were obtained by thermal decomposition of an oxalate precursor $\text{Ce}_{1.8}\text{Gd}_{0.2}(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$. Such parameters as particles' sizes, agglomerates' sizes and shape, specific surface area were controlled by changing conditions of dehydration and oxidation of the precursor. The obtained powders of GDC were compacted and sintered using different sintering protocols: conventional sintering, SPS and also conventional sintering combined with SPS. The obtained ceramics were investigated by different methods. Influence of the powders morphology and sintering protocols on the properties of final ceramics (ionic conductivity, grain size, density) is discussed.

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W.Y.O.S.2.

The BaTiO₃ nano-scale coated morphology influence on electronic properties and ceramics fractal nature frontiers

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The BaTiO₃ ceramics applications based on electronic properties have very high gradient scientific and industrial-technological interests. Our scientific research has been based on nano BaTiO₃ with MOD-Y salts and also on Y₂O₃. The samples have been consolidated at sintering interval 1200 – 1350 °C. We demonstrate the new frontiers for different electronic properties between the layers of BaTiO₃ grains. As a research target we had GB composite, Nano size metal oxide dispersions, AC-DC safety capacitance, nano scale grain boundary control, capacitance, GB control mobility in DC BS operation voltage. We applied all related characterizations and especially SEM. Fractal nature characterization and corrections include influences grains and pores surface and Brownian motions of particles. We established relation with all of this characteristics and temperature. Throw this experiments and results and fractals characterization, we opened new perspectives for higher electronic properties integrations between the grains and practically established the control within the processing, morphological structures and designing the properties. This is very important, new approach towards further miniaturization-fractal miniaturization and related, advanced technologies.

W.Y.O.S.3.

Sintering process optimization for Cu-Al₂O₃ powders synthesized by novel method

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This paper presents sintered materials for use as contacts produced via novel synthesis method of starting powders by combination of explored conventional routes of thermochemical synthesis and mechanical alloying.

Starting raw materials for powder synthesis by thermochemical route were soluble salts, nitrates of copper and aluminum of p.a. quality, dissolved in distilled water (50wt.% solution) in suitable ratio for final powder to contain 50wt.% of Al₂O₃ in structure. Nitrate solution was spray dried and subjected to heat treatment (900 °C/1h). Obtained oxides were reduced in hydrogen atmosphere (flow rate 20L/h at 350 °C for 1h) in order to obtain composite of Cu-Al₂O₃. Produced powders were used for mechanical alloying of atomized copper (5h, 300 min⁻¹). Final amount of alumina Al₂O₃ in composite powder were 1, 1.5 and 2 wt.%. After mechanical alloying obtained powders were compacted by a uniaxial pressing (8×32×3mm, 500 kN). Sintering of samples was performed in hydrogen atmosphere in isothermal conditions at five different temperatures in the range from 725-925 °C for 15 to 120 min.

Results of characterization show, that increase of Al₂O₃ content has more noticeable effect on the electrical conductivity and hardness than sintering temperature and time. With increase of Al₂O₃ from 1 to 1.5 wt.% there is a slight decrease in both investigated properties, while with increase up to 2 wt.% Al₂O₃ significant decrease in electrical conductivity and hardness of sintered samples is observed.

According to achieved results optimum sintering parameters for composite materials produced by novel synthesis method based on copper with dispersed 1% Al₂O₃ are 875 °C/60 min.

Based on the achieved results, this method provides production of contact materials with good combination of electrical and mechanical properties, but with estimated lower production costs.

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W.Y.O.S.4.

The effect of severe plastic deformation (SPD) via high pressure torsion (HPT) on physical and mechanical properties of thermoelectric materials

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Clathrates, but especially skutterudites and Half-Heusler alloys are known as promising candidates to serve as leg materials for thermoelectric (TE) generators, which can directly convert waste heat into electricity. They are not only environmentally friendly, but can be used in a wide temperature range and the starting material is available and cheap.

Since recently, it is known that SPD-processing of thermoelectrics can enhance the values of the figure of merit, ZT , due to the ultra fine grained microstructure in combination with a high level of point, linear and surface lattice defects, which significantly enhance the scattering of the phonons, thus leading to a minimum of lattice thermal conductivity.

Especially for skutterudites, high-pressure torsion, as one of the major techniques of SPD processes, is a great tool to either enhance ZT of hot pressed samples or to directly produce fast and easily high ZT thermoelectric bulks. A still unsurpassed highlight is the enhancement of ZT from 1.6 to almost 2 at 825 K for an n-type skutterudite.

Whilst for thermoelectric clathrates so far little success was reported, HPT treatment of Heusler and Half-Heusler phases in some cases was able to boost ZT .

As concerns mechanical properties, the application of SPD methods significantly raises the strength although the density becomes slightly lower, while leaving the elastic moduli more or less unchanged.

W.Y.O.S.5.

G-quadruplex DNA oligomer for electrochemical sensing of insulin

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Certain guanine-rich DNA oligomers form G-quadruplex structure and bind hemin inside. Such DNA oligomers are called hemin-binding DNA aptamer. Guanine-rich DNA oligomer with the sequence of 5'-GTGGTGGGGGGGTTGGTAGGGTGTCTTC- 3' was reported to bind insulin selectively and named IGA3. In this study, we investigated the application of DNA aptamer IGA3 as sensing material for insulin detection. IGA3 forms anti-parallel G-quadruplex folding single strand DNA. It was reported that some anti-parallel G-quadruplex bind hemin and show peroxidase activity by spectroscopic observation. In this study peroxidase activity of IGA3 with hemin was confirmed by spectroscopic measurement using 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) as an electron donor, and the activity was 2.75 times higher than hemin itself. IGA3 showed the selectivity against glucagon, which is hormone and related to carbohydrate metabolism as well as insulin.

Then IGA3 was immobilized onto a gold electrode to determine its activity electrochemically and to examine insulin binding-effect to the activity. Peroxidase activity of immobilized IGA3 with hemin was determined by Cyclic Voltammetry using H_2O_2 as substrate. Cathodic current was observed through electron transfer. Cathodic peak current around -0.4V of the electrode showed the dependence on the concentration of H_2O_2 up to 30 μM and at higher concentration the current reached steady state. Thus the peroxidase activity of IGA3 was confirmed electrochemically without ABTS as a donor. At the range of concentration 20-30 μM of H_2O_2 , the cathodic peak current decreased by addition of insulin. The decrease depended on the concentration of insulin at the range of 1-5 μM . As a result we demonstrated the usability of IGA3 DNA oligomer for electrochemical sensing of insulin.

W.Y.O.S.6.

Smart composites with combined caloric and magnetoelectric effects

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Recently, the great scientific interest has focused on the design of smart materials, which exhibit large caloric effects (CE) combined with strong magnetoelectric (ME) coupling, for biomedicine and energy efficient technologies.

The two types of SMART composites with large magnetocaloric and ME effects around room temperature were fabricated, their structure, magnetic and ME properties were studied:

1) Layered composites, consisted from the layer of magnetocaloric alloy Fe₄₈Rh₅₂ with thicknesses of 50-150 nm, deposited on a ceramic piezoelectric substrate of lead zirconate– lead titanate PZT

2) Flexible polymeric composites FeRh / PVDF and GdGeSi / PVDF, consisting of magnetocaloric microparticles Fe₅₀Rh₅₀ and Gd₅Ge_{1.6}Si_{2.4} embedded into a piezopolymer matrix of poly(vinylidene fluoride) (PVDF) in mass ratios from 2 to 40%.

The technological conditions for fabrication bulk samples of Fe-Rh alloys and film composites based on them were developed to obtain samples with optimal magnetic characteristics for these materials and a sharper type of magnetic phase transition and the strong ME effect around magnetic phase transition were observed. The methodics for fabrication of flexible polymer magnetoelectric composites based on magnetocaloric microparticles were developed, their structure and basic physical characteristics were studied in detail. Preliminary experiments on samples with mass fractions of the magnetic phase of 2 and 12% observed the presence of a magnetoelectric interaction in the vicinity of the magnetic phase transition temperature of the magnetocaloric component of the composite, which can be used for further functionalization of “smart” composites.

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W.Y.O.S.7.

Temperature dependence of graphene transport coefficients

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General expressions for energy dependencies of transport coefficients are obtained by solving the Boltzmann transport equation. The paper presents their temperature dependencies in graphene. Coefficient of electrical conductivity, coefficient of electronic thermal conductivity, Zebek coefficient and Lorence function in graphene were analyzed. The expressions for all transport coefficients were found analytically in the low temperature range ~ 50 -100 K, and then presented graphically as well.

W.Y.O.S.8.

Control of structure and thermo-reversible gelation of networks with reversible covalent Diels-Adler crosslinks

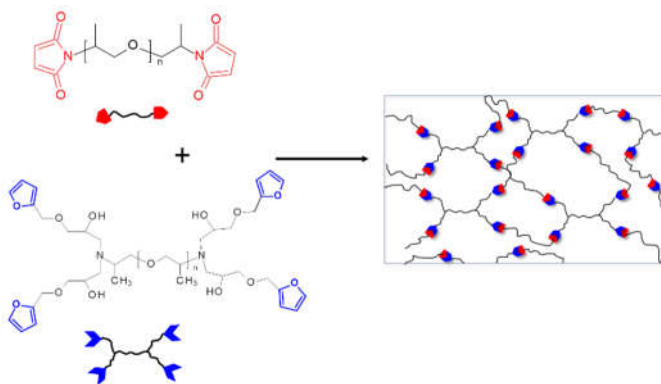
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The reversible Diels-Alder reaction is becoming an increasingly popular route for obtaining thermo-sensitive polymer networks, which could display self-healing or shape memory properties.

In this contribution, networks were investigated (see Scheme 1), which were based on different types of maleimides combined with furan-bearing macro-monomers. The latter were obtained by end-group-modification of Jeffamine D2000 with furan derivatives. The tested maleimide monomers exhibited different functionality and structure, including bifunctional and trifunctional, aliphatic-, aromatic-, as well as polyether-type. The structure of the bismaleimides was found to strongly affect the thermodynamics and kinetics of the Diels-Alder reaction. Hence, also the gelation process, the stability, crosslinking density, as well as the dynamics of the thermoreversible crosslinking were controlled by the structure of the maleimide monomers.

The best of the studied systems showed a good promise as self-healing materials.



Scheme 1. Chemical structures of multifunctional furan and maleimide compounds used for building-up self-healing polymeric materials.

Acknowledgement: The authors acknowledge the financial support of the Grant Agency of the Czech Republic (Project 17-13103S).

Y.O.S.II.1.

The structure and electrochemical properties of fayalite Fe_2SiO_4

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Fayalite has been found various applications in many fields. Here is presented its use as anode material for lithium ion batteries. The syntheses of Fe_2SiO_4 and its composite with carbon are conducted through solid-state reaction at 850 °C under inert atmosphere of argon, using cheap and abundant precursors ($\text{Fe}(\text{NO}_3)_3 \times 9\text{H}_2\text{O}$ and amorphous silica). Citric acid served as carbon source. The phase-purity of synthesized powders is checked by X-ray powder diffraction. The crystal structure of the powders is refined in orthorhombic Pbnm space group. Half-cell configuration, with lithium metal as counter electrode and fayalite as working electrode, is used for electrochemical measurements: galvanostatic cycling and electrochemical impedance spectroscopy.

Y.O.S.II.2.

Fabrication of graphene/Cu flexible electrode with excellent mechanical reliability and electrical performance

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Flexible electrode is an indispensable component of emerging portable, flexible and wearable electronic devices. Although various flexible electrodes with different dimensions and functions have been explored, developing a new electrode material with excellent mechanical reliability and superior electrical performance remains challenge. In this talk, we present a new graphene-covered Cu composite electrode film with a total thickness of ~100 nm, which was successfully fabricated onto a flexible polyimide substrate by means of a series of assembly methods including physical vapor deposition, chemical vapor deposition and transfer technique. The composite electrode film on the flexible substrate exhibits evidently enhanced tensile strength, monotonic bending and repeatedly bending fatigue reliability as well as electrical performance compared with that of the bared Cu electrode film. Such excellent mechanical performances were attributed to the role of the graphene coating in suppressing fatigue damage formation and preventing crack advance. It is expected that the synthesized graphene-covered Cu composite electrode would extend the potential ultrathin metal film electrode as the innovative electrode material for next-generation flexible electronic devices.

Y.O.S.II.3.

PLD growth of STO/PZT thin films on graphene oxide-buffered Si (001) surfaceZoran Jovanović^{1,2}, Urška Gabor¹, Elena Tchernychova³, Danilo Suvorov¹, Matjaž Spreitzer¹¹Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia; ²Laboratory of Physics, Vinča Institute of Nuclear Sciences, Belgrade, Serbia; ³National Institute of Chemistry, Ljubljana, Slovenia

Epitaxial integration of complex oxides with semiconductors is often limited by lattice mismatch between the two material systems and their dissimilar chemical properties. However, in case of 2D materials the strict requirements of traditional epitaxy can be alleviated by the weak van der Waals interactions. As a result, a 2D material, such as graphene, can allow remote epitaxial registry with a substrate at a long distances or act as a template by itself. In the present work, we investigated the potential of graphene oxide (GO) to act as a template for pulsed-laser deposition (PLD) growth of SrTiO₃ (STO) on Si(001)/SiO₂ surface. For this purpose, the GO was spin-coated on silicon surface to coverages of ~ 50 %, ~ 80 % and ~ 100 %, annealed in vacuum at 600 °C for 3h, after which STO was deposited in vacuum at 700 °C. The results revealed that GO can direct the growth of STO to a smooth, compact and pinhole-free layer, with mostly (001) out-of-plane orientation. When this was combined with SrO-assisted deoxidation of silicon surface, a partially epitaxial, highly crystalline STO film, with exclusively (001) out-of-plane orientation, was obtained. Thanks to high-quality, as-grown STO was used as a pseudo-substrate for piezoelectric integration Pb[Zr_{0.52}Ti_{0.48}]O₃ (PZT), that exerted properties comparable to ones obtained in more complex integration methods. Our results suggest that GO can be used as a template for integration of complex oxides with silicon in a way that is less demanding in terms on interface control and vacuum conditions, which are important advantages for development of large area PLD processes.

Y.O.S.II.4.

Deposition of nanocomposite organosilicon thin films under dusty plasma conditions

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During the past decades nanocomposite polymer coatings have attracted increasing attention because of their unique optical, mechanical, magnetic and optoelectronic properties arising from the combination of organic matrix and inorganic nanoparticles. Combinations of the attractive functionalities of both components at the nanolevel acquired from organic polymers and inorganic nanoparticles, are expected to exhibit synergistically improved material properties. Among the numerous nanocomposite preparation methods, the deposition under dusty plasma condition is one of the most attractive tools, which could be successfully applied in many industrial and technological applications, ranging from microelectronic industry to aerospace industry and biomedical applications. In the present work plasma-polymer nanocomposite thin films were prepared under dusty plasma conditions. Due to their nanocomposite structure, the films showed very interesting mechanical properties, for example high elastic recovery resulting in behaviour similar to superelasticity. Variation of the deposition conditions enabled to vary the surface composition and structure of the deposited films. The surface structure of the films influenced their surface free energy in a wide range, therefore it was possible to prepare films with hydrophilic as well as hydrophobic properties.

X-ray Photoelectron Spectroscopy (XPS), Fourier Transform Infrared Spectroscopy (FTIR) and Rutherford Backscattering Spectroscopy (RBS) combined with Elastic Recoil Detection Analysis (ERDA) were used to study the atomic composition and chemical structure of the films. The mechanical properties of the films were studied using nanoindentation technique and the surface structure was studied using atomic force microscopy.

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Y.O.S.II.5.

Photovoltaic perovskites for high sensitive X-ray detection

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$\text{CH}_3\text{NH}_3\text{PbI}_3$ is a perovskite material which has proven to be highly efficient in photovoltaics, and it has high potentials in other applications like light-emitting diodes, thermoelectrics, water splitting, magnetic memories, various detectors and else. It has turned out that not only visible light but all kinds of irradiations generate a high concentration of photoelectrons in this material, suitable for detection purposes.

Due to the strong impact of high energy photons on living matter, it is highly important to reduce the X-ray flux in medical imaging techniques, like X-ray computed tomography (CT) or else. We have developed a lithographically defined heterostructure, where the deposition of the perovskite on graphene substrate further amplifies the detection capabilities (going down to single photon sensitivity). Translating this observation to a viable device architecture (large scale production of X-ray detectors), Aerosol Jet Printing technology was applied, which gave excellent results: more than four orders of magnitude higher sensitivity than the best, commercially used α selenium detectors. The market potentials of this cheap, highly performant X-ray detector will also be presented.

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Y.O.S.II.6.

Effect of graphite reinforcements on the tribological properties of Al_2O_3 coatings deposited by plasma spraying

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Plasma spraying is an advanced surface engineering technology, which allows to deposit various materials including hard ceramic materials and composites. Al_2O_3 and its composite coatings are the most commonly used industrial-materials due to high hardness, good strength and toughness, excellent tribological properties etc. The addition of graphite into Al_2O_3 allows to create novel self-lubricating coatings with improved tribological properties.

Al_2O_3 and Al_2O_3 -graphite coatings were deposited on steel substrates by atmospheric plasma spraying. The plasma was created using air and hydrogen gas. The influence of graphite content and process parameters on the surface morphology, structure and tribological properties of the Al_2O_3 coatings were investigated. The surface morphology was determined by a scanning electron microscope. The elemental composition of the coatings was determined by energy dispersive X-ray spectroscopy. The roughness was measured using a Mitutoyo SurfTest-SJ-210-Ver2.00 profilometer. The structure of the coatings was analyzed by X-ray diffraction. Tribological properties were inspected using a CETR-UMT-2 ball-on-disc tribometer. The investigations indicated that the surface morphology and roughness for the alumina-composite coatings depended on the graphite content in the feedstock powders and the process parameters. It was obtained that the graphite reinforcements changed the structure and reduced the friction coefficient of the as-sprayed coatings. Meanwhile the wear rate was slightly reduced or remained unchanged.

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Y.O.S.II.7.

Optical and structural properties of tin oxide thin films doped with fluorine obtained by USP technique

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FTO films were deposited on glass substrates by ultrasonic spray pyrolysis technique (USP). These films are obtained using tin chloride pentahydrate SnCl_4 dissolved in ethanol to obtain SnO_2 , and a solution of ammonium fluoride NH_4F dissolved in deionized water H_2O_{DI} to dope it. The deposition is carried out at 450 °C with variation of time of 10, 12 and 14 minutes. The films thickness was obtained by profilometry technique. The applied deposition time allowed to control the increase in thickness of 300 nm between each sample, and this was possible due to the films are uniform and reproducible. The X-ray diffraction (XRD) showed the crystalline structure with a tetragonal rutile phase in the preference plane (211). The crystallite size slightly varies from 40 to 42 nm. The effect in the optical properties was analyzed by UV-visible spectroscopy (UV-Vis), the films have an optical transmittance in the visible range between 60 and 70 %. The average of energy band gap is around 3.88 eV. Using the effect Hall technique, electrical properties of the samples were studied. The minimum resistivity obtained was $6.5 \times 10^{-4} \Omega\text{cm}$ for a thickness of 800 nm which correspond to time deposited of 12 minutes. The highest conductivity was $1.5 \times 10^3 \text{ 1}/\Omega\text{cm}$ for a thickness of 800 to 1100 nm, with times of 12 and 14 minutes.

Y.O.S.II.8.

Photoluminescence enhancement of Dy³⁺-doped tellurite glasses through nanoparticle doping for solid-state lighting applicationsAli Erçin Ersundu, Orhan Kibrisli, Miray Çelikkilek Ersundu

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Dy³⁺ offers promising features for solid-state lighting applications owing to its narrow emission bands located at yellow and blue region of the visible spectrum. The proper combination of blue and yellow emissions from Dy³⁺ ions generates white light upon UV or blue excitation. The position of rare earth energy levels is identical for different host materials; however, the intensity of emissions dramatically changes with the phonon energy and the local crystal field of the host matrix. Among different host materials, tellurite glasses are considered as promising luminescent materials for solid-state lighting applications due to their relatively low phonon energy, high rare earth solubility, good non-linear optical properties, low scattering and absorption losses, high refractive index, good thermal and chemical stability. Recent studies have shown that Dy³⁺-doped tellurite glasses reveal promising features for solid-state lighting applications, but shielded f-f transitions of rare earth ions with low absorption and emission cross-sections requires additional improvement for better luminescence properties. It is well-known that doping of nanoparticles into glass matrix along with rare earth ions enhances luminescence properties due to nanoparticle-light interactions induced by the surface plasmon resonance. Therefore, in this study, the effect of nanoparticle doping (ZnSe and CdSe) on color properties and luminescence efficacy of Dy³⁺-doped tellurite glasses were investigated. Accordingly, conventional melt-quenching technique was used to synthesize glass samples and controlled heat-treatment procedures were applied for the growth of nanoparticles. For characterization studies, UV-Vis-NIR absorption, photoluminescence, X-Ray diffraction techniques were applied. Consequently, CIE color coordinates, lifetime values and J-O parameters were determined for the investigation of nanoparticle doping on luminescence enhancement of tellurite glasses for their use as solid-state lighting materials. The authors gratefully acknowledge The Scientific & Technological Research Council of Turkey (TUBITAK) for the financial support under the project numbered 117M206.

Y.O.S.II.9.

Point defect-enhanced optical and photoelectrochemical water splitting activity of nanostructured $\text{Zn}_{1-x}\text{Fe}_y\text{O}_{(1-x+1.5y)}$

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Even has been under study since 1935, zinc oxide (ZnO) based materials still attract a huge scientific attention. Owing to a wide band gap energy (3.37 eV at room temperature) and a large exciton binding energy (60 meV) ZnO has a variety of application, e.g. in electronics, optoelectronics, spintronics and photocatalysis. Besides, it has been shown that zinc oxide-based materials have a great potential as photoelectrocatalysts in the processes of water splitting, yielding an increased both photocurrent density and photoconversion efficiency. However, with a band gap energy of 3.37 eV, ZnO is restricted to absorb UV light only. This restriction can be overcome by modifying optical properties of zinc oxide particles. During the years different approaches have been applied to modify the visible light photocatalytic activity of ZnO materials, for example: (1) metal and nonmetal ion doping, (2) hydrogenation, (3) the incorporation of crystalline defects in the form of vacancies and interstitials, (4) the modification of particles morphology and surface topology, etc.

In this study we employed 3d metal ion substitution to improve visible light-driven photoactivity of zinc oxide particles. We investigated the influence of Fe concentration in $\text{Zn}_{1-x}\text{Fe}_y\text{O}_{(1-x+1.5y)}$ nanoparticles on crystal structure, textural, optical and photoelectrocatalytic properties. $\text{Zn}_{1-x}\text{Fe}_y\text{O}_{(1-x+1.5y)}$ nanoparticles with nominally 5, 10, 15 and 20 at.% of Fe ions were synthesized by microwave processing of a precipitate. The crystal structure and phase purity of the samples were investigated by X-ray diffraction, Raman and ATR-FTIR spectroscopy. Mössbauer spectroscopy was carried out to clarify the valence state of the iron ions in the ZnO crystal structure. Effects of the iron ions concentration on particles morphology and texture properties were observed with field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM) with elemental mapping, and nitrogen adsorption-desorption isotherm, respectively. The optical properties were studied using UV-Vis diffuse reflectance and photoluminescence (PL) spectroscopy. Photoelectrochemical activity of the $\text{Zn}_{1-x}\text{Fe}_y\text{O}_{(1-x+1.5y)}$ samples as anode material was evaluated by linear sweep voltammetry in Na_2SO_4 electrolyte; the oxygen evolution kinetics were determined and compared. In addition, a series of first principles calculations were performed to address the influence of the iron concentration on the electronic structure of $\text{Zn}_{1-x}\text{Fe}_y\text{O}_{(1-x+1.5y)}$ samples.

Y.O.S.II.10.

Development of new functional materials and 3D nanocomposites for applications in THz optics

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Significant interest to the development of materials for THz optics is observed what is demanded by the progress in THz communications and biophotonics. Polymers and crystalline media are used for making THz optics elements, however, existing THz materials characterized by significant dispersion of optical properties, high absorption, low refractive index and heat resistance.

A prospective approach for the development of THz optics materials we associate with use of nanostructured composite media, the optical properties of which could be tuned in relatively wide limits by changing their composition, porosity and 3D structure. Particularly, the monolithic blocks of porous alumina could be a promising material for the further design. The original laboratory technology of growing highly porous monolithic nanomaterials at the surface of liquid alloys Me-Al (Me = Hg, Ga, In, Bi...) has been progressively developing. Currently, highly porous monolithic blocks possessing 3D structure consisting of network of alumina nanofibrils ($\varnothing \sim 4-7$ nm) can be grown with the volume up to several liters. Annealing at the temperatures of 400 – 1700 °C allows to obtain materials with the density ~ 0.02 to ≤ 3 g/cm³ and open porosity from 99.3 to $\sim 25\%$. Annealing decreases the samples dimensions isotropically, but integrity and open porous 3D structure preserved.

Porous 3D structure allows to apply various methods of chemical modification in order to create new nanocomposites and hybrid structures. The simplest chemical modification made by filling the pores with liquid solutions of salts, polymers, colloids or suspensions. The solvents were removed after impregnation and nanoparticles precipitates inside. Nanocomposites Al₂O₃-TiO₂(or -ZrO₂ and -CeO₂) were obtained. Nanocomposite Al₂O₃-Ni was obtained by NiO nanoparticles reduction in hydrogen during annealing.

The chemical modification of the alumina nanocomposites with transition metal monophthalocyanates (MePc) and rare-earth sandwich complexes opens up new possibilities for creating functional hybrid 3D materials and heterostructures with nonlinear electrodynamic and optical characteristics.

Y.O.S.II.11.

Electron holography examination of FeSiB ribbons crystallized by using interference pulsed laser heating

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The magnetic nature of soft magnetic FeSiB ribbon after interference pulsed laser heating, using variable pulse energy and number of consecutive pulses, is investigated. Performed laser treatment succeeded in periodically distributed, crystallized micro-areas (dots), ~10 μm in diameter, in the remaining amorphous matrix. SEM, TEM and HRTEM observations indicate that pulsed laser interference heating involves structural transformations in the subsurface layer up to ~300 μm . Images of holography fringes carrying information about phase shift of electron wave interacting with a sample. The phase shift consists of contributions introduced by electric and magnetic fields. Certainly, in the laser crystallized FeSiB amorphous ribbon, the detailed distribution of lines of magnetic flux at a nanometer scale are visualized. In the absence of external magnetic field phase shift contours were parallel to the edge in the amorphous matrix, while $\alpha\text{-Fe}(\text{Si})$ crystallites involves visible shift of magnetic lines. Interestingly, phase shift contours, after switching on external magnetic field, drastically altered their configuration. It is clearly seen that external magnetic field, perpendicular to the sample surface, rotates the phase shift contours by almost 90 degrees in the surface plane of the sample. These and other results obtained for FeSiB alloy samples will be presented and discussed.

Y.O.S.II.12.

Acoustically tuned quantum light emission from atom-like defects in hexagonal boron nitride

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Owing to their unique mechanical, electronic and optical properties, two-dimensional semiconductors have recently emerged as the leading physical system for quantum photonics. Among these, monolayers, multilayers and crystals of hexagonal boron nitride (h-BN) have been shown to host robust, high-temperature and ultra-bright multicolor single photon emitters (SPEs), which are most likely originating from midgap vacancy-related localized defects [1,2]. Identifying the exact nature of SPEs still remains a challenge for any future practical applications of h-BN. Furthermore, on-chip solutions require deterministic SPEs that can be operated on-demand and with the possibility for in-situ control of the photon emission wavelength. To date, spectral tuning of the optical emission from h-BN has only been demonstrated experimentally over a few meV range by static strain. Here, we report on the dynamic control of SPEs in h-BN using radio frequency surface acoustic waves (SAWs). The SAWs are excited on the surface of a LiNbO₃ crystal equipped with an acoustic delay line, onto which flakes of multilayer h-BN were mechanically transferred. Luminescent intrinsic defects are identified using spatially, polarization- and time-resolved micro-photoluminescence spectroscopy. They exhibit a pronounced antibunching signature of single photon emission in the photon correlation experiments. The dynamic real-time control of the photon emission wavelength is demonstrated on individual defect-related radiative transitions whose emission energy, when subjected to the propagating SAW, is periodically modulated over a ~2 meV bandwidth by the acousto-mechanical coupling [3] at the acoustic frequency of ~330 MHz. The SAW-induced modulation is further combined with spectral detection filtering for temporal control of the emitted photons [3]. This study opens the door to the use of sound for scalable integration of h-BN emitters in nanophotonic and quantum information technologies.

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Y.O.S.II.13.

Mechanical properties of 1T-TaS₂

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Transition Metal Dichalcogenides (TMD), as exfoliable, layered materials are in the focus of basic and applied research because of their potential application in novel electronics. They are foreseen to be essential building block in artificial heterostructured materials, consisting of Graphene/TMD units. In such architectures, knowing their response to mechanical stress is very important. We have addressed this issue in archetypical charge density wave compound 1T-TaS₂.

The bulk crystals and ultrathin flakes of various thickness were investigated by three different methods: atomic force microscopy (AFM), nano-indentation and mechanical spectroscopy (vibrating reed). In the case of AFM measurements ultrathin, high quality membranes were exfoliated and transferred onto a substrate with prefabricated circular nanoholes. From AFM based method the average value of the in-plane Young's modulus of 236 GPa was obtained. For the large macroscopic samples the vibrating reed method gave 103 GPa presumably due to the shear forces between the layers. In addition, the weak interlayer coupling the indentation gave even lower apparent Young's modulus of 49 GPa and 63 GPa for indents normal and parallel to the layers, respectively. Our theoretical modelling gave a coherent description of the observations, including the effects of dislocations and point defects, as well.

Y.O.S.III.1.

Effects of annealing on the physical properties of various metallic oxides

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In this study, we analyze the effects of thermal annealing on the physical properties of indium tin oxide (ITO) thin films deposited by RF-magnetron sputtering. We discuss the induced changes by two types of thermal treatments, e.g. *in-situ* and *ex-situ*. The *in-situ* annealing consisted of the heating of the substrate during deposition at 100 °C, 200 °C, 300 °C, and 400 °C, while the *ex-situ* one was made using an oven, in air, at 200 °C, 300 °C and 400 °C, respectively. The X-ray diffraction investigations demonstrated that the *ex-situ* thermal treatment increased the number of oxygen vacancies and this led to an increase of electrical conductivity. All prepared samples have good transparency, larger than 75%, in the visible domain, and have a relatively smooth and uniform surface. Roughness average, root mean square roughness and Skewness parameter were calculated by atomic force microscopy and were discuss in terms of annealing conditions and temperature. For the purposes of comparison, the obtained results for pristine grown ITO thin films are given.

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Y.O.S.III.2.

Cryo-deformation by upsetting-extrusion: effect on microstructure and mechanical properties of CoCrFeMnNi high-entropy alloy

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Severe plastic deformation methods are widely used for effective control microstructure and properties of metallic materials. One of such methods is to use upsetting- extrusion (or extrusion - upsetting) processing, that can repeat many times (cyclically). This method was developed at National Science Center Kharkov Institute of Physics and Technology of NAS of Ukraine [1] and has proven its efficiency in preparing ultra-fine grain materials with unique physical and mechanical characteristics in laboratory conditions as well as in industrial conditions [1,2]. Note that the process of upsetting and extrusion is usually carried out at room or elevated temperatures. It is interesting to carry out this process at cryogenic temperatures, the deformation at which more intensive refine the grains [3].

CoCrFeMnNi high-entropy alloy (known as Cantor’s alloy) which exhibits remarkable ductility at cryogenic temperature was chosen as an object for performing such experiments. The initial billet of the alloy in the form of a cylinder with a diameter of 10 mm and a height of 20 mm was extruded by barocryodeforming [3] at 77 K by 22%, followed by upsetting by the same extent at 77 K. Such cycle was repeated twice, and samples for electron microscopic analysis and microhardness measurements were cut off perpendicular to cylinder axe after each pass. Features of formed microstructure were studied and a significant rise in hardness during upsetting – extrusion processing at cryo temperatures was found.

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Y.O.S.III.3.

Microstructure and mechanical property of solid–phase joints formed by EP975 superalloy and VKNA-25 type intermetallic alloys

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This paper is devoted to the study of the pressure welding (PW) and heat treatment (HT) influence on solid-phase joint (SPJ) formation of EP975 nickel-based (superalloy) with VKNA-25 type intermetallic Ni₃Al-based alloy. PW was performed in vacuum under EP975 high-temperature superplasticity conditions. HT included high-temperature heating to the single-phase region of the superalloy and subsequent aging. The SPJ strength was estimated by tensile testing at room temperature. It was established, that there was a visible interface between the materials joined. In the adjacent zone of SPJ on the side of EP975 visible changes in the structure were not detected. The structure of EP975 was grains of gamma and gamma-prime phases. The microstructure of the VKNA-25 side was intermediate between the structure of the original material and the raft structure which is usually formed in single crystals of nickel and intermetallic alloys. The energy-dispersive analysis results showed that after PW, a transition diffusion zone up to 40 microns thick is formed between dissimilar nickel alloys. After HT on the side of the superalloy, the microstructure became coarse-grained, with an average grain size of the γ -phase up to 150 microns. The γ' -phase of 150-500 nm appeared inside the gamma grains. VKNA-25 alloy retained its single-crystal structure. But in the zone adjacent to the joining zone, thickening of the gamma-phase interlayers increased to 500 nm. No embrittling intermetallic particles were found in the SPJ. The SPJ strength increased after HT and reached 0.9 of the intermetallic alloy strength. The investigation results show that pressure welding under the high-temperature superplasticity conditions of EP975 superalloy is an efficient method to obtain quality solid-phase joints of EP975 superalloy with intermetallic VKNA-25 alloy.

The work was supported by the Russian Science Foundation (Grant No. 18-19-00685)

Y.O.S.III.4.

Synthesis and catalytic properties of Co-Pt, Cu-Pd, Ni-Pt nanoalloys

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Platinum-based nanoalloys have a number of interesting physical and chemical properties due to the size effect. Mixing platinum metals with other transition elements allows to reduce the content of the noble metal in the alloy and modify the electronic structure of the active particles. Such materials have high catalytic activity, exhibit plasmon resonance, in some cases demonstrate outstanding magnetic properties. Therefore, the production of platinum metal nanoalloys is one of the important areas of research and development in the preparation of catalysts and new functional materials.

One of the ways to modify the properties of nanoalloys is the formation of an ordered superstructure in their crystal lattice. Thus, a number of works have shown that intermetallic compounds possess catalytic activity exceeding the activity of disordered alloyed particles.

The aim of the present work is to create methods for the preparation and testing of catalysts based on Cu-Pd, Ni-Pt, Co-Pt intermetallic nanoalloys, including on the surface of the active support. In this work, thermolysis of multicomponent precursors was used to obtain nanoalloys. Samples of catalysts were prepared, whose active centers are alloyed ordered and disordered particles. Their catalytic activity was tested in the oxygen reduction reaction (ORR), the reactions of decomposition of 1,2-dichloroethane and ethylene to produce carbon nanofibers. Impregnation of the carbon support (Vulcan XC-72) with the double complex salts $[\text{Co}(\text{H}_2\text{O})_6][\text{Pt}(\text{NO}_2)_4] \cdot 2\text{H}_2\text{O}$, $[\text{Ni}(\text{H}_2\text{O})_6][\text{Pt}(\text{NO}_2)_4] \cdot 2\text{H}_2\text{O}$ and further reductive thermolysis allowed to get supported CoPt/C and NiPt/C ordered nanoalloys which have electrochemical activity and stability comparable to commercial Pt/C (20%) in the ORR.

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Y.O.S.III.5.

Peculiarities of impurity effect on the oxygen adsorption on the $\text{Ti}_3\text{Al}(0001)$ and $\text{TiAl}(100)$ surfaces

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Titanium aluminides are considered as ones of the most promising high temperature structural materials for aero-engine components. They have good mechanical properties such as high specific strength and melting point, low density and stable moderate temperatures properties. However, the Ti_3Al and TiAl alloys are characterized by an insufficient high temperature corrosion resistance that limits their applications. Despite intensive experimental and theoretical studies over the past decades, these alloys remain attractive for researchers from both technological and fundamental point of view. It is known that the impurity segregation influences on the oxygen adsorption on the Ti-Al surfaces and also affects the oxidation kinetics. In order to obtain information about the initial stage of oxidation of the Ti-Al alloy surface at a microscopic level, the *ab-initio* methods within the density functional theory (DFT) are used. These methods allow to calculate the oxygen binding and adsorption energies for different positions on the alloy surface in dependence on its orientation and composition.

In present work the microscopic mechanisms of oxygen adsorption on the doped $\text{Ti}_3\text{Al}(0001)$ and $\text{TiAl}(100)$ surfaces is investigated by the projector augmented-wave method. It is shown that transition metal impurities occupying the Ti-sublattice lead to decrease of the O adsorption energy (E_{ads}) in the most preferred sites on surfaces of both alloys. The adsorption energy is increased by impurities of the beginning of $4d$ -period such as Y, Zr, Nb and Mo, if they occupy the Al-sublattice on the $\text{Ti}_3\text{Al}(0001)$ surface, while the impurities of the second half of $4d$ -period result in E_{ads} decreasing. At the same time, substitution of Al atom on the $\text{TiAl}(100)$ surface by almost all $4d$ impurities leads to increase of the oxygen adsorption energy. The dominant structural and electronic factors which are responsible for the change of the O adsorption energy are determined. The increase/decrease of the adsorption energy in the specific position is determined by competition of ionic and covalent contributions to oxygen binding energy as follows from analysis of electronic properties of systems under question.

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Y.O.S.III.6.

Screen-printed thin smooth nanostructured BaTiO₃ films for printed electronics

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Printed electronics is an all-encompassing field for production of electronic devices by printing on a variety of substrates. Printed electronics have become secure, flexible and cost-effective, all of which make it appealing to a broad range of industries. Despite its status as a fast-growing field, there are some challenges in printed electronics. Particularly, modern technologies of printed electronics for MLCC, SOFC, DSSC, electroanalytical sensors require developing of appropriate structures in form of thin layers with smooth interface. This problem can be solved by the development of a new technologies and modernization of traditional methods or by the development of new raw materials for printing. For example, using of nanopowders instead micron-sized particles allow to form dense homogeneous thin films by screen-printing method. During screen-printing, the functional material in the form of suspension of solid particles with suitable properties and morphology takes the appropriate configuration on the substrate. Such printing settings as squeegee load, squeegee speed and the snap-off distance determine the thickness and defectiveness of prints edges and can be controlled during printing process. However, pastes rheology plays a crucial role for production of high quality films because screen-printing involves tangential stress on the paste, the paste falling through the mesh and its recovery on a substrate. In the case understanding the physical-chemical features of interactions between polymer molecules and nanoparticles allow to develop a new foundation for the traditional lithographic processes of colloidal formation through designing the morphology of structural elements under directed flow for specific object and the formation processes.

Y.O.S.III.7.

Mechanism of topochemical conversion of $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ in SrTiO_3 nanoplates under hydrothermal conditions

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The topochemical conversion mechanism of $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ template plates in SrTiO_3 plates was studied under hydrothermal conditions. SrTiO_3 plates can be further used as a substrate for epitaxial growth of other MTiO_3 ($M = \text{Ba}, \text{Ca}$) perovskites and for the preparation of the composite plates which are expected to express enhanced piezoelectric, ferroelectric and photocatalytic properties. $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ template plates (side length: 1 μm , thickness: 70 nm) were synthesized in the molten salt of NaCl/KCl at 800 °C. X-ray diffractometry, energy-dispersive X-ray spectroscopy, electron microscopy (SEM, TEM, STEM) and differential scanning calorimetry analyses were performed to disclose the pathway and mechanism of the transformation. We observed that $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ templates are terminated by atomically flat layer of $[\text{Bi}_2\text{O}_2]^{2+}$. Moreover, $[\text{Bi}_2\text{O}_2]^{2+}$ and $[\text{Bi}_2\text{Ti}_3\text{O}_{10}]^{2-}$ layers are perfectly aligned throughout the whole plate and no defect is observed. The transformation starts at the edges of the $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ plate and continues laterally to the center of the plate. During the transformation, Sr^{2+} and Bi^{3+} ions exchange through „exchange channels” which are formed and disappears as the $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ is converted in SrTiO_3 . SrTiO_3 nucleates at many sites and as a result, SrTiO_3 mesocrystalline plates with the preserved shape of the template are formed. Negligible remains of bismuth are still present. Understanding this mechanism is important for preparation of other MTiO_3 ($M = \text{Ba}, \text{Ca}$) perovskite nano-plates using the same template and synthesis method.

Y.O.S.III.8.

Synthesis of anodic alumina membrane with defined pore diameters

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Porous anodic aluminum oxide membranes were fabricated by two step anodization of aluminum in 0.3M oxalic, 0.3M sulphuric and 0.17M orthophosphoric acid solutions. The parameters of oxide film such as: pore diameter, interpore distance, porosity, pore density can be fully controlled by operating conditions of anodization. Additional, the pore diameters and pore density can be controlled by chemical treatment (pore opening/widening process). The effect of anodizing conditions such as applied voltage, type of electrolyte and purity of the substrate on the rate of porous oxide growth were discussed. The obtained results were compared with theoretical predictions and data reported in the literature.

Y.O.S.III.9.

Mechanical behavior of nanocrystalline Ni-Mo layers processed by electrodeposition

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This research was undertaken to study the mechanical properties of nickel alloy thin films fabricated by electrodeposition. Ni-Mo layers with low (~0.4 at.%) and high (~5.3 at.%) Mo contents were processed by electrodeposition and then annealed by differential scanning calorimetry (DSC) to the characteristic temperatures. The influence of saccharin addition to the electrolyte bath on the mechanical behaviour of Ni layers with low and high Mo contents was also studied. The variation in hardness with increasing Mo content was compared with the values obtained for ultrafine-grained Ni-Mo alloys with similar compositions but processed by severe plastic deformation (SPD). It was found that the addition of Mo and saccharin enhanced the hardness in nickel alloy layers, however, no annealing-induced hardening effect could be observed, unlike SPD processed layers with similar composition. Moreover, along with hardness measurements, micropillar compression tests were performed to further probe the mechanical properties of the layers. For this purpose, uniaxial compression was applied on focused ion beam (FIB) manufactured micropillars with dimensions of $3\mu\text{m} \times 3\mu\text{m} \times 6\mu\text{m}$ on as-deposited layers with varying Mo and saccharine contents. The size effect in the micropillar compression experiments was negligible and therefore could be ignored. Finally, the results obtained by studying the mechanical behavior of the layers were correlated with the microstructural parameters including grain size and dislocation density determined from the previous study on the same specimens.

Y.O.S.III.10.

Prediction of the temper of hardening in the free and bounded bending of long-length, low-alloyed copper billets under high-cycle processing conditions

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At present, of the known technical approaches that provide noticeable hardening of lengthy blanks with a slight change in their cross section in the process of high-cycle processing, ECAP conforms are actively used. Despite the high efficiency of this method in the formation of the UFG structure and strengthening of the workpieces, there are a number of problems and aspects, mainly tribological, restraining the development of this method. As an alternative, improving manufacturability during hardening in conditions of continuous plastic processing of lengthy workpieces and a slight change in their cross section, the effect of deformation by bending around a rotating roller was investigated. The study was conducted using the software DEFORM 3D for the conditions of free and constrained alternating bending at 90 degrees with the analysis of the parameters of the stress-strain state.

It has been established that after 4 cycles of bending, the workpiece is rotated 90 degrees around the longitudinal axis before each successive cycle, the gradient character of the accumulated deformation is formed in the workpiece. The maximum values are noted in the surface layers of the workpiece, the minimum in the central region. The constrained bend reduces the level of tensile stresses on the surface, other things being equal. Free bending is most rational to use in conditions of small accumulations of deformation per treatment cycle, which in total provides for the accumulation of a high level of deformation at acceptable levels of tensile stresses. The obtained information allows forecasting the level of hardening of blanks with free and constrained bending of long-length low-alloyed copper blanks. Verification studies on the Cu-0.5% Cr alloy show good convergence of virtual studies.

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Y.O.S.III.11.

Development and characterization of carbon nanotube reinforced natural rubber composite for prosthetic foot application

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This research is motivated by the desire to develop low specific weight, high strength material that will compete favourably with existing foreign foot prosthetics in restoring quality of life to transtibial amputees in Africa. The study uses multi-walled carbon nanotube (MWCNT) reinforced natural rubber (NR) polymer nanocomposite (PNC) for prosthetic foot application because of its weight advantage coupled with manufacturing cost and affordability. The CNT was synthesised via catalytic chemical vapour deposition (CCVD) technique. The synthesised CNT was purified and functionalised by the dual actions of nitric acid and 1.2 mM sodium dodecylbenzene sulfonate to open up active sites for adhesion of constituent parts of the nanocomposite (NC) and homogeneous dispersion. The optimum reinforcement fraction was established at 3 wt percentage MWCNT. Characterization was carried out using Dynamic mechanical analysis (DMA) and thermal analysis (DTA). The characterised sample was used to produce anthropomorphic prosthetic foot using compression moulding technique. The field test conducted was assessed using modified revised Trinity Amputation and Prosthesis Experience Scale (TAPES-R). Results from gait score confirmed good compliance with international standard.

Y.O.S.III.12.

Effects of cooling rate during casting on the corrosion resistance of 6xxx aluminium alloy

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6xxx aluminium alloy, despite its good mechanical properties do undergo corrosion attack thereby reducing the lifespan of the alloy and increasing liability in its application. This study investigates the effects of cooling rate during casting process on microstructure, mechanical properties and corrosion behaviour of 6xxx aluminium alloy. Aluminium ingot was melted in a muffle furnace and cast into rods. The cooling rate was controlled by holding the moulds at different temperatures. Microstructural characteristics were examined by optical microscopy. Mechanical properties such as impact strength, hardness, and tensile strength were analysed using standard methods. Corrosion behaviour was evaluated by potentiodynamic polarization. It was found that increasing cooling rate resulted in a significant improvement in mechanical properties and corrosion resistance of the 6xxx alloy. The findings were explained in terms of microstructural refinement and chemical homogeneity of the alloy.

Y.O.S.IV.1.

Hemodialysis composite membranes with functionalized graphene

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Polymeric membranes are widely used for various biomedical applications like proteins concentration [1], osseointegration [2] or substitutes as technological solutions for various organs, like artificial lung – oxygenator [3] or artificial kidney – haemodialysis [4]. This work presents the principle for synthesis of a new generation of composite polymeric membranes with functionalized graphene for haemodialysis. Citric acid was covalent immobilized on graphene in order to increase the anticoagulant activity, to selectivity and specificity for removing targeted compounds for specific medical conditions associated with chronic renal disease. In the second stage of synthesis, functionalized and derivatized graphene are used for obtaining composite polymeric membranes with controlled porosity for hemodialysis. Fully structural and morphological characterization of synthesized materials is presented and hydrodynamic and separation properties. Also, haemotoxicity tests were performed in order to study and prove the non-cytotoxic character of synthesised membranes.

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Y.O.S.IV.2.

Supercritical CO₂ utilization in preparation of poorly soluble drugs solid dispersions

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Formulation of solid dispersions is one of the most feasible strategies for overcoming the poor drugs' solubility – one of the major issues affecting drug bioavailability and therapeutic outcomes. Since traditional methods used for preparation of solid dispersions often require usage of organic solvents, it is of great importance to seek for more environment-friendly methods. It has been demonstrated that supercritical (sc) CO₂ may be effectively utilized for dispersion of drugs into the suitable carrier (polymer), thus obtaining solid dispersions with the improved drug dissolution rate. The aim of the presented study was to investigate the potential of scCO₂ for preparation of poorly soluble antihypertensive drugs (carvedilol and valsartan) solid dispersions in the conventional pharmaceutical polymers (polyvinylpyrrolidone-PVP and hypromellose-HPMC). Prepared solid dispersions were characterized by scanning electron microscopy, differential scanning calorimetry and Fourier-transform infrared spectroscopy; their porosity and density were determined and drug dissolution rate was assessed and compared to the results obtained from solid dispersions prepared by the traditional solvent casting method. Selected samples were tested for their tableting properties as well. It has been demonstrated that scCO₂ may be successfully applied for preparation of carvedilol or valsartan solid dispersions with the improved drug dissolution rate. Further characterization revealed the nature of interactions between the drugs and selected polymers. Due to the low density (and high porosity), some of the prepared solid dispersions may be used for further development of the floating dosage forms. It has also been demonstrated that some of the prepared dispersions have excellent compressibility and compactibility, which is of great importance for further development of solid dosage forms. The obtained results provide framework for further development of environment-friendly methods in pharmaceutical development and production.

Financial support of this work from the Ministry of Education, Science and Technological Development of the Republic of Serbia (Projects TR 34007 and III 45017) is gratefully acknowledged.

Y.O.S.IV.3.

New agents for nitric oxide (NO) chemotherapy of bacterial infections

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This work presents first data on new-generation antibacterial prodrugs design based on structural analogues of natural nitric oxide donors, namely, low-molecular nitrosyl iron complexes of the “g= 2.03 family”.

Nitrosyl iron complexes with functional ligands, viz. thioanalogues of pyridine DNA bases, aliphatic thioamines, thioureas and thiotriazoles were synthesized and studied by physicochemical methods in the solid phase and in solutions. NO-donor activity of synthesized compounds and their polymer composites has been screened. The cytotoxicity of synthesized complexes was studied *in vitro* on Vero cell culture (African green monkey, kidney). Complexes with low cytotoxicity have been identified.

The antibacterial activity of synthesized NO donors has been studied on strains of gram-negative and gram-positive bacteria. Nitrosyl iron complexes of different structural types possess antibacterial activity comparable or superior to that of some known antibiotics. It has been established that the antibacterial effectiveness of the complexes is comparable, and in some cases exceeds the antibacterial effect of NO donors of other families (okothilol nitroxyl derivatives [1], sodium nitroprusside [2], furoxan derivatives [3], NONOats [4] and other). The effect of new NO donors on the formation of biofilms of gram-positive bacteria was studied too.

Toxicity and antibacterial efficacy of composites of synthesized water-soluble NO donors with polyvinylpyrrolidone (as a prototype of the dosage form) were experimentally established.

This approach aimed on antibacterial NO-generating tools application and creating of the technology of surface and bulk processing of medical materials has been proposed for the first time. The work has been performed with financial support from the RFBR (Grant No.17-03-00837)

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Y.O.S.IV.4.

Controllable release of oxaprozin from hydroxyapatite nano-particles

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Inflammatory response is an integral phase of bone healing, and is beneficial if acute and well controlled. However, if it progresses into a chronic state, it can exert an adverse influence on healing. Therefore, bone tissue engineering scaffolds should provide an integrated ability to control the inflammation. In this research, we investigated the possibility of nano-hydroxyapatite (HA) to bond, and deliver in a controlled manner, a non-steroidal anti-inflammatory drug – oxaprozin. HA was synthesized by hydrothermal method, while the adsorption was carried out by controlled mixing of HA with oxaprozin/ethanol solution. The adsorption was optimized by varying the concentration of the solution, temperature and time. FTIR, TG/DTG and SEM characterization confirmed the adsorption of oxaprozin on HA, while drug release experiment demonstrated favorable kinetics with over 2 days of continuous release, making the obtained powder suitable as a potential filler for biocomposites with anti-inflammatory properties, for bone defects treatment.

Y.O.S.IV.5.

Polysaccharide-coated polylactide microparticles with controlled surface structure

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Polylactide microparticles are widely proposed as biodegradable materials for tissue engineering in a form of injectable cell microcarriers or building blocks for 3D scaffold fabrication, which requires a profound control over its surface properties. This work was aimed at evaluation of possibility to control surface structure and morphology of the microparticles in a course of their fabrication via oil/water solvent evaporation technique by modification of emulsifiers in aqueous phase. Surface characteristics of polylactide microparticles were controlled by modification of (1) chemical structure of emulsifier in aqueous phase or (2) form of these emulsifiers, i.e. as macromolecular solutions or nanoparticles. In the frame of the first approach, a variety of chitosan's derivatives and graft-copolymers were used to stabilize oil/water emulsion during the microparticles fabrication process. As a function of hydrophilic-hydrophobic balance modified by variation of degree of substitution and degree of polymerization of grafted fragments, the microparticle's total yield, a mean size and size distribution could be controlled. Macromolecular emulsifier used for the microparticle stabilization could enrich a thin surface layer formed, while application of macromolecules in a form of nanoparticles allowed to fabricate core-shell microparticles via oil/water Pickering emulsion technique. Polysaccharide nanoparticles used for emulsion stabilization were prepared through bottom-up or top-down method to form polyelectrolyte nanoparticles or polysaccharide nanocrystals, respectively.

The reported study was funded by grant (MK-1974.2019.3) of the President of the Russian Federation (in a part of microparticle fabrication and optimization) and by RFBR (№18-29-17050) (in a part of synthesis of chitosan's derivatives and copolymers). The authors are grateful to Wallonie-Bruxelles International (WBI) for support of this Russia-Belgium collaboration.

Y.O.S.IV.6.

Hydroxyapatite/ β -tricalcium phosphate granules enriched with strontium induce improved bone regeneration in osteoporotic bone: comparison between 11 different bone conditions

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The aim of our study was to compare 11 different groups of bone samples obtained from rabbits' femoral neck, as it is the most common osteoporotic fracture in postmenopausal women. Methods: Study was composed of osteoporotic (n=36) and healthy (n=10) female rabbits. Osteoporotic bone defects (n=30) in femoral neck area were filled with hydroxyapatite 30% (HA) and tricalcium phosphate 70% (TCP), 5% Sr-enriched HA₃₀/TCP₇₀, HA₇₀/TCP₃₀, or Sr-HA₇₀/TCP₃₀ granules and were compared to intact leg (n=36), sham surgery (n=6) and healthy non-operated bone. Expression of osteoprotegerin (OPG), nuclear factor kappa beta 105 (NFkB-105), osteocalcin (OC), bone morphogenetic protein 2/4 (BMP-2/4), collagen I (Col-1 α), matrix metalloproteinase 2 (MMP-2), tissue inhibitor of matrix metalloproteinase 2 (TIMP-2), interleukin 1 (IL-1) and interleukin 10 (IL-10) was analyzed by histomorphometry, immunohistochemistry and evaluated semi quantitatively 12 weeks after surgery. Results: Our study showed that Sr-HA₇₀/TCP₃₀ induced higher expression of all above-mentioned factors compared to intact leg and even higher expression of OC, MMP-2 and NFkB-105 compared to Sr-HA₃₀/TCP₇₀. HA₇₀/TCP₃₀ induced higher level of NFkB-105 and IL-1 compared to HA₃₀/TCP₇₀. Sham group showed higher expression of only Col-1 α compared to operated leg. Conclusion: Sr-enriched biomaterials improve bone regeneration at molecular level in osteoporotic femoral neck bone and induced activity of the factors responsible for cellular activity, new bone formation, bone mineralization and extracellular matrix was higher than after pure ceramic, sham or even healthy rabbits.

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Y.O.S.IV.7.

Hydroxyapatite nano particles doped with Gd^{3+} , Yb^{3+}/Tm^{3+} and Eu^{3+} as lumino-magnetic multimodal contrast agents

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Hydroxyapatite (HAp) has been widely used as bone reconstruction materials due to their similarity to bone tissue. The improvement of HAp properties was achieved by doping its crystal lattice with different ions. Lanthanides, i.e. Rare Earth Elements (RE) are also suitable for doping HAp. The aim of the presented research was to investigate the possibility of creating lumino-magnetic particles of HAp doped with gadolinium (Gd^{3+}) ions and co-doped with ytterbium/thulium (Yb^{3+}/Tm^{3+}) or europium (Eu^{3+}) ions for potential use in multimodal imaging (MI).

Pure HAp ($Ca_5(PO_4)_3(OH)$), magnetic HAp:Gd ($Ca_{4.85}Gd_{0.15}(PO_4)_3(OH)$), and lumino-magnetic HAp:Gd/Yb/Tm ($Ca_{4.85}Gd_{0.03}Yb_{0.1}Tm_{0.02}(PO_4)_3(OH)$) and HAp:Gd/Eu ($Ca_{4.94}Gd_{0.02}Eu_{0.04}(PO_4)_3(OH)$) particles were synthesized using emulsification process and hydrothermal processing. All synthesized particles had an elongated shape and exhibited a paramagnetic behavior. Reduction of the unit cell volume as a result of replacement of Ca^{2+} ions by ions with a smaller ionic radius (Gd^{3+} , Yb^{3+} , Tm^{3+} , Eu^{3+}) confirmed by using XRD and Rietveld refined plots. The energy band gap values of the synthesized samples range from 4.93 to 3.18 eV and decrease in the following order: HAp:Gd > HAp:Gd/Eu > HAp:Gd/Yb/Tm. The results of photoluminescence emission spectra of HAp:Gd/Yb/Tm and HAp:Gd/Eu particles showed characteristic transitions of Tm^{3+} and Eu^{3+} , respectively.

Y.O.S.IV.8.

The effect of Ga-substitution on magneto-structural properties of cobalt ferrite nanoparticles

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In the last two decades cobalt ferrite (CoFe_2O_4 , CFO) has attracted considerable attention due to its potential applications in catalysis, energy, environment, and in particular, biomedicine. To further extend applicability and improve understanding of fundamental processes, the present work investigates the influence of heteroatoms on physicochemical properties of CFO. The partial substitution of Fe^{3+} ions with gallium ions (Ga^{3+}) has been proposed in order to tune the magnetic properties of solvothermally derived CFO nanoparticles ($\text{CoGa}_x\text{Fe}_{(2-x)}\text{O}_4$; $x=0, 0.1, 0.2, 0.3, 0.4$ and 0.5). The XRD measurements confirms the presence of pure cubic spinel phase in all samples. The obtained particles are sphere-like in shape with a mean diameter of $\sim 6 \pm 1$ nm extracted by TEM. The amount of adsorbed oleic acid on the surface of the nanoparticles was determined by TG analysis, while the presence of oleic acid on the surface of the nanoparticles and the nature of the bonding with the metal atoms on the surface of the NPs was confirmed by the FT-IR analysis. Also, a fingerprint region in FT-IR spectrum of metal–oxygen (Me–O, Me = Co, Fe, Ga) stretching modes of spinel ferrites was used to obtain information on the inorganic phase. By adding gallium in CFO structure the Me–O stretching mode of the tetrahedral sites moved towards higher values, indicating a gradual substitution of iron ions by gallium ones. Magnetic measurements at 5 K indicate that the insertion of Ga^{3+} ions within the inverse spinel structure leads to increase of the saturation magnetization and decrease of the magnetic anisotropy with respect to the non-substituted sample. Mössbauer spectra has been recorded at low temperature (10 K) under an intense magnetic field (8T) in order to study the influence of Ga content on the magnetic structure. These measurements evidenced the modification of inversion degree, with the content of iron in tetrahedral site decreasing with the increase of Ga content.

Y.O.S.IV.9.

Materials properties modification *via* nanotechnology approach

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Due to dramatic influence of the nanostructuration process on the basic physical-chemical parameters of the organic and inorganic materials, in the current paper the two aspects in this area will be discussed. The first approach is connected with the laser oriented deposition technique use in order to improve the spectra, refractive features, mechanical hardness and wetting angle of the optical inorganic structures such as LiF, KBr, Sc, Cu, ITO, etc. materials. The second approach will be connected with the doping process influence on the refractive and photoconductive characteristics of the organic materials. The comparative results will be shown for the liquid crystal materials and some doped polymer materials. Moreover, the dependence of the content of the nanoparticles on the wetting angle of the solid organic films surface will be shown. The mechanisms responsible for the dynamic properties improvement will be discussed.

Partially, the observed phenomena have been previously published in the papers [1-3].

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Y.O.S.V.1.

Solvent-free mechanochemical reactions of chitosan: a green chemistry approach

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A solvent-free method of synthesizing of chitosan derivatives via reactive twin-screw extrusion is described. This simple one-step procedure allows to produce chitosan, its salts of different acids, acyl, alkyl (including unsaturated substituents) derivatives, as well as amphiphilic copolymers. The mechanochemical organic reactions are currently receiving a great deal of interest. They have numerous advantages since are high-concentration reactions and proceed much more efficiently and faster than solution reactions in many cases. High conversion of chitosan functional groups can be achieved by variations of temperature, screw speed, and residence time. The technique is based on a variety of chemical and physical transformations of polymeric solids at conditions of plastic flow, which are realized by applying external mechanical energy. The main working elements of extruder screws perform compression and continuous shear deformation of the material. Solvent-free technique can be considered as one of the promising trends in modern chemistry of chitosan that provides a powerful means to promote new biological activities and to modify chitosan ability be processed into new materials. The obtained derivatives has been investigated as potential scaffolds for tissue engineering.

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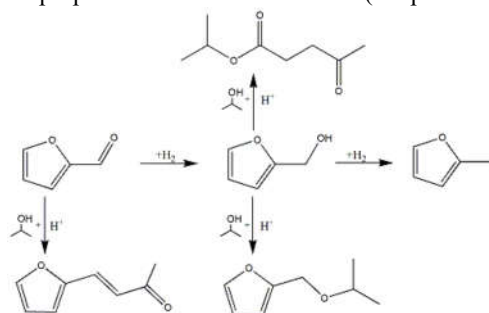
Y.O.S.V.2.

Characterization and application of molybdenum-oxides in liquid-phase hydrodeoxygenation of furfural

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Lignocellulosic biomass represents the most promising substitution for fossil energy in ever-demanding production of fuels and chemicals. Unlike petroleum, biomass is over-functionalized, mostly with oxygen, whose removal is essential for increasing the energy density. One of the possible routes is by hydrodeoxygenation (HDO) over molybdenum-oxide catalysts. Thorough characterization of active catalysts is of uttermost importance towards explaining the surface chemistry of chosen reaction system. This study had an aim of characterizing various molybdenum-oxide catalysts utilizing physisorption, chemisorption, DRIFT, SEM, TEM, EDX, XPS, XRD. Despite their relatively low specific surface areas ($2.0 \pm 0.9 \text{ m}^2 \text{ g}^{-1}$) compared to that of alumina-supported molybdenum ($192 \text{ m}^2 \text{ g}^{-1}$), various unsupported molybdenum(VI)- and molybdenum(IV)-oxides have shown to be active for liquid-phase HDO of 10% furfural in isopropanol under mild conditions (temperature below 225°C and H_2 pressure up to 50 bar).



reactions during the hydrotreatment of furfural.

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Based on GC-MS analyses (Shimadzu 2010 Ultra), a reaction pathway has been proposed and the data was utilized in mikrokinetic modelling. Results suggested hydrogenation reaction taking place without the catalyst while ring-opening to levulinic acid in presence of the catalyst. Results presented at the conference will show an influence of structural and textural properties of Mo-based catalysts on the activity and selectivity of hydrogenation, dehydroxylation, esterification and ring-opening

Y.O.S.V.3.

Zero waste recovery of mining and industrial waste

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Raw materials are vital for everyday life and crucial for development of innovative technologies which play a major role in the solutions for present challenges. Slovenian National Building and Civil Engineering Institute is a „core partner“ in the EIT Raw Materials initiative, which has the vision to develop raw materials into a major strength for Europe through supporting innovation, education and entrepreneurship over a versatile portfolio of funded projects.

Slovenian National Building and Civil Engineering Institute is coordinating and participating in several EIT Raw Materials projects, targeting the needs and challenges in the field of raw materials in the South East Europe region. The scope of the projects is on the circular economy principles and zero-waste paradigm in several types of waste materials, which are generated through industrial or mining/metallurgical activities and usually possess high threat for the ecosystem. Furthermore, the increasing costs of landfilling and strict environmental policies are urging the waste/tailings owners to seek for other possible solutions. On the other hand, these waste materials are a potential source of *Critical Raw Materials* with a high supply risk and could be extracted by innovative technological methods and the remaining material can be utilized in the construction industry.

Through several projects, these issues are addressed and solutions are properly presented in the pilot demonstrations. Projects are also oriented towards the establishment of network across the entire raw materials value chain, including all three sides of the knowledge triangle (education, research, industry), bringing good practices and supporting innovativeness in the South East Europe region.

Y.O.S.V.4.

Influence of the sintering temperature on the microstructure of belite-sulfoaluminate cement clinkersMartina Cvetković¹, Lea Žibret¹, Andrej Ipavec², Sabina Kramar¹¹Slovenian National Building and Civil Engineering Institute, Dimičeva ulica 12, SI-1000 Ljubljana, Slovenia; ²Salonit Anhovo d.d., Anhovo 1, SI-5210 Deskle, Slovenia

Cement clinker reactivity depends greatly on its phase compositions and microstructure, which can be controlled by changing the heating conditions during the clinkering process. In this study the influence of different heating regimes on the microstructure of belite-sulfoaluminate clinkers, a low-carbon and low-energy alternative to the ordinary Portland clinker, was explored. As an additional sustainable and green opportunity, different secondary waste raw materials were used in the clinker synthesis to substitute one part of natural raw materials. Three clinker mixtures consisting of (i) waste brick, (ii) waste concrete and (iii) the combination of waste brick and concrete, having two different targeted phase compositions (different proportions of the main phases - belite, ferrite and ye'elimite), were heated to three different sintering temperatures: 1200 °C, 1250 °C and 1300°C. The formed phases were studied using the X-ray powder diffraction and the Rietveld quantitative analysis, while the microstructure and morphology of the phases, as well as the incorporation of foreign ions in the main phases were characterized by the scanning electron microscopy with energy dispersive spectroscopy. Results showed that there was a slight difference in the phase composition between the cement clinkers depending on the secondary raw material used. For instance, the amount of belite in both mixtures with waste bricks was close to the targeted amount, whereas in the mixtures with waste concrete, the amount of belite was lower than targeted. Moreover, the samples with waste concrete also contained a considerably higher amount of the minor phase periclase with respect to the samples containing waste brick. There were also considerable differences in the microstructure between the mixtures depending on the sintering temperature, in the way that samples achieved better defined phases when they were heated to higher temperatures. When it comes to the secondary raw materials used, the difference in the microstructures was particularly noticeable with respect to the size and the shape of grains of the phases.

Y.O.S.V.5.

Dielectric loss factor of jute woven fabrics: effect of alkali treatment conditions

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In this investigation, the influence of alkali treatment conditions on the dielectric loss factor of jute woven fabric was studied. In that purpose, jute fabric has been alkali treated with NaOH solution (1%, 5% and 17.5%) at room temperature for different periods of time (5 min and 30 min). The jute woven fabric is a heterogeneous three-phase ("fiber-moisture-air") system, which implies the need for investigation of jute fabric chemical composition, moisture sorption, crystallinity index and structural parameters. The obtained results showed that with increasing the alkali treatment severity, the hemicelluloses content decreased for 14.4-43.3%. In addition, the alkali penetration induced fiber swelling and disrupting of the crystalline regions which result in a decreased crystallinity index. Hemicelluloses removal together with the decreased crystallinity index contributed to the higher availability of cellulose hydroxyl groups which in turns increases the moisture sorption values of alkali treated jute fabrics (for 7.2-21.0%) compared to the untreated fabric. With increasing the alkali treatment severity, the fabric thickness and fabric weight increased, while the fabric porosity decreased. All mentioned properties influence the dielectric loss factor, which is an important fabric parameter related to the ability of the fabric to dissipate electric energy or to convert the electric energy to heat. On such way, the obtained increase of the dielectric loss factor after the alkali treatments (for 2.5-9.2 times) can be attributed to the changes in the fabric structural characteristics and decrease in the content of hemicelluloses and crystallinity index, as well as the increased ability for moisture sorption.

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Y.O.S.V.6.

A novel type of building material derived from the by-products of steel making industry

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Electric arc furnace slag (EAFS) and electric arc furnace dust (EAFD) are the waste materials generated during the iron and steel scrap remelting in electric arc furnace. EAFS is non-hazardous material which has found its application in different field of civil engineering. On the other hand, EAFD is classified as hazardous materials due to the presence of heavy metals (Zn, Pb, Cu, Cr and Cd) and their potential leaching into environment.

Stabilization/solidification (S/S) of toxic waste is a widely investigated as simply method for production of stable product. Cement binder was mainly used for this purpose but important shift in the use of different waste materials as a cement replacement was observed.

The aim of this study was to investigate the possibility of S/S of heavy metals from EAFD using the alkali activated binders based on EAFS. The alkali activated slag with a different content of EAFS was synthesised and characterized using the SEM/EDS, XRD, FTIR. The binding of Zn into the reaction product of slag alkali activation was founded. The immobilization efficacy was evaluated using TCLP Method No. 1311 (USEPA) and EN 12457-2 (EULFD) leaching tests.

Y.O.S.V.7.

Comparative studies on electrodeposition of metals from gluconate solutions

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Electrodeposited cobalt and nickel, their alloys and composites are widely applied for various purposes ranging from magnetic films to corrosion protection coatings. Properties of the electroplated metals depend on the composition and pH of the bath, temperature, current/potential conditions. Various solutions were used for cobalt or nickel electrodeposition. Among them simple salt acidic baths are used most often, while complex salt solutions are usually environmentally friendly, show better buffering properties and enable to produce adherent and smooth coatings. The work reports comparative investigations of a new type of the electrolyte for the deposition of metals. The solutions contained sodium gluconate as a cheap and biologically safe additive, which can form soluble complexes with many metal cations in either acidic or alkaline baths. Presentation shows detailed characteristics of cobalt and nickel electrodeposition from weakly acidic gluconate solutions containing two types of anions: chloride or sulphate. It was shown that speciation of the solutions can affect the nucleation stage, electrochemical characteristics and morphology of the deposits, which, in turn, determine properties of the coatings. Cyclic voltammetry and potentiostatic measurements confirmed inhibition of the cathodic processes by free sulphate ions. Improved buffer capacity of gluconate baths in the presence of sulphate ions protected against contamination of the metal deposits by products of salt hydrolysis. Mathematical models of the metal nucleation were verified indicating progressive mode responsible for the formation of both metal phases. Diffusion coefficients of metal species were also determined using various approaches. Thickness, morphology, structure and cathodic current efficiencies of cobalt or nickel potentiostatic deposition were also discussed.

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Y.O.S.V.8.

Conditions of non-cryogenic brittle fracture of different starch grains under their mechanical treatment

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Recently, great interest has been shown in nanocrystalline starch (NCS), which is used in materials science for biodegradable polymers manufacturing, for producing NCS-based nanocomposites, for creating materials with water sensitivity and barrier properties. The source of NCS is a grain of natural starch, which, as well known, is an abundant bio-renewable resource and is extracted from various plants. Starch grains consist of alternating amorphous and crystalline regions, and the surface of the starch is always covered with a stable crystalline shell. NCS is extracted using acid or enzymatic hydrolysis and the extraction process takes from several hours to several days. The smaller the size of the nano-crystalline, the longer isolation from starch grain. Therefore, it is clear that the intensification of the NCS isolation process is on the front burner. Mechanical treatment is one of the most common methods to facilitate solid phase processes. In fact, pretreatment in mills accelerates the hydrolysis of starch several times. However, in the mills, the deformation of starch grains between the two faces occurs. Such processing is accompanied by plastic deformation of starch grains, which leads to a decrease in the yield of NCS. We have found that a free impact, which is realized in jet mills and disintegrators at a certain speed results in brittle destruction of starch with a characteristic glassy fracture surface. It is known, brittle fracture occurs with minimal plastic deformation and is not accompanied by heating of the material. As a result of the brittle crack, the crystalline phase of the grain is preserved and amorphous areas with higher reactivity are opened. It was shown that the crack of starch grain reveals threshold nature, which corresponds to the theory of the brittle destruction of Griffiths and depends on the moisture content of the grain and its origin. Thus, at a humidity of about 10%, corn starch grain is destroyed at an impact velocity of 100–120 m/s, which corresponds to a mechanical energy density of 0.8–1.0 J/cm³. The corresponding values for potato starch grain are 60–80 m/s and 0.3–0.5 J/cm³. The yield of fractured grains at these conditions is 20 – 25 %.

Y.O.S.V.9.

Heterogeneous enzymatic hydrolysis of non-cryogenic brittle fractured starchValeria Vasikhovskaya¹, Anatoly Politov^{1,2}¹Novosibirsk State University, Novosibirsk, Russia, ²Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia

On depending on their origin, grains of natural starch range in size from 2-8 microns (rice starch) to 250 microns (yam starch). It is believed that all grains of starch have a layered structure in which amorphous and crystalline layers alternate, and the crystalline layer is on the surface providing the relative chemical stability of starch grains to acid and enzymatic hydrolysis at temperatures of 30-40 °C. The study of the influence of various factors on the heterogeneous kinetics of the catalytic hydrolysis of starch at low temperatures is extremely important. This is due to the fact that at low temperatures starch digestion occurs in many living organisms and it is often necessary to control this process. On the other hand, at temperatures below the gelatinization temperature, nanocrystalline starch can be isolated, which is highly demanded in the production of various modern materials. In the present work, the effect of preliminary mechanical processing of potato starch on the kinetics of its subsequent enzymatic hydrolysis has been studied. It was shown that after both viscous and brittle destruction of starch grains, a multiple increase in the rate of enzymatic hydrolysis occurs at 40 °C. Thus, during hydrolysis by amylolytic enzymes, conversion of hydrolysis of brittle destroyed starch increases by 4-5 times in 4-6 hours compared to hydrolysis of native starch under the same conditions. It is found that the energy efficiency of brittle starch damage is several times higher than viscous damage. During the hydrolysis, attention was also paid to the mechanical denaturation of enzymes. Mechanisms of the observed phenomena are also proposed.

Y.O.S.V.10.

Making a curved part with LAMP technology using two synchronized robots, without using a physical mandrel

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Laser-Assisted Tape Placement (LAMP) technology is complex and dependent on a variety of conditions. It is carried out using a machine consisted of a robot with a mounted TTH head (Thermoplastic Tape Head), which contains a flexible compaction roller and a place for setting up of one thermoplastic prepreg spool with 25 mm width. This technology is most commonly used for tape placement on a physical mandrel for production of composite parts, but in this research instead a physical mandrel, another auxiliary robot is used as a support during the tape lay-up, which moves synchronized together with the first one.

For realization of this project, it is necessary to implement certain steps in order to achieve synchronized work of both robots. These initial steps consist of: physical connection of the two controllers, installation of Robo Team software, calibration of both robots in order to generate matrix of the relation between the two coordinate systems, replacement of the CNC with KRL code and template defining for the KRL code, adjustment of the KRL code and program design.

By performing all these initial preparations, the goal is to obtain correct and precise thermoplastic tape placement for manufacturing of a composite curved part, without using a physical surface pad.

Poster Presentation

P.S.A.1.

Physicochemical properties of cobalt ferrite nanoparticles synthesized by using linear surfactants and non-planar stereogenic-at-metal complexes

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In the overwhelming number of cases the synthesis of substituted cobalt ferrites is carried out using of the Co^{2+} precursor salts and the linear surfactants molecules. The most commonly used surface capping agents are oleic acid, citric acid, polyethylen glycole (PEG), polyvinylpyrrolidone (PVP), sucrose, dextran or other planar polysaccharides. In the general case the nucleation of nanoparticles (NP) in the presence of a surfactant takes place on a seed that is electrostatically (or, in other words, via an ionic bond) attached to a terminal charged group of a surfactant molecule. Thus, in the process of nucleation, we always have a multiple nucleation centers attached to the one surfactant molecule.

The present work investigates the physicochemical properties of cobalt ferrite nanoparticles formed on the seeds of Co ions, which are covalently bounded to the chiral complex with a propeller-shaped arrangement of the tridentate ligands structure around metal center. . This structure was obtained by the method of asymmetric synthesis and it serves simultaneously as the surfactant, center of nucleation (due to its electrostatic charge and) and precursor of Co ions. Thus, using this stereogenic-at-metal enantiomeric complexes as a “glue” for the formation of magnetic NP, we characterised the differences in the morphological and magnetic properties between cobalt ferrite samples synthesized without surfactants, using new non-planar complexes and usual used linear surfactants.

P.S.A.2.

Hall-Petch relation in harmonic structure designed Ni compactsHiroki Hino¹, Bhupndra Sharma², Mie Kawabata², Kei Ameyama²¹Graduate School of Science and Engineering, Ritsumeikan University; ²Faculty of Science and Engineering, Ritsumeikan University, Shiga, Japan

The Harmonic Structure (HS) is an attractive candidate materials design to achieve high strength and high ductility at the same time. Fig.1 demonstrates a general concept of the HS design. As opposed to the Homogeneous (Homo) ultra-fine grained (UFG) or coarse grained (CG) materials, the “HS” materials have a unique heterogeneous “Three-dimensionally (3D) Gradient Microstructure” wherein the UFG areas (“Shell”) form an interconnected 3D network surrounding the CG regions (“Core”), and Core and Shell areas are periodically arranged in all the directions. In the present study, the HS-Ni is fabricated by powder metallurgy route consisting of mechanical milling (MM) of Plasma Rotated Electrode Processed (PREP) pure-Ni powder and subsequent sintering by Spark Plasma Sintering (SPS). The plastic deformation at powder particle surface increases with increasing MM time. As a result, after sintering, shell fraction also increases in the HS-Ni. The relation between strength and grain size, i.e., Hall-Petch relation, of the HS-Ni is shown in Fig.2. An unusual Hall-Petch relationship was observed for HS-Ni, which is one of the anomalous deformation behavior of HS Ni. The HS-Ni indicates significantly large slope of “proof strength - $d^{-0.5}$ ” line as compared to the Homo-Ni samples. The grain size of HS-Ni is measured by total average grain size which includes Shell and Core areas. As can be seen, the results indicated in Fig.2 are presumably able to be understood not by the extra hardening, but by other microstructural factors.

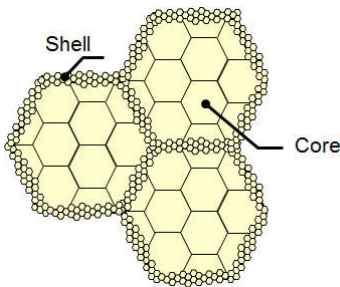


Fig. 1

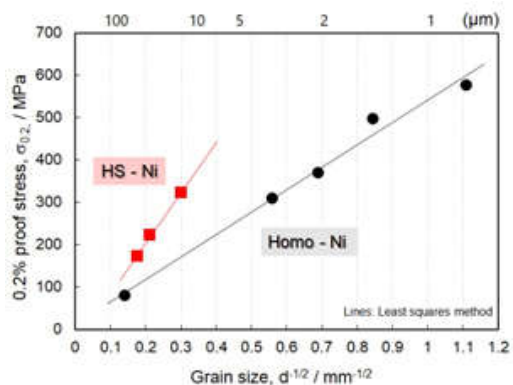


Fig. 2

P.S.A.3.

Preferential recrystallization by thermo-mechanical processing in pure titanium with harmonic structure

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The improvement in strength is usually accompanied by ductility loss, due to the plastic instability in the early stage of the deformation, in the structural materials, which is a long-standing conflict referred as the strength-ductility trade-off. Recently, a novel heterogeneous bimodal microstructure design called Harmonic Structure (HS), in which coarse grains (“Core”) are surrounded by continuously connected network of ultra-fine grains (“Shell”), has been introduced. The structural materials with HS microstructure exhibit improved mechanical properties as compared to the conventional homogeneous counterparts. In the present study, Thermo Mechanical Processing (TMP) is applied to harmonic structured commercially pure titanium (Ti-HS). The TMP process involves; cold-rolling (CR) of as-fabricated Ti-HS compacts from 10% to 30%, followed by annealing at the temperature of 873 K for 1.8 ks. The TMP processed HS-Ti exhibited higher tensile strength than the as-fabricated HS-Ti, without sacrificing in ductility (as shown in Fig.1). Fig.2 show EBSD image of TMP processed (10% CR + 873 K, 1.8 ks) HS-Ti. Remarkable is that both Shell fraction and mean grain size increases after TMP process. This strongly suggests that concentration of deformation was given mainly to the Shell region, and hence, it leads to a predominant recrystallization in the Shell. Our results demonstrate that the mechanical properties of HS designed titanium can be effectively improved by simple thermomechanical treatments. The proposed process of “HS+TMP” offers a design strategy towards a new generation of high-strength and high-ductility titanium based materials.

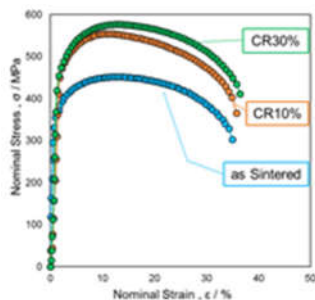


Fig.1 Tensile test of Harmonic structure and HS-TMP

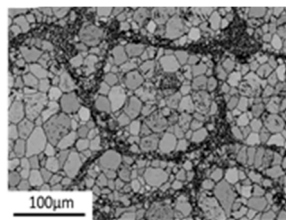


Fig.2 EBSD image of a HS-Ti after TMP.
(10%CR+873K, 1.8 ks)

P.S.A.4.

Microstructure and mechanical properties of harmonic structure designed Cu-9 at% Ge alloy

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In general, increasing strength by grain refinement leads to the poor ductility whereas improving ductility by increasing grain size leads to poor strength. Therefore, because of the strength-ductility trade-off problem, it remains a challenge to achieve a good combination of strength and ductility by varying grain size. In order to optimize the balance of coarse grains and fine grains in the microstructure matrix, a novel heterogeneous microstructure design process called "Harmonic Structure (HS)" has been introduced. The HS materials have a heterogeneous microstructure consisting of bimodal grain size together with a controlled and specific topological distribution of ultra-fine grains (UFG) area ("Shell") and coarse grains area ("Core"). The Harmonic Structured materials have the potential to be widely adopted for the various structural materials design with better mechanical properties than that of the similar materials with conventional homogeneous microstructures. In our previous studies, it has been shown that the HS materials exhibit a good combination of both high strength and high ductility compared to the homogeneous counterparts. However, the deformation behavior and relationship with stacking fault energy (SFE) in HS materials are not reported. Therefore, in this study, we applied the HS design to Cu-Ge alloy and investigate the relationship between the deformation mechanism and low SFE in harmonic structured Cu-Ge alloy. The HS Cu-9.0 at% Ge alloy was fabricated by pre-alloyed plasma rotating electrode process (PREP) powder of Cu-9.0 at% Ge alloy. Since Cu-9.0at% Ge alloy has lower SFE of 8 mJ/m² compared to that of pure-Cu of 55 mJ/m², the Cu-9.0at% Ge alloy powder is easier to be deformed in the surface region. In other words, compared to pure-Cu, the mechanical milling process is more efficient in the Cu-9.0at% Ge alloy powder. The microstructure and mechanical properties were analyzed by EBSD and tensile tests, respectively.

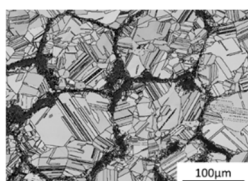


Fig. 1 EBSD Grain boundary and Band contrast Map of Cu-9.0at%Ge HS.

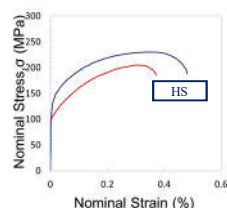


Fig. 2 Stress-strain curves of Homo and HS materials.

P.S.A.5.

Effect of UFG structure on mechanical properties in harmonic structure designed pure-NiTaiki Kambara¹, Masaya Nagata², Bhupendra Sharma³, Mie Kawabata³, Kei Ameyama³¹Graduate School of Science and Engineering Ritsumeikan University, Kusatsu/Shiga, Japan;²Japan Patent Office, Tokyo, Japan; ³Department of Mechanical Engineering Ritsumeikan University, Kusatsu/Shiga, Japan

Refining grain size in structural materials by Severe Plastic Deformation is an efficient way to increase strength, but it concurrently causes a reduction in ductility. One of the best solutions to solve this problem is the formation of a novel heterogeneous microstructure design called “Harmonic Structure” (HS). The HS materials consist of the islands of coarse grains (“Core”) surrounded by a continuous 3D network of ultra-fine grains (“Shell”). Such a unique arrangement of Coarse grains (CG) and ultra-fine grains (UFG) in the microstructure matrix can be achieved via a ‘powder metallurgy’ route allowing full control over different grain fraction along with their topological distribution. The HS materials exhibit superior mechanical properties as compared to the homogeneous (Homo) counterparts. However, the change in mechanical properties can be expected by a change in the fraction and distribution of CG and UFG areas in the matrix. Therefore, tailor-made mechanical properties, as per the requirement of applications, can be obtained for the HS materials. In the present research, we focused on the effect of UFG distribution on the mechanical properties of Pure-Ni. Fig.1 shows EBSD BC/GB images of Homo and HS Pure-Ni compacts. Fig.2 shows the stress-strain curve of Homo and HS Pure-Ni. The HS Pure-Ni demonstrates the higher 0.2% proof stress and higher strain hardening rate than that of the Homo pure-Ni. HS Pure-Ni shows higher ultimate tensile strength and large uniform elongation as compared to the Homo Pure-Ni. This strength-ductility synergy in HS Pure-Ni comes from high strain hardening rate and it delays the initiation of necking.

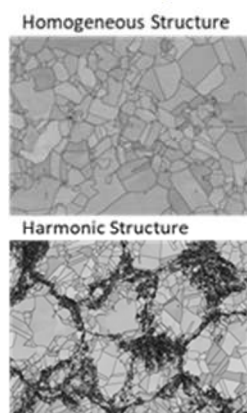


Fig. 1

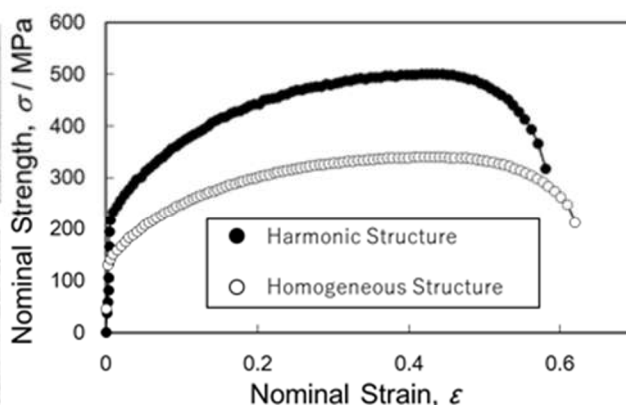


Fig. 2

P.S.A.6.

Harmonic structure design of Co-Cr-Mo alloy and its mechanical properties

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Over many years, ultra-fine grained (UFG) metals have been proved to be attractive structural materials because of superior strength, especially when compared to their coarse-grained (CG) counterparts. However, the downside of homogeneous UFG materials is typically in a low elongation because of the plastic instability in the early stage of deformation. Therefore, fabrication of materials with superior combinations of high strength and high elongation remains a hot issue in material engineering. The Harmonic Structure (HS) design can be a candidate materials design, which combines high strength with high ductility at the same time. Fig.1 demonstrates a concept of the HS design. As opposed to a “Homogeneous-UFG” material, “HS” material has a unique heterogeneous “Three-dimensionally (3D) Gradient Microstructure” wherein the UFG areas form an interconnected three-dimensional network surrounding CG regions, and CG and UFG areas are periodically arranged in all the directions. In the present study, the HS design was applied to a Co-Cr-Mo Alloy (CCM). The CCM is widely used as structural materials for biomedical applications, such as coronary stent, hip and knee replacements and dental implants, due to their excellent biocompatibility, wear resistance, corrosion and mechanical properties. Mechanical milling was used to produce ultra-fine grain region on the surface of powder by controlling the milling conditions, leading to bimodal structure in the milled powder. Subsequently, the MM bimodal powder was sintered by Spark Plasma Sintering (SPS). Sintered compacts of milled powder exhibited “Harmonic structure” and they demonstrated outstanding mechanical properties compared to Initial powder compacts. Thermo-mechanical processing is also applied to the CCM-HS compacts.

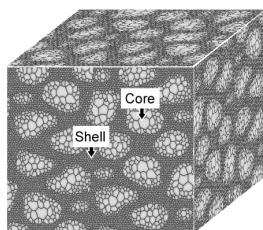


Fig.1 Concept of the HS Design

P.S.A.7.

Improvement of mechanical properties of harmonic structure SUS304L by thermo-mechanical process

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The Harmonic Structure (HS) has a heterogeneous microstructure consisting of bimodal grain size together with a controlled and specific topological distribution of ultra-fine grains (“Shell”) and coarse grains (“Core”). An increasing volume fraction of a Shell area leads to a higher strength without losing considerable ductility. The improved mechanical properties of HS materials is attributed to the continuously connected ultra-fine grain (UFG) “Shell”. It is assumed that the characteristic “micro-scale stress concentration” and “macro-scale stress dispersion”, by a network-type Shell structure, leads to a large work hardening and a constraint of the deformation localization. In the present work, the HS designed SUS304L austenitic stainless steel (HS-SUS304L) was prepared via a powder metallurgy process. The thermo-mechanical processing (cold rolling and annealing at 1173 K for 1.8 ks) has been applied to the as-fabricated HS-SUS304L. The thermo-mechanical processing (TMP) treatment to the HS-SUS304L material resulted in more developed Shell structure and a further improvement in mechanical properties. Fig.1 shows tensile test results of the HS and homogeneous (Homo) SUS304L after TMP. It is noteworthy that the TMP HS-SUS304L exhibited a superior combination of strength and ductility as compared to the Homo counterpart. Improvement of the mechanical properties via TMP is attributed to a strain-induced martensite transformation by the cold rolling and the reverse transformation to finer austenite grains by subsequent annealing. That is, even a slight cold rolling easily led to a martensite transformation because of the stress concentration to the Shell. Therefore, subsequent annealing resulted in an evolution of fine grain structure in the Shell region.

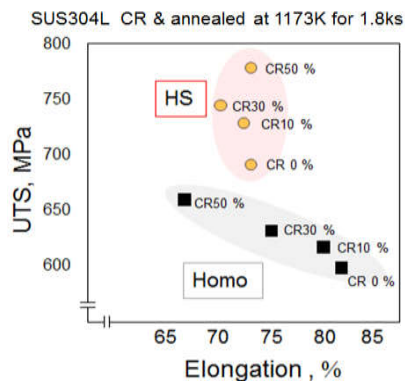


Fig.1 Tensile test results of the HS and homogeneous (Homo) SUS304L after TMP

P.S.A.8.

Plasma electrolysis oxidation using a pulsed unipolar power supply to improve electrochemical behavior of 316L austenitic steel

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The candidate materials for Generation IV nuclear power reactors include modified stainless steels as 316L in order to improve corrosion resistance in extreme conditions.

Ceramic-like aluminum oxide layers were developed on 316L austenitic steel by Plasma Electrolysis Oxidation (PEO) in aqueous solution of 30g/L NaAlO₂ using a pulsed unipolar power supply.

The necessary conditions (preliminary surface treatment, working parameters) for forming the barrier layer necessary to establish the microarc oxidation regime were determined.. The obtained layers were characterized by XPS, SEM, EDS, XRD analysis and electrochemical techniques (Electrochemical Impedance Spectroscopy, Tafel polarization curves).

The obtained results are compared with previous results obtained using a DC power supply [1].

[1] V.A.Andrei, E.Coaca, M.Mihalache, V.Malinovski, M.Patrascu-Minca, Surf.Interface Anal.2016, 48, 654-659

P.S.A.9.

Synthesis of titanium nitride via hybrid polymeric composites

Anca Dumitru¹, Sorina Ifimie¹, Anita Radu², Andreea Miron², Andrei Sarbu², Cristian Panaiotu¹,
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This study presents the developing of titanium nitride ceramic materials via hybrid polymeric composites starting from a synthesized porous inorganic structure. The hybrid polymeric composites were obtained by radical polymerization of a vinyl monomer in pre-synthesized porous TiO₂. In order to obtain TiN ceramic materials, the hybrid composites have been subsequently subjected to four-step thermal treatments at 290, 550, 1000 and 1400 °C, under nitrogen atmosphere. The thermal treatment at 290 °C and 550 °C involves the stabilization and thermal pyrolysis of polyacrylonitrile from the hybrid composite. The thermal treatment of hybrids at 1000 °C leads to the carbonization of polyacrylonitrile and the phase transition of TiO₂ from anatase to rutile. In the last step of the thermal treatment, TiN ceramic powder was obtained via carbothermal reaction at 1400 °C under nitrogen flow.

The synthesized hybrid polymeric composites were characterized using Fourier-Transform Infrared spectroscopy (FT-IR) and Thermal Gravimetric Analysis (TGA). The X-ray diffraction (XRD) proved the conversion of hybrid composites to TiN ceramic materials after carbothermal reaction.

Acknowledgements: This work was financially supported by *The Romanian National Authority for Scientific Research*, UEFISCDI, Project No. 40PCCDI/2018, Project Component no. 1-BIOTiN.

P.S.A.10.

Synthesis, structural modelling and functional properties of amorphous transition metal polysulfides

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Transition metal polysulfides are sulfur-rich inorganic compounds with layered or chain-type structures, such as TiS_3 , VS_4 , MoS_3 , etc. Among them, there are ones that exist only in the amorphous state (MoS_3 , MoS_5 , CrS_3 , etc.), which makes them interesting objects due to their developed surface, surface dichalcogenide groups (S-S), and significant numbers of unsaturated defect sites, that is important for catalytic and electrochemical processes.

We synthesize and perform a comparative analysis of the physico-chemical characteristics of transition metal polysulfides, including MoS_3 and MoS_5 . XRD, IR, TGA, XPS, ICP, and SEM data were complemented by DFT calculations revealing the causes of amorphization of these compounds, their globular morphology and non-stoichiometry. Finally, we demonstrate great promise of transition metal polysulfides as advanced electrode materials of Li-ion batteries with enhanced capacities and stable performance.

Acknowledgements: This work is supported by the Russian Foundation for Basic Research (Project #18-33-20006). E. D. G. is grateful to the President of Russia for the scholarship awarded (CII-140.2018.1).

P.S.A.11.

Application of high intensity ultrasound for obtaining magnesium hydroxide from seawater

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Magnesium hydroxide in nano sized forms is a very important chemical with good physical and chemical properties and it has wide application in the paper industry, production of refractory materials, as a catalyst, additive. Various methods have been developed to synthesize nano magnesium hydroxide but the precipitation crystallization method is the most economic one for industrial continuous production, having a simple process and low energy consumption. In this paper magnesium hydroxide has been obtained from seawater by a well-known industrial process. The process involves the chemical reaction between magnesium ions of seawater with dolomite lime to produce the magnesium hydroxide precipitate. The purpose of this paper was to modify the precipitate of magnesium hydroxide by ultrasound of high intensity. The purpose was to obtain magnesium hydroxide with high purity, and reduced particle size without agglomeration. High intensity ultrasound was used during the precipitation of magnesium hydroxide (80% precipitation) and after the drying process to eliminate the agglomerates. The precipitated magnesium hydroxide is characterized by the particle size distribution determined by the laser scattering method in the range of 20 nm to 200 nm, and by the SEM/EDS analysis. The contents of MgO and CaO in the samples of the magnesium hydroxide product (80% precipitation) were: 65.28 wt % MgO, and 2.07 wt % CaO. The EDS analysis confirmed the chemical composition of the samples. It has been observed from the SEM analysis that particles of magnesium hydroxide can easily aggregate during the drying process which was carried out in an air dryer at 40 °C / 10h. The particle size of magnesium hydroxide in agglomerates is in the range of 130-250 nm. In order to eliminate agglomerates, ultrasound was used for 20, 40 60, 140, and 160 s after the drying process. The optimum time of using high intensity ultrasound is 140 s because after that time no changes were observed in samples by measuring the particle size distribution. After that the size of magnesium hydroxide agglomerates was in the range from 3 to 6 µm. The application of the ultrasonic generator at the examined operating conditions in the precipitation process is sufficient to reduce the particle size of precipitated magnesium hydroxide but is not sufficient to reduce the agglomerates after drying process.

P.S.A.12.

Thin films for multilayer devices by tape casting method

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Creation of thin BaTiO₃ tapes always was a challenging goal because is the most efficient way to increase an MLCC capacity. The use of nanopowders as the basis for tapes is promising because it allows obtaining of films with low thickness and roughness close to the linear dimensions of one nanoparticle. It is a guarantee of improving the performance of multilayer devices without increasing their size, which is consistent with the tendency of miniaturization. Adaptation of high productive film formation method like tape casting to create layers of less than 1 μm is a promising and challenging goal.

The BaTiO₃ nanopowder was used to create tapes of dielectric layers and a mix of Ni/NiO powders was used for conductive layers. Tapes with the thickness from 5 μm to less than 1 μm were created by the tape casting method. The rheological behavior of all casting suspension was studied and casted tapes were characterized. Surface roughness comparable with the diameter of 1 particle was achieved. From obtained tapes, a few types of multi-layer composites with different layers thickness were assembled using isostatic lamination. Obtained multi-layer composites were successfully annealed and sintered without cracking or delamination.

P.S.A.13.

Investigation of ZrN-ZrB₂ composition synthesis by spark plasma sintering method

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ZrN-ZrB₂ composition can be used for the manufacture of parts of jet engines, armored plates, parts of hypersonic aircraft, cutting tools, crucibles, electrodes for plasma arc devices due to the fact, that its compounds have a number of unique properties.

The initial ZrH₂+BN mixture of powders was used for the purpose of synthesizing the ZrN-ZrB₂ composition containing 35 wt. % ZrB₂. Sintering was carried out using a pulsating current on the Dr. Sinter® 1050 arrangement in a vacuum of 10-60 Pa. There was no exposure at sintering temperatures of 900-1500 °C, the exposure was 3 min at 1600-1900 °C.

During sintering, gas evolution was observed in the interval of T=520-1500 °C. The first significant peak on the curve of the residual pressure in the chamber versus the sintering time was observed at 650-680 °C. This could be due to the decomposition of a partially hydrated B₂O₃ oxide layer located on the BN surface. This layer consisted of H₃BO₃ and decomposed by endothermic reactions. The presence of the second small peak at T=700 °C was associated with the start of the dehydrogenation process, which was also endothermic. The peaks in the power curve versus time, that accompanied the gas evolution peaks, confirmed the endothermicity of the above processes. During the heating to T=900 °C, dehydrogenation led to the transition of the ZrH₂ dihydride into hydride phases with a lower hydrogen content (ZrH_{1.66}, ZrH, ZrH_{1.801}), ZrB₂, ZrO_{0.35} and ZrC_{0.32}H_{1.20} phases formation. When heated to T=1100 °C, activation of carbon diffusion into the crystal lattice of hydrides occurred with an increase in the relative amount of zirconium carbohydride ZrC_{0.32}H_{1.20}, and dehydrogenation took place with a decrease in the hydrogen content in the sample. Dehydrogenation was accompanied by a small wide 3rd peak (T=1020-1030 °C) on the curve of the residual pressure in the chamber versus time. There was also the formation of ZrN and an increase in the relative amount of ZrO_{0.35}. When heated to T=1300 °C, zirconium carbohydride ZrC_{0.32}H_{1.20} decomposed, ZrC carbide was oxidized with residual oxygen, zirconium was reduced from ZrO_{0.35} oxide, further dehydrogenation and the formation of zirconium nitrohydride ZrN_{0.4}H_{1.10} occurred. At T=1100 °C, a sharp increase in the residual pressure in the chamber began due to the large amount of evolved gases. The maximum of the 4th largest peak was reached at T=1370-1380 °C. Heating to T=1500 °C led to the decomposition of zirconium nitrohydride with the formation of ZrN. As a result, ZrN+ZrB₂ composition was formed with a small residual impurity of the original boron nitride. Sintering at T=1600-1700 °C with a holding time of 3 min did not completely eliminate the residual BN. An increase of temperature to 1800-1900 °C led to the obtaining of the composition without impurities.

P.S.A.14.

Synthesis, crystal structures and magnetic properties of mono and dinuclear Cu(II) complexes with the condensation product of 2-acetylpyridine and Girard's T reagent

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The ligand (**HLCI**), (*E*)-*N,N,N*-trimethyl-2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl)ethan-1-aminium-chloride, was obtained in the condensation reaction of 2-acetylpyridine and Girard's T reagent. In the reaction of the ligand **HLCI** with Cu(ClO₄)₂·6H₂O in a 1 : 1 molar ratio in methanol, mononuclear Cu(II) complex (**1**), with the composition [CuLCl]ClO₄, was obtained. The square-planar complex cation consists of a Cu(II) center coordinated with the NNO donor set of the tridentate zwitterionic hydrazone ligand and the Cl⁻ ion at the fourth coordination site.

Reaction of **HLCI** with Cu(ClO₄)₂·6H₂O and NaN₃ in a 1 : 1 : 3 molar ratio, in a mixture of methanol/water, gives dinuclear double end-on azido bridged Cu(II) complex (**2**), with composition [Cu₂L₂(μ_{-1,1}-N₃)₂](ClO₄)₂. In the dinuclear complex, each Cu(II) centre is coordinated to pyridine nitrogen, azomethine nitrogen and carbonyl oxygen atoms from the deprotonated hydrazone ligand, and two N atoms belonging to two bridging azido ligands.

Magnetic measurements for dinuclear Cu(II) complex showed intra-dimer ferromagnetic coupling between Cu(II) ions ($J = 7.4 \text{ cm}^{-1}$).

P.S.A.15.

Development of sugarcane bagasse reinforced onibode clay composite for high voltage insulation

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In this study, sugarcane bagasse (SCB) reinforced Onibode clay composite suitable for high voltage insulation was developed via slip casting technique. Clay samples from Onibode, Ogun state, Nigeria was collected at depth of 5 meters beneath the earth surface. Sugarcane bagasse was collected from a local market in Alaba-rago, Nigeria. Onibode clay – sugarcane bagasse composite samples were developed from a mixture of fine clay particles ($<150\ \mu\text{m}$) and SCB reinforcement particles (fine - $<150\ \mu\text{m}$; coarse – $300\ \mu\text{m}$) of 0 – 6 %wt with a constant 53 %wt moisture and five drops of sodium silicate. The samples were fired at a temperature of $1150\ ^\circ\text{C}$ and held for 1 hour. Properties such as thermal conductivity, linear shrinkage, bulk density, and apparent porosity of the samples were evaluated. Results show that sample with a fired shrinkage of 4.03%, apparent porosity of 31.22%, bulk density of 1.73g/cm^3 and thermal conductivity of $0.0143\ \text{W/mK}$ possessed the optimum refractory properties suitable for high voltage insulation.

P.S.B.1.

Cost effective alloys based catalysts for alkaline fuel cells application

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Alkaline fuel cells (AFCs) have recently become attractive as environmental friendly future power sources. It was really important having in mind that in alkaline media less expensive non noble catalysts could be used. Namely, successful alkaline anion exchange membrane development enabled benefits of faster kinetics of oxygen reduction reaction in alkaline solutions.

In this study electrodeposited silver-palladium alloys of various composition were investigated and tested as the prospective catalysts for direct ethanol fuel cells application. All samples were characterized by scanning electron microscopy, energy dispersive spectroscopy, X-ray photoelectron spectroscopy, as well as by electrochemical techniques: cyclic voltammetry, polarization measurements at rotating disc electrode. The electrochemical active surface area was determined from the charge values corresponding to the reduction of Pd (II) oxide, assuming 420 μC for full oxide monolayer coverage. The optimal alloy composition showing the best catalytic activity for oxygen reduction and ethanol oxidation, with as much as possible lower content of Pd, was determined. It was found that it could be possible to obtain alloys containing only $\sim 20\%$ of more noble metal – palladium, showing high activity for both anode and cathode reaction. The stability testing gave very promising results, as well.

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P.S.B.2.

Polyanionic cathode material $\text{Na}_4\text{Fe}_3(\text{PO}_4)_2\text{P}_2\text{O}_7/\text{C}$ for aqueous sodium-ion batteries

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Sodium-ion batteries can be a promising power sources for large-scale energy storage systems, due to the huge availability of sodium and its low price. Different mixed polyanionic phosphates with 3D framework have the potential to be promising and low cost cathode materials for sodium-ion batteries. For the first time, the iron-based mixed polyanionic nanocomposite of $\text{Na}_4\text{Fe}_3(\text{PO}_4)_2\text{P}_2\text{O}_7/\text{C}$ was synthesized through a simple and fast sol-gel process, which starts from the divalent salt of iron and citric acid, followed by a heat treatment at 500 °C under Ar/5% H_2 atmosphere. During the synthesis the sucrose was added as an additional source of carbon. The structure of the synthesized powder was indentified by X-ray diffraction and the presence of another phase $\text{Na}_2\text{FeP}_2\text{O}_7$ was noticed. Infrared and Raman spectroscopy were used to further characterize the structure of the material. Thermogravimetric analysis revealed the total carbon content of ~20 wt. %, of which ~6 wt. % originates from sucrose. Its addition significantly increased the value of specific capacity. The capacity and rate capability of $\text{Na}_4\text{Fe}_3(\text{PO}_4)_2\text{P}_2\text{O}_7/\text{C}$ nanocomposite were investigated by cyclic voltammetry and chronopotentiometry. The ability of this material to intercalate/deintercalate sodium ions in 6M NaNO_3 aqueous solution was demonstrated. The high specific capacity of 90.17 mAh g^{-1} was measured at a 1.25 A g^{-1} (9.68 C) using galvanostatic method.

P.S.B.3.

Thermolysis prepared Co_3O_4 carbon paste electrode decorated with single wall nanotubes as voltammetric sensor for determination of antioxidant α -lipoic acid

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The novel carbon material modified with Co_3O_4 particles, prepared by calcination and mixed with single wall carbon nanotubes, was characterized and used for sensing of prominent antioxidant α -lipoic acid (LA). The new material was prepared by thermolysis of Novolac phenol-formaldehyde resin and cobalt(III) nitrate mixed with graphite powder, producing mostly glassy carbon decorated with cobalt oxide. XRD and SEM measurements were used to study composition, structure and morphology of cobalt oxide modified carbon material. Impedance spectroscopy measurements indicate higher conductivity of thermolysis prepared Co_3O_4 carbon paste electrode with single wall carbon nanotubes (TPC Co_3O_4 CPE/SWCNT) compare to material without nanotubes (TPC Co_3O_4 CPE), while the best voltammetric response of LA was also recorded at TPC Co_3O_4 CPE/SWCNT. In order to find optimal conditions and investigate electrode process, effect of Co content in electrode material, influence of pH and scan rate were studied. The quantification of α -lipoic acid was done by sensitive square-wave voltammetric technique (SWV). Under the optimized SWV parameters, in Britton Robinson buffer solution at pH 6, the linear range was recorded from 2 to 100 μM of LA. TPC Co_3O_4 CPE/SWCNT electrode exhibits good stability and reputability, too. This new combination of carbon materials, partially self-made, with incorporated Co oxide particles, could be interesting platform for determination of α -lipoic acid in dietary supplements and pharmaceutical formulations, with sensitivity and selectivity comparable and even better than determinations of this analyte at commercially available carbon electrodes and reported modified electrodes.

P.S.B.4.

Special application possibilities of metakaolin based geopolymer foams

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Nowadays one of the biggest problems is the global climate change, the main cause of which is greenhouse gases emission. One of the biggest emitters of CO₂ is the cement industry. The raw material demand for cement production is enormous. It is no coincidence that today several research aimed at the production of non-cement based binders. These new binders are collectively called geopolymers or alkali activated inorganic polymers (AAIPs). Besides that AAIPs can be used to replace cement-based traditional binders due to their high strength, these materials can also easily be well foamed. These foams are eco-friendly porous materials, which have good mechanical and chemical stability, high temperature resistance, etc. The foams with sufficiently high open porosity (~ 70 vol %) and adequate strength (>1.5 MPa) can be used as catalyst supports for photocatalytic sewage treatment processes.

The aim of this work was to investigate the photochemical activity of metakaolin based geopolymer foams. These foams were produced by gelcasting/saponification/peroxide decomposition (GSP) combined method using sunflower oil as surfactant and H₂O₂ as foaming agent. The organic matter content of the samples is a major problem, which can be reduced by the reduction of oil content and by calcining the specimen with appropriate firing parameters. The changes in curing temperature and treatment time have critical influence on the cracking tendency, especially in the early-stage of geopolymerization reaction. The produced crack-free foams can be used either alone or as catalyst supports in photochemical decomposition processes. The UV resistance of organic matter free samples were investigated. Results show that the foams have different photochemical activity. The reason for this phenomenon may be that the temperature distribution in the furnace space is not uniform during the firing of the samples. Experiments show that the pore structure formed by GSP combined method is sensitive to temperature changes. Furthermore the relationship between photochemical activity and structure was investigated, using XRD, FT-IR, SEM and NMR. Samples that are not photochemically active can be used as catalyst supports, if TiO₂ is immobilized on their surface.

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P.S.B.5.

Ultra-fast volume-responsive temperature- and pH-sensitive poly(N-isopropylacrylamide) hydrogels

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Dually Temperature- and pH-sensitive super-porous hybrid nanocomposite hydrogels based on poly(N-isopropylacrylamide)/nano-SiO₂ were prepared and characterized, which might be of interest for actuator applications. The gels display a very fast volume response to both stimuli, namely in the 10s range to Temperature (symmetric response) and 10 min / 200 min (slower re-swelling) to pH. The pH-responsiveness of the gels was achieved by incorporating sodium metacrylate (SMA) as co-monomer, in the amount of several mol%. The interconnecting super-porosity, which enabled fast volume response to stimuli, was obtained via conducting the synthesis as cryo-polymerization. The ultra-fast and symmetric response to Temperature as well as the mechanical strength of the gels was achieved by incorporating 8 wt.% of nano-SiO₂ (approximately spherical particles sized ca. 10 nm) generated in-situ via hydrolysis/condensation of tetramethoxysilane during the polymerization. This nano-reinforcement is resistant against dissolution in acidic and neutral solution, which was the operating environment of the studied gels (the pH-induced volume change occurs near pH = 4). The amplitude of the Temperature- and pH-responsiveness was varied in a wide range by changing the amount of incorporated SMA co-monomer. For best dual responsiveness, SMA-contents in the range of 3–5 mol% were found to be optimal. The difference in the rate of response to pH- and T-stimuli appears to be a result of ionic effects (diffusion of the pH stimulus) and did not depend on the SMA amount.

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P.S.B.6.

X-ray spectra, electron structure and physical properties of the Ce_2ScSi_2 and CeScSi compounds

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Energy structure of the valence band of the Ce_2ScSi_2 and CeScSi compounds was studied by the methods of the high-energy spectroscopy (XPS, XES and XAS). Dependence of magnetic susceptibility $\chi(\mathbf{T})$ of the Ce_2ScSi_2 compound within wide temperature range corresponds to the Curie-Weiss law. Based upon temperature dependences $\chi(\mathbf{T})$ and $\alpha(\mathbf{T})$, together with calculated valence of Ce by the data of the absorption L_{III} –spectroscopy, a conclusion has been made on the existence of the fluctuating transition, «State of intermediate valence - Condo-systems", in the Ce_2ScSi_2 compound. The calculations of electron energy bands $E(k)$ and partial DOS for Ce_2ScSi_2 and CeScSi compounds were performed by the semi relativistic linear muffin-tin orbital method without considerations of spin-orbit interactions A satisfactory agreement between theoretical and experimental data is achieved.

P.S.B.7.

Theory and experiment - Slowing probe and conjugate pulses in potassium vapor using Four Wave Mixing

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We used four-way mixing (FWM) phenomena to slow light pulses in hot potassium vapor. The atomic scheme for FWM was off-resonant double-Lambda scheme that was previously used to study slow light in Rb [1] and Na vapors [2]. At high atom density and strong pump laser power, this atomic system is a parametric amplifier which generates probe and conjugate photons with gain. The goal of this work was to find how fractional delays and pulse broadenings obtained in K vapor compare with those obtained in other alkali vapors.

We measured and calculated fractional delays and pulse broadening of probe and conjugate for different gas densities, different pump one photon detuning, and two photon Raman detuning. In the experiment phase matching was established at the small angle between probe and pump at the entrance. Probe and conjugate waveforms are detected and placed on the time scale whose zero corresponds to the maximum of the reference pulse. Theoretically we calculated waveforms of transmitted probe and conjugate by solving optical Bloch-Maxwell equations for the four-level system.

We present fractional delays and broadening, and gains of probe and conjugate, as a function of two photon detuning for incident probe pulse between 20 and 120 ns, at K densities between 10^{11} and 10^{12} cm⁻³, for several values of one photon (pump) detuning. Parameters for optimum results will be discussed and will be compared to those reported for Rb and Na.

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P.S.B.8.

Cup anemometer friction torque and classification according IEC standard

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The cup anemometer operational uncertainty is defined in the new IEC standard 61400-12-1: 2017. In this standard, the cup anemometers are classified in four classes of local terrain and climate conditions according the range of changes of influence parameters: the air temperature, air density, air flow inclination angle and turbulence. The anemometer transfer function is determined from wind tunnel calibration in stationary state and at well defined conditions and gives a linear relation between the horizontal wind speed and the anemometer rotor rotation frequency. Since cup anemometers operate at the open field conditions which differ strongly from the wind tunnel calibration environment, the recorded wind speed deviates from the actual value. The classification procedure includes computer simulation that results in determination of the classification index k which is used to calculate the anemometer operation uncertainty. The simulation is based on the dynamic balance of the resulting aerodynamic, friction and output signal conversion system torques. We analyzed the existing data of several commercial cup anemometers and found that the friction torque is dependent on the inclination angle and that the anemometer inclination angle characteristic depends on the temperature. These relations are not included in the simulation model used for an anemometer classification. The cup anemometers are intended for long term measurements at open field including cold climate regions so that the wear at shaft-bearing contact is also important. We concluded that the challenges of revised IEC standard application are the modification of the theoretical model, development of new laboratory tests necessary for modelling the cup anemometer operation and improvement of the instrument tribology characteristics.

P.S.B.9.

Laser welding of similar materials

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The work presents laser welding of materials in such configurations: steel – steel (X8CrNi19-11). The system is of interest because such welding is beneficial in improving surface related properties, joining of different materials which will be applied in modern power boilers industry. The paper describes the microstructure and properties (phase and chemical composition, microhardness, corrosion resistance) of the laser welded parts used in the form eg. pipes. Depending on the proces parameters (such as: pipe rotation speed, laser energy density, focusing of the laser beam) the joint were with or without welding incompatibilities. Two zones are generated in the processed material due to the process: fusion zone and a heat-affected zone. Due to solidification, in the area of weld face and weld axis Cr, Mn, Nb rich paricipates were analysed. Examination of the chemical composition of cross-sections of joints showed homogeneous distribution of the alloying element. Crystallisation of the welded joints, in the case of X8CrNi19-11 steel, showed the increasing of the hardness of the fused zone (about 150 HV1), in heat affected zone 181 HV1 and base material about 191 HV1.

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P.S.B.10.

Corrosion resistance of high Al and MgSi Zinc alloys for batch hot dip galvanizing

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The corrosion resistance of hot dip galvanizing coatings is determined by their thickness and structure. In the initial period of coating operation in conditions of aggressive corrosive environment, protection is provided by the outer layer. Its corrosion resistance directly depends on the chemical composition of the hot dip galvanizing bath. The paper presents research results determining the effect of addition of aluminium and magnesium to zinc alloys for hot dip galvanizing process. The tests were carried out on zinc alloys with addition of 5-15% wt. Al and 0.5-3% wt. Mg. Corrosion resistance of tested alloys was compared with corrosion resistance of the traditional zinc bath alloy. Corrosion resistance of the alloys was defined by comparative methods in two standard corrosion tests in neutral salt spray and in moist atmosphere containing SO₂. It has been found that the addition of aluminium to the zinc alloy improves the corrosion resistance. In addition, the corrosion resistance improves the addition up to 1% wt. Mg. Higher Mg additives up to 3% cause decreasing the corrosion resistance.

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P.S.B.11.

The properties of ZnAlMgSi alloys for batch hot dip galvanizing

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The temperature of a metal bath and the dissolution rate of iron influences the structure and thickness of the coating and its properties and it determines the producibility of the batch hot dip metallization process. In zinc-aluminium baths an increase in the content of Al causes an increase of alloy melting point and the dissolution rate of iron. In such conditions intense dissolution of iron takes place and the bath loses its producibility. As a result the possibilities of using Zn-Al alloys for batch hot dip metallization process are limited. In the paper the melting point of Zn-Al alloys with the addition of Mg has been determined, based on solidification curves. The spinning disk method determined the effect of the addition of Mg and Si on the constant of iron dissolution rate. Alloys containing 23 and 31 % wt. Al with the addition of 3 and 6 % wt. Mg were under investigation. It has been determined that the solidification temperature of the ZnAlMg alloy is a synergistic effect of the Al and Mg contents. In baths with higher contents of Al the addition of Mg causes a decrease of the melting point. The additives to the zinc bath affected the constant of the iron dissolution rate. Magnesium causes a slight decrease in the constant dissolution rate, but unit mass losses are comparable to the unit losses observed in baths without Mg. A significant reduction in unit mass losses and a constant dissolution rate occurs after the introduction of the Si additive into the bath.

P.S.B.12.

The effect of a single shock processing on mechanical properties Al-Li 2099 (T-83) alloy

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Al-Li alloys are widely used in aerospace engineering due to the unique combination of low density, required strength and extremely high elastic moduli compared to other aluminum alloys – each 1% lithium reduces the alloy density by 3% and increases the Young's modulus by 5%. The Al-Li 2099 (T-83) alloy has an improved corrosion and fatigue crack development characteristics compared to other alloys of this alloying system.

In this work, we study the effect of shock processing on the mechanical properties of Al-Li alloy 2099 modification T-83. A one-time shock processing was carried out with a weight of 10 kg falling from a height of 1 m to deform samples by 5% and 15 kg to deform samples by 12%. The shock processing was performed at room and liquid nitrogen temperature.

The microhardness was measured before and after processing. The deformation at the room temperature leads to an increase in the microhardness h_v by 70% with the degree of deformation $\varepsilon=5.5\%$ and by 47% with $\varepsilon=12.5\%$. As a result of processing at the temperature of liquid nitrogen, the microhardness h_v is increased not so significantly: by 28.5% with the degree of deformation $\varepsilon=5.7\%$ and by 35.5% with $\varepsilon=10.8\%$.

The yield strength and tensile strength under uniaxial tension were measured for the Al-Li 2099 (T-83) alloy in the initial state and after shock processing at different temperatures. Yield stress increased up to 7.5% and tensile stress increased to 6.25% at $\varepsilon=12.5\%$ (room temperature processing). At liquid nitrogen temperature processing the yield stress increased to 6.9% and tensile stress increased to 4% at $\varepsilon=5.7\%$.

The values of yield strength and tensile strength at tensile of the initial Al-Li alloy of the T-83 modification coincide with the alloy characteristics passport. The shock mechanical processing at room temperature leads to an increase of the dislocation density to Al-Li 2099 alloy (T-83) and, accordingly, the mechanical characteristics (microhardness, yield strength and tensile stress) increase.

The mechanical properties of Al-Li 2099 alloy after shock treatment at liquid nitrogen temperature change nonlinearly with increasing degree of deformation. This may be due to a change in the hardening mechanism at a lower temperature.

P.S.B.13.

Influence of the impurity segregation on the adhesion properties of $\text{Al}_2\text{O}_3/\text{Ti}_3\text{Al}$ interface

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Intermetallic Ti-Al alloys have high technological importance due to unique mechanical properties. However, poor oxidation resistance of titanium aluminides restricts their application at high temperatures. Experimental studies have shown that this is connected with a growth of mixed oxide layers containing titanium and aluminum oxides. It has been established that in spite of the initial oxidation stages of titanium aluminides may differ depending on the aluminum content in Ti-Al alloys, at the later stages internal and external oxidation takes place simultaneously. The outer oxide film is mainly formed by TiO_2 , whereas Al_2O_3 is formed at the alloy–oxide interface. The impurity segregation can influence on the stability and the strength of the internal $\text{Al}_2\text{O}_3/\text{Ti}_3\text{Al}$ interface, which is formed due to Al depletion of interface Ti-Al layers. The aim of present work is to study the properties of this $\text{Al}_2\text{O}_3/\text{Ti}_3\text{Al}$ interface and to reveal the effect of impurity segregation on its adhesion properties.

Using the projector augmented-wave method within density functional theory it is shown that the $\text{Al}_2\text{O}_3(0001)_\text{o}/\text{Ti}_3\text{Al}(0001)$ interface is characterized by the highest adhesion energy of 9.3–11.0 J/m² in dependence on its configuration. The largest values of the adhesion energy are due to the ionic contribution to the chemical bonding at the interface. For other terminations (by one or two Al layers) of $\text{Al}_2\text{O}_3(0001)$ surface the adhesion energy is significant smaller, 0.89–3.18 J/m². The effect of transition metal impurities on the adhesion at the $\text{Al}_2\text{O}_3/\text{Ti}_3\text{Al}$ interface is investigated. It is found that the impurities of IIIB and IVB groups on the Ti-sublattice result in a decrease of the adhesion energy by 0.06–0.23 J/m² while the detrimental effect of Al antisite is more pronounced (0.30 J/m²). At the same time, the Ti antisites and some impurities on the Al-sublattice can lead to interface strengthening. The electronic structure of doped and undoped interface is analyzed in dependence on its configurations and composition of interfacial layers. The role of electronic structure of impurity atoms in a change of the adhesion energy is discussed.

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P.S.B.14.

Localized plastic deformation autowaves under tension of nitinol specimens

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The paper studies the evolution of deformation fields in nitinol specimens under uniaxial tension. Specimens of 55.76 wt. % Ni + 44.24 wt. % Ti composition were quenched in water from a temperature of 1073 K. At room temperature, they were in the R-phase state and had superelastic behavior. In the process of tension, macrodeformation localization zones were visualized by digital image correlation (DIC) method. Under deformation, the metastable R-phase underwent a phase transition to the B19' state. On the load curve, this process was represented by a yield plateau with a well-shaped sharp yield point. In some cases, the first stress drop was followed by another one. It has been established that deformation-induced phase transformation is realized through the formation and movement of two localized deformation fronts that originate at the borders of the specimen gauge. The fronts move towards each other and annihilate when they meet. Front velocities are interrelated and the sum of their modules remains constant. It is determined by the yield plateau duration and increases with the increasing traverse speed of the tensile testing machine movable grip. Changing the last one during deformation made it possible to establish that the dependence on the loading rate is not linear. In this respect, phase transition fronts behavior is fully similar to Lüders band (LB) front kinetics in low-carbon steel and can be considered as a switching autowave of localized deformation. The main difference between these phenomena is that the degree of strain localization at the phase transformation front is an order of magnitude less than that at the LB front. In addition, it was found that phase transformation front has a more complex structure than LB front. It is the place for changes in all three distortion tensor components: local elongations, local shear and local rotations.

Meaningful results were obtained in the process of unloading the specimen at a constant speed of the testing machine grip. Although the specimen size and shape are not fully recovered, moving fronts of B19' → B2 reverse phase transformation are formed. Reverse phase transformation front velocities are greater than velocities of direct phase transformation fronts, while the fronts themselves are very blurry and characterized by low amplitudes.

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P.S.B.15.

DMA and TMA study of glass transition in Cu-Zr based bulk metallic glasses

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Using dynamic mechanical analysis (DMA) and thermal mechanical analysis (TMA) techniques we have studied different CuZr-based bulk metallic glasses (BMGs), i.e. $\text{Cu}_{46}\text{Zr}_{46}\text{Al}_8$, $\text{Cu}_{44}\text{Zr}_{44}\text{Al}_8\text{Hf}_2\text{Co}_2$, $\text{Cu}_{44}\text{Zr}_{44}\text{Al}_8\text{Hf}_4$ and $\text{Cu}_{44}\text{Zr}_{44}\text{Al}_8\text{Co}_4$ in a wide temperature region (150 K – 870 K). DMA experiments were performed at different frequencies in the range 0.1 Hz to 15 Hz at a heating rate of 10 K/min. During the experiments, we have observed sharp changes in the storage modulus with corresponding peaks in loss modulus for all samples in the glass transition region. The glass transition temperature (T_g) changed with frequency in a systematic way according to an Arrhenius law. From DMA and TMA experiments, we found clear shifts of the T_g by adding different alloying elements to $\text{Cu}_{46}\text{Zr}_{46}\text{Al}_8$. In all investigated alloys we found a stiffening behavior of the elastic modulus prior to the glass transition. This might be related to structural rearrangements triggered by dynamic relaxation processes such as the beta transition. The results clearly highlight the importance of microalloying and its influence on the microstructure-property relationships in CuZr-based BMGs.

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P.S.B.16.

High-temperature phase relations in the $\text{Bi}_2\text{O}_3\text{-Mn}_2\text{O}_3\text{-M}_2\text{O}_3$ ($\text{M}=\text{Fe, Ga, Al}$) pseudo-ternary systems

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Ceramics that contain Bi_2O_3 exhibit various very interesting physical properties and are widely investigated in last decade. In the present investigation a subsolidus high-temperature phase relations in air were determined in the systems: (1) $\text{Bi}_2\text{O}_3\text{-Mn}_2\text{O}_3\text{-Fe}_2\text{O}_3$, (2) $\text{Bi}_2\text{O}_3\text{-Mn}_2\text{O}_3\text{-Ga}_2\text{O}_3$ and (3) $\text{Bi}_2\text{O}_3\text{-Mn}_2\text{O}_3\text{-Al}_2\text{O}_3$. The samples were prepared by wet method from nitrates and/or acetate in order to obtain well homogenized starting material. The samples were equilibrated at temperatures 760-790 °C. Based on microstructural and X-ray powder diffraction analysis relevant phase diagrams were constructed. In all three systems a $\gamma\text{-Bi}_2\text{O}_3$ was confirmed as well as a solid solution in entire compositional range based on Sillenite phases. In the perovskite BiFeO_3 crystal structure, which forms in the system $\text{Bi}_2\text{O}_3\text{-Mn}_2\text{O}_3\text{-Fe}_2\text{O}_3$ up to 15 % of Fe can be substituted by Mn and thus formed solid solution lies on the $\text{BiFeO}_3\text{-"BiMnO}_3\text{"}$ compositional line, however the BiMnO_3 can not be prepared at environmental pressure. In the systems the mullite-type compounds $\text{Bi}_2\text{M}_{14}\text{O}_{9+\delta}$ ($\text{M}=\text{Mn, Fe, Ga, Al}$) form solid solutions in limited range, and their extension depends on the system.

P.S.B.17.

Low-temperature superplasticity of Ek61 and Ep975 superalloys with ultrafine-grained structure

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Superalloys are difficult to deform and have a low technological plasticity. Therefore, in the technological processes of manufacturing parts from superalloys, the application of the superplasticity (SP) effect is promising. This can be achieved due to the formation of semi-finished products from superalloys having ultrafine-grained (UFG) and nanocrystalline structures [1,2]. The aim of this work is to study the superplastic characteristics of deformable EK61 and EP975 superalloys with UFG structure. The UFG microstructure was formed by thermomechanical processing in double-phase region of superalloys. It is shown that as a result of deformation and heat treatment in the EK61 superalloy a UFG microstructure with an average grain size of the γ -phase $\sim 0.8 \mu\text{m}$ and δ -phase $\sim 0.75 \mu\text{m}$ can be formed. Such microstructure provides a manifestation of SP effect in the EK61 superalloy in the temperature range of 700 ... 900 °C. The maximum value of the relative elongation at a temperature of 800 °C was 1431% and the coefficient of strain rate sensitivity m is 0.4. At a lower temperature of 700 °C, SP effect was also detected ($\delta = 292\%$; $m = 0.31$). In the EP975 alloy, a UFG structure is formed with an average grain size of the γ -phase $\sim 0.8 \div 2 \mu\text{m}$. At the same time, large particles of the γ' phase (up to $3 \div 5 \mu\text{m}$) are preserved in the superalloy. The SP effect for EP975 superalloy in the temperature range of 850 $\div$ 1000 °C was observed for the first time. The maximum value of the relative elongation was 1490% at a temperature of 950 °C (the m is 0.44).

In summary, it was demonstrated that the formation of ultrafine-grained microstructure of superalloys facilitates the effect of low-temperature SP.

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P.S.B.18.

Mechanical and microstructural properties of TRIP-matrix composites studied by neutron scattering methods

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The main parameters of the microstructure of TRIP (TRansformation Induced Plasticity) composites with an austenitic matrix and a ZrO₂ zirconium-dioxide reinforcing phase subjected to plastic deformation of different degrees (compressive uniaxial load) are studied by neutron diffraction and small-angle neutron scattering methods. A series of TRIP-matrix composite samples with different contents of the ZrO₂ ceramic phase (0, 10, 20, 30, and 100 wt %) are prepared by the powder metallurgy method using hot pressing. In the region of plastic deformation at load values above 650 MPa, two additional phases are observed in the austenitic matrix: cubic α' -martensite and hexagonal ϵ -martensite. Data on the crystal lattice strains of the observed phases, dislocation density in the austenitic matrix, and characteristic sizes of the martensitic-phase particles are obtained.

P.S.C.1.

Microstructure of Half-Heusler thermoelectric alloys after severe plastic deformation

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Half Heusler (HH) alloys are a broad class of materials with promising thermoelectric (TE) properties. They can be used in TE generators for conversion of waste heat into electricity. The complex crystal structure of HH alloys with three sublattices makes it possible to improve their TE efficiency by tuning electronic properties via changing the chemical composition on individual sublattices. Further enhancement of TE properties can be achieved by nanostructuring [1, 2].

In this work, we characterize the microstructure of p-type NbFeSb and $\text{Ti}_{0.15}\text{Nb}_{0.85}\text{FeSb}$ TE materials prepared by ball milling and hot pressing (BM+HP) and examine the effects of additional high pressure torsion (HPT). Fracture surfaces of the processed samples were studied in a Tescan LYRA 3XMU SEM×FIB scanning electron microscope (SEM). Thin cross sectional lamellae were prepared by a focused ion beam in SEM and inspected in a Philips CM12 STEM transmission electron microscope (TEM) and a JEOL JEM 2100F high resolution TEM with an X-Max80 Oxford Instruments energy dispersive X-ray analytical system. Dramatic changes in grain size and dislocation density caused by HPT processing were quantified.

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P.S.C.2.

Multiple twinning and stacking faults in silver dendrites

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Detailed defect structure of dendrite formation was studied in order to connect the mesoscopic with the atomistic structure. It was demonstrated that twinning and stacking fault formation play a central role in the growth of electrodeposited Ag dendrites. The broad faces and main trunk growth directions were found to be $(\bar{1}11)$ and $[\bar{1}1\bar{2}]$, respectively. Dendrite branches were elucidated to grow from the main trunk, parallel to the $[12\bar{1}]$ and $[\bar{2}\bar{1}\bar{1}]$ crystallographic directions. Twins and stacking faults were found to reside on the $\{111\}$ crystallographic planes, as expected for a face centered cubic Ag crystal. Using electron back scattered diffraction (EBSD) two variants of in-plane 60° rotational twin domains were found in the $(\bar{1}11)$ broad dendrite surface plane. The intersections of twins and stacking faults with dendrite branch surfaces were found to be perpendicular to the $\langle 112 \rangle$ branch growth directions. However, occasionally twins on $\{111\}$ planes parallel to the $\langle 112 \rangle$ branch growth directions were also observed. Although defect assisted dendrite growth is facilitated by twinning and stacking fault formation on $\{111\}$ planes, the growth directions of the trunk and branches are not of $\langle 111 \rangle$ type, but rather close to $\langle 112 \rangle$, maintained by breaking dendrite facets into thermodynamically stable 111 and 200 steps and structural ledges of various length.

P.S.C.3.

HPHT synthesis of nano-sized diamonds doped with Si or ^{13}C for biological and medical applications

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Nanodiamonds (NDs) with negatively charged silicon vacancy (SiV^-) centers have recently attracted attention as potential high performance bioimaging probes and nanoscale thermometry. The NDs doped with ^{13}C and having the negatively charged nitrogen-vacancy centers (NV^-) offer possibilities as novel hyperpolarized probes for magnetic resonance imaging (MRI). We demonstrate here the growing of NDs (20 to 200 nm) containing a multi bright NV^- and SiV^- colour centres using the high pressure high temperature (HPHT) method of synthesis based on hydrocarbon growth systems. Detonation nanodiamonds (DNDs) with the size of 3-4 nm were incorporated in the initial hydrocarbon growth systems for enhancement of the content of nano-size diamond fraction in the products of synthesis. Naphthalene (C_{10}H_8), hexamethylenetetramine ($\text{C}_6\text{H}_{12}\text{N}_4$), tetrakis(trimethylsilyl)silane ($\text{C}_{12}\text{H}_{36}\text{Si}_5$), benzoic acid ($^{13}\text{C}_6\text{H}_5^{12}\text{COOH}$) were used as the main hydrocarbon and N, Si and ^{13}C doping components the growth systems. HPHT treatment of the samples was carried out in "Toroid" type apparatus. The experimental procedure consisted of loading the high pressure apparatus to 8.0 GPa, heating the samples to synthesis temperature (about 1400 °C) and short (1-3 s) isothermal exposure. Raman and PL spectroscopies, SEM and TEM microscopies were used for characterization of synthesized diamond materials. ^{13}C enriched NDs were obtained with 4 different concentrations: 5%, 14%, 20% and 30% confirmed using Raman spectra analysis. The obtained NDs-Si were tested for all-optical thermometry. Thermometers made with our NDs-Si show exceptional sensitivity and can detect a 0.4 °C change of temperature in a measurement taking only 0.001 second due to their high SiV^- concentration. The NDs with ^{13}C are currently under study on these hyperpolarization properties.

P.S.C.4.

Oxygen storage capacity versus catalytic activity of ceria–zirconia solid solutions in CO and HCl oxidation

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Oxygen storage in solid catalyst is very important for industrial oxidation reactions such as HCl oxidation reaction (Deacon process). Ceria nanoparticles act as promising catalysts for HCl oxidation reaction. Ceria possesses high OSC (oxygen storage capacity) which is a measure of the oxygen quantity that material can store and release. This makes ceria suitable for redox reactions which usually follow Mars-van Krevelen mechanism (surface oxygen atoms directly involved in reactions). $\text{Ce}_x\text{Zr}_{1-x}\text{O}_2$ solid solutions were prepared as a function of the composition x with constant specific surface area in order to explore the relationship between oxygen storage capacity (OSC) and activity of the oxidation reactions of CO and HCl. The as-prepared $\text{Ce}_x\text{Zr}_{1-x}\text{O}_2$ solid solutions were characterized by X-ray diffraction (XRD), Raman spectroscopy (Raman), and X-ray photoelectron spectroscopy (XPS). The complete (or total) oxygen storage capacity ("complete" OSC: OSCc) at 430 °C is shown to be linearly correlated to the CO oxidation activity at 430 °C as a function of the Ce concentration x , thus being compatible with the expected Mars–van-Krevelen mechanism. For the catalytic HCl oxidation reaction at 430 °C the activity is also shown to be linearly correlated to the OSCc with a maximum activity realized with $\text{Ce}_{0.8}\text{Zr}_{0.2}\text{O}_2$. From the linear relationship of oxidation activity of HCl and OSCc (that in turn is linear to the activity of CO oxidation) we conclude that the HCl oxidation reaction over $\text{Ce}_x\text{Zr}_{1-x}\text{O}_2$ solid solutions proceeds via the Mars–Van-Krevelen mechanism with the reduction of $\text{Ce}_x\text{Zr}_{1-x}\text{O}_2$ being rate-determining.

P.S.C.5.

Structure, morphology and photocatalytic properties of $\text{Co}_x\text{Mg}_{1-x}\text{Fe}_2\text{O}_4$ ($0 < x < 1$) spinel ferrites obtained by sol-gel synthesis

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Nanocrystalline cobalt magnesium ferrites with varying cobalt and magnesium content ($\text{Co}_x\text{Mg}_{1-x}\text{Fe}_2\text{O}_4$, $0 < x < 1$) were synthesized using the sol-gel self-combustion method with citric acid as fuel, followed by calcination at 700 °C for 2 hours. Structural characterization was performed using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and Raman spectroscopy. It confirmed the formation of agglomerated nanocrystalline ferrites with an inverse cubic spinel structure. The optical band gap energy was determined using UV/Vis spectrophotometry. It reduced with increased Co content. Visible light photocatalytic activity was tested using natural and artificial light sources through a series of experimental degradations of the methylene blue (MB) solution.

P.S.C.6.

High-performance supercapacitors based on core-shell structured carbon fibers@spinel oxide composites

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Core-shell structured carbon fibers@spinel composites have been synthesized by a facile two-step procedure. In the first step, phase-separated polymer solutions with various quantities of metal precursors were electrospun into hybrid fibers. In the second step, these fibers were converted into composites by using the specific heat treatment. Scanning transmission electron microscopy (STEM) in combination with energy dispersive X-ray spectroscopy (EDS) of cross-sections of composite structures revealed that carbon occupies inner part inside spinel rings. The X-ray diffraction (XRD) patterns indicated that formation of spinel phases can be controlled by changing the molar ratio of metal precursors. Thin-layer composite electrodes delivered high specific capacities in alkaline solutions with excellent capacity retention and cyclic stability. The improved electrochemical properties are ascribed to the complex structures with the abundance of surface redox sites combined with conductive carbon backbone which provides fast transport of electrons ensuring the mechanical stability of composites. Benefiting from these unique properties, synthesized materials are highly attractive for high-performance supercapacitor electrodes.

P.S.C.7.

Citrate assisted solvothermal synthesis of β -NaYF₄: Yb, Er up-converting nanoparticles

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Thanks to the unique optical properties, up-converting nanoparticles (UCNPs) have a wide application in optoelectronics, forensics, security and biomedicine. The synthesis of the most efficient hexagonal β -NaYF₄: Yb/Er phase is usually performed through thermal decomposition of organic precursors which could cause the UCNP cytotoxicity. Since cubic polymorph is kinetically more stable than hexagonal, we used citric acid and Na-citrate for the nucleation of hexagonal NaYF₄: Yb, Er phase in nanosized particles. Additionally, effect of different precipitation agents (NaF, NH₄F and NH₄HF₂) used during solvothermal synthesis is explored. The XRPD analysis showed that using of citric acid led to a product composed from mixture of cubic and hexagonal NaYF₄: Yb/Er phase, while the presence of Na-citrate influences the nucleation of well crystallized hexagonal β -NaYF₄: Yb/Er phase, regardless of precipitation agents used. All samples are composed of polycrystalline spherical particles which size is influenced by the precursor chemistry. UCNPs emit intense green emission due to the (²H_{11/2}, ⁴S_{3/2}) → ⁴I_{15/2} electronic transitions, after been excited with infrared light (λ =978 nm).

P.S.C.8.

Effect of rare earth elements (Eu^{3+} , Sm^{3+} , $\text{Yb}^{3+}/\text{Er}^{3+}$) doping on luminescence properties of Y_2MoO_6

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Phosphors are materials which emit radiation when exposed to various types of excitation (ultraviolet radiation, X-rays, electron beam, etc.). They are comprised of a host lattice with dopant as an activator. One of the extensively investigated host lattices is monoclinic Y_2MoO_6 with rare earth elements (REE) as dopants. The REE are used as activators since they have a $4f$ shell which is not entirely occupied and its electrons are thereby screened by the electrons from the outer shells. As a result, they emit different wavelengths from the number of discrete energy levels, providing possibility for various applications.

In this study, we report successful synthesis of Y_2MoO_6 powders doped with rare earth elements (5at% Eu^{3+} , 2at% Sm^{3+} , and 2.5at% $\text{Yb}^{3+}/0.5\text{at}\% \text{Er}^{3+}$) by a self-propagating method followed by annealing at various temperatures (600-1400 °C) for 4h. Obtained powders were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and luminescence emission and excitation spectra. All obtained powders were single phase $\text{Y}_2\text{MoO}_6\text{:REE}$, where particle size varied from nanorange (annealed at 600 and 800 °C) to microrange (annealed in the range 1000 - 1400 °C) i.e. particle size increased with increase of annealing temperature. Y_2MoO_6 doped with Eu^{3+} or Sm^{3+} exhibited a broad absorption line in the 324-425 nm interval; sharp emission peak of Eu^{3+} was observed at 611 nm, and an emission peak of Sm^{3+} was observed around 652 nm. Since both materials show absorption in the near-UV part of spectrum, and emission in the red part, they can be considered promising materials for red phosphors in light emitting diodes (LEDs). On the other hand, $\text{Yb}^{3+}/\text{Er}^{3+}$ doped Y_2MoO_6 has double emitting luminescence at around 655 and 546 nm, and could therefore be applied in lasers and devices for optical communications due to the infrared-to-visible light conversion.

P.S.C.9.

The effect of pH on visible-light photocatalytic properties of pseudobrookite nanoparticles

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In this study, pseudobrookite (Fe_2TiO_5) nanoparticles were fabricated by a modified sol-gel method using $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and $\text{Ti}(\text{OC}_3\text{H}_7)_4$ as starting reagents and ethanol as solvent. Oxalic acid was used as a chelating agent while cetyltrimethylammonium bromide (CTAB) and citric monohydrate were used as surfactants. Structural and morphological characterization using X-Ray Diffraction (XRD) and Field Emission Scanning Electron Microscopy (FESEM) analysis confirmed the formation of pseudobrookite nanoparticles. As synthesized Fe_2TiO_5 nanoparticles were utilized as photocatalysts for decolorisation of Methylene blue (MB) under visible light irradiation. It was observed that the adsorption of MB onto Fe_2TiO_5 nanoparticles is strongly dependent on the solution pH. Maximum decolorization was observed for Fe_2TiO_5 nanoparticles prepared with CTAB under alkaline conditions ($\text{pH}=10.5$).

P.S.C.10.

Ion-irradiation of ZrNb nanoscale multilayers

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ZrNb nanometric multilayer films having periodicity (L) from 6 to 167 nm were irradiated at ambient temperature by carbon and silicon ions with low and high fluences. The implanted ion profiles, mechanical properties, and irradiation damage were studied by secondary ion mass spectrometry (SIMS), nanoindentation, X-ray diffraction (XRD), and scanning transmission electron microscopy (STEM). The carbon and silicon concentration profiles obtained from SIMS were not affected by the periodicity of the nanolayers, but Nb layers captured more ions due to higher Nb density. This result was confirmed by Stopping and Range of Ions in Matter (SRIM) simulations. The damaged region is clearly visible on STEM cross-section micrographs on the surface side of the multilayer. The most damaged and disordered zone is located close to the maximum ion concentration. A structural evolution in relation to L was found using XRD and electron diffraction. After irradiation, Zr (0002) and Nb (110) reflexions overlap for L = 6 nm. For L > 6 nm the Zr (0002) peak is shifted to higher angles and Nb (110) peak to lower angles. This indicates positive and negative out-of-plane stresses in Zr and Nb individual layers induced by irradiation.

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P.S.C.11.

Orientation dependence of microstructure formation in Cu-8% at. Al single crystals

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The present experiments were conducted using a Cu-8% at. Al single crystals with an initial orientations: $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$. The samples were deformed by cold drawing with a total strain of $\varepsilon = 2,2$. Microstructure analyses were performed using a transmission (TEM). The refined microstructures were examined qualitatively and quantitatively by the stereological methods. The changes of mechanical properties was carried out using Vickers micro hardness and compression testing. The aim of this study is to understand how an initial orientation affects the microstructure formation of Cu-8.5%at. Al single crystals subjected to drawing process. In order to accurately characterize the microstructure evaluation of examined single crystals after deformation, formed shear bands (SB) were divided in two groups: macroscale SB (MSB) and microscale SB (MicSB). The width of both was measured

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P.S.C.12.

Utilizing ion beam irradiation for structural modification of 12-tungstophosphoric acid

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Properties of heteropolyacids strongly depend on their structure. In this work we utilized ion beam irradiation as a tool for structural modification of 12-tungstophosphoric acid (WPA). WPA was spin-coated from the ethanol solution onto platinized silicon substrate and irradiated with 10 keV C⁺ ions at fluences between 5×10^{14} and 2.5×10^{15} ions/cm². The samples were characterized by attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR), Raman spectroscopy, UV-Vis diffuse reflectance spectroscopy (UV-VIS DRS), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM) and atomic force microscopy (AFM). Investigation of morphology showed agglomeration of WPA grains with irradiation. ATR-FTIR and Raman spectra showed shifts and widening of vibration bands. Also, changes of electronic structure of irradiated samples were manifested as peak shifts in O1s and W1f XPS spectra and as appearance of new absorption bands in UV-VIS DRS spectra. Results indicate that up to (5×10^{14}) ions/cm² the Keggin structure is partially modified while at higher fluences the transformation of WPA to phosphate tungstate bronzes occurs.

P.S.C.13.

Rapid reaction of Mo₂N nanowires with Pb²⁺ ions in water and its use for production of PbMoO₄ nanoparticlesAleš Mrzel¹, Damjan Vengust¹, Matejka Podlogar^{1,2}, Mojca Vilfan¹¹J. Stefan Institute, Jamova 39, 1000, Ljubljana, Slovenia; ²National Institute of Chemistry, Hajdrihova 19, 1000, Ljubljana, Slovenia

Molybdenum nitrides, which are used as hard coatings or corrosion and abrasion resistant layers, are in general considered as having good chemical resistance. We find, however, that molybdenum nitride Mo₂N nanowires promptly react with lead nitrate in water at room temperature, resulting in formation of lead molybdate nanoparticles. Depending on the initial concentrations, the resulting material are either hybrid nanowires decorated with individual lead molybdate nanoparticles, or solely lead molybdate nanoparticles. The synthesised nanoparticles are fairly uniform in size, with diameters of up to a hundred nanometres. We find that the particle size is practically independent of the initial concentrations that we used. The performed one-step reaction, which is very fast and requires no additional reagents, clearly shows chemical reactivity of molybdenum nitrides and opens a new use for molybdenum nitrides as starting materials in a variety of chemical reactions. At the same time, the demonstrated reaction presents a new method for synthesis of lead molybdate nanoparticles or hybrid materials using molybdenum nitride nanowires as the starting material.

P.S.C.14.

Consequences of confinement conditions on absorption in molecular nanofilms

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The model of the ultrathin (nano) film as spatially very confined (along one direction majorly narrowed) of molecular crystal structures is presented here. The theoretical analysis of the dielectric and optical properties of such samples was carried out using the Frenkel's exciton model and the Green's function method. The four-layered dielectric nanofilms with different boundary conditions on surfaces were researched and some discrete resonant absorption lines were obtained as a consequence of appearance of localized states in the surface layers. Their number and frequency position depend on the boundary parameter values. Practically monochromatic absorption may occur. Unlike the corresponding bulk-samples which are total absorbers throughout the near IR region, in ultrathin films will appear selective and discrete reflection and larger transparent region. These results can greatly contribute to optical nanoengineering, especially in the design of new photon equipment in nanomedicine to monitoring the movement of nanoparticles – drug carriers/deliverers.

P.S.C.15.

Structural investigations of alloyed Al with TiCN nanopowder under load and tensile

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The nano-powder introduction in the molten metal leads to microstructure, mechanical and some electrochemical properties alternation of the crystallized metal. The amendment is expressed in grain refinement, microstructure components modifying, increase in the microhardness, and mechanical and electrochemical properties improvement when nano-powder is introduced through appropriate way and volume fraction in the molten material [1,2].

Our previous results [3-5] showed the possibility of improvement of the mechanical properties by introduction of TiCN nanoparticles into Al matrix by means of electron beam surface modification. The microhardness of the formed layer is 16-22 times greater in comparison with the base Al substrate.

The alloying of Al with TiCN nanoparticles is able to improve significantly the functional properties and to introduce these materials for novel applications in the modern industry. However, the structure and mechanical performance of the discussed materials under different load (pressure) or tensile are not yet studied.

The aim of this study is to investigate the changes in the structure (lattice strain, microstrain, phases content) of alloyed Al with TiCN by means of extrusion of powders as a function of the applied load (at room temperature) and the concentration of the nanoparticles.

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P.S.C.16.

Cubic silver nanoparticles fixed on TiO₂ nanotubes as a simple and efficient substrates for surface enhanced Raman scatteringRobert Ambroziak¹, Marcin Hołdyński², Tomasz Płociński³, Marcin Pisarek², Andrzej Kudelski¹¹Faculty of Chemistry, University of Warsaw, Pasteur Str. 1, 02-093 Warsaw, Poland; ²Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka Str. 44/52, 01-224 Warsaw, Poland;³Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507, Warsaw, Poland

In this work we show that ordered freestanding titanium oxide nanotubes may be used as substrates for the simple and efficient immobilization of anisotropic plasmonic nanoparticles. This is important because anisotropic plasmonic nanostructures give usually greater spectral enhancement than do spherical nanoparticles [1]. The size of the pores in a layer of titanium oxide nanotubes can be easily fitted to the size of many silver plasmonic nanoparticles highly active in SERS (surface-enhanced Raman scattering) spectroscopy (for example, silver nanocubes with an edge length of ca. 45 nm), and hence, the plasmonic nanoparticles deposited can be strongly anchored in such a titanium oxide substrate. The tubular morphology of the TiO₂ substrate used allows a specific arrangement of the silver plasmonic nanoparticles that may create many so-called SERS hot spots [2]. The SERS activity of a layer of cubic Ag nanoparticles deposited on a tubular TiO₂ substrate is about 8 times higher than that of the standard electrochemically nanostructured surface of a silver electrode (produced by oxidation reduction cycling). Furthermore, a super hydrophilic surface of TiO₂ nanotubes [3] allows a uniform distribution of Ag CNPs on the nanotubes, which are deposited from an aqueous suspension [4]. The new Ag CNPs/TiO₂ NT/Ti hybrid layer ensure a good reproducibility of SERS measurements and exhibit a higher temporal stability of the achievable total SERS enhancement factor, one that is far better than standard SERS silver substrates [2]. To characterize the morphology and structure of such evidently improved SERS platforms thus received, we applied microscopic techniques (SEM, STEM) and surface analytical techniques (AES, XPS).

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P.S.C.17.

Formation of borides, silicides and boride-silicide powder composite materials by mechanical alloying

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The combination of titanium diboride with metal silicides of IV – VI groups makes it possible to produce the materials with high heat resistance, wear resistance, hardness, high tribological properties and moderate fracture toughness.

An aim of the present work is to obtain $\text{TiB}_2\text{--MeSi}_2$ highly disperse composite powders by the method of mechanochemical synthesis, which makes it possible to provide an uniform distribution of different phases in the nanostate in contrast to the method of mechanical mixing of ready-made corresponding borides and silicides.

The composite nano-sized powders of boride-silicide system were prepared by the method of mechanochemical synthesis. Pre-products were Ti, V, Nb, Ta metallic powders, amorphous boron, and electrolytic Si. Mechanical treatment was conducted in an AIR-type planetary mill with centrifugal effort of 25g in the steel drums charged by silicon and boron. The mixtures were calculated for the preparation of powders of composition $0.8 \text{ TiB}_2\text{--}0.2 \text{ MeSi}_2$.

The features of the phase composition and structure of the resulting powders with a particle size of 40 – 70 nm were studied. The initiating effect of TiB_2 on the formation of silicide phases in the process of cooperative mechanosynthesis was shown.

The obtained electrolytic coatings of the composition $\text{Ni--TiB}_2\text{--MoSi}_2$ showed high wear resistance under sliding friction conditions and can be recommended for hardening and restoring the surfaces of machine parts and mechanisms.

P.S.C.18.

Preparation of polylactide-kaolinite nanocomposite

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Nowadays, the plastics are widely used because of their favourable manufacturing possibilities and application properties. The increasing plastic consumption produces large amounts of plastic waste which cause serious environmental problems. The use of biodegradable polymer-polylactide (PLA) can reduce the application of hydrocarbon based polymers (e.g. polyethylene (PE)) which are essentially undegradable in the natural environment. But the mechanical properties of PLA are not so advantageous, and it should be improved by addition of various organic or inorganic particles. In this work, we investigated the preparation and properties of PLA-kaolinite nanocomposite. Our high-efficient one-pot technique was used to produce kaolinite nanoscrolls. These nanoscrolls have a polar siloxane surface; therefore no surface treatments were used on the nanoscrolls. The mechanical properties and the structure of the PLA-kaolinite nanocomposite were investigated using Charpy impact and tensile strength test, X-ray diffraction (XRD) and scanning electron microscopy (SEM), respectively.

P.S.D.1.

Identification and evaluation of changes and migration mechanisms of petroleum pollutant in the environment using the alkane fraction biological markers (river Vrbas, Bosnia and Herzegovina)

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Organic geochemical knowledge about the origin and degree of thermal maturation of petroleum can also be applied to a large extent in environmental chemistry. Based on the composition of the oil, primarily on the basis of distribution and abundance of biological markers (normal alkanes, isoprenoid aliphatic alkanes, and polycyclic alkanes of the sterane and terpane type), it is possible to distinguish the anthropogenic organic substance from the native, then it is possible to estimate the intensity of pollutant changes in different segments of the environment, and finally it is possible to estimate the way, i.e. the mechanism of migration of oil pollutant through the soil or through some similar recent sedimentary formations. In this paper the river sediments of Vrbas (Banja Luka, Bosnia and Herzegovina) contaminated with oil pollutants were investigated. The aim was to identify and characterize the pollutant in terms of the intensity of biodegradation and the mechanism of water-based migration using organic geochemical approaches.

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P.S.D.2.

Potential application of activated carbonaceous materials for removing residual contaminants from complex biochemical and pharmacological mixtures

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To date, carbon-based materials are widely studied in different biomedical fields (implants, antimicrobial properties). In the recent years, the immobilization of DNA on carbon-based materials has become an important issue in different fields ranging from medicine to analytical chemistry, DNA chips and lab-on-a-chips based on micro fluidic techniques as well as molecular electronics. In this study, we examined the possibility to immobilize DNA on active carbonaceous materials obtained by hydrothermal carbonization process. The aim of the study is to remove residual DNA from different pharmacological and biotech formulations. Our preliminary data suggest that, our newly synthesized and examined materials might be the powerful and safe tool for removing the residual DNA from complex biochemical mixtures.

P.S.D.3

The influence of modification and the particle size of the montmorillonite on the hydrolytic stability of urea-formaldehyde composite

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Urea-formaldehyde (UF) resin adhesive is a polymeric condensation product of formaldehyde with urea and is considered as one of the most important wood adhesives. In spite of some advantages such as lower cost, fast curing, good performance in the panel, water solubility and being colorless, UF resin adhesives also possess a critical disadvantage: formaldehyde (FA) emission from the panels. Exposure to FA may occur by breathing contaminated indoor air, tobacco smoke, or ambient urban air. Furthermore, the FA emission from the panels used for interior applications is known as one of the main factors causing sick building syndrome in an indoor environment.

Montmorillonite (MMT) clays are of great importance for processes such as adsorption and catalysis and polymer composites fabrication. The textural properties of this filler can be modified to increase its application. In this study, the hydrolytic stability of modified UF resins with modified and unmodified montmorillonites as scavengers of FA, with a different particle size (K10 and KSF), was studied. Five UF composite materials of F/U 0.8 ratio with MMT and Na-MMT were synthesized by the same method. The sensitivity to the hydrolysis of the crosslinked UF resin depends on its chemical nature and the degree of cross-linking. The hydrolytic stability of the investigated modified UF resin was determined by measuring the loss of weight and the concentration of released formaldehyde from the modified UF resin after acid hydrolysis. The obtained results showed improved hydrolytic stability of the modified resin containing unmodified KSF as a scavenger of FA.

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P.S.D.4.

Group chase and escape in the presence of obstacles

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We study a stochastic lattice model describing the dynamics of a group chasing and escaping between two species in an environment that contains obstacles. The Monte Carlo simulations are carried out on a two-dimensional square lattice. Obstacles are represented by non-overlapping lattice shapes that are randomly placed on the lattice. The model includes smart pursuit (chasers to targets) and evasion (targets from chasers). Both species can affect their movement by visual perception within their finite sighting range σ . We concentrate here on the role that density and shape of the obstacles plays in the time evolution of the number of targets, $NT(t)$. Temporal evolution of the number of targets $NT(t)$ is found to be stretched-exponential, of the form $NT(t) = NT(0) - \delta NT(\infty) [1 - \exp[-(t/\tau)^\beta]]$, regardless of whether the obstacles are present or not. The characteristic timescale τ is found to decrease with the initial density of targets ρ_{T0} according to a power-law, i.e., $\tau \propto (\rho_{T0})^{-\gamma}$. Furthermore, temporal dependences of the number of targets $NT(t)$ are compared for various combinations of chasers and targets with different sighting ranges, $\sigma = 1, 2$, in order to analyze the relationship between the ability of species and the capture dynamics in the presence of obstacles.

P.S.D.5

Regulation of lipid production of *Torulaspora globosa* yeast, cultivated in the medium with ethanol as a carbon sourceNadezda N. Stepanova¹, Grigorii I. Morgunov², and Svetlana V. Kamzolova¹¹G.K. Skryabin Institute of Biochemistry and Physiology of Microorganisms, Federal Research Center "Pushchino Center for Biological Research of the Russian Academy of Sciences", Pushchino, Moscow region, 142290 Russia²Peoples' Friendship University of Russia (RUDN University), Moscow, 117198 Russia

Lipids are an important group of practically valuable products that can be obtained by microbiological synthesis.

The aim of the work was to study the effect of various cultivation factors on the biosynthesis of lipids in yeast *Torulaspora globosa*, grown in the medium with an environmentally friendly substrate - ethanol.

In the course of the work, the cultivation parameters were determined in order to develop the ecotechnology of lipid production by in *T. globosa* VKPM Y-953 yeast: temperature 28 °C; pH = 5.5; aeration 60% of saturation. It has been established that the nature of the growth-limiting component (C/N ratio) has a significant effect on lipid synthesis: under conditions of limitation of cell growth by nitrogen, a higher accumulation of lipids was observed (43.8%) compared to an energy substrate deficiency (27.8%). The effect of different concentrations of zinc ions on the rates of *T. globosa* growth and lipid synthesis has been studied. It was found the correlation between the content of protein, lipids and macroelements in the biomass. Under conditions of zinc increase from 0.001 to 2.8 mg/L, the proportion of lipids was also increased by 67%, which correlated with an increase in the proportion of carbon by 16.7% and hydrogen by 13.4%. At the same time, when zinc was increased from 0.001 to 2.8 mg/L, the protein content was decreased by 65%, which correlated with a decrease in the proportion of nitrogen by 68.1%. The oxygen mass transfer in flasks was evaluated. The necessity of regulation of the oxygen mass transfer by fermentation phases has been established: in the phase of intensive growth (up to 12 h), the producer requires 0.36 mmol O₂/L·min, and in the phase of lipid synthesis (from 12 to 48 h) it increases up to 0.14 mmol O₂/L·min. Under optimal conditions, a high content of palmitoleic acid (up to 41.7%), the novel lipokine, was observed in the fatty acid composition of lipids.

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P.S.E.1.

Development of a 3D system for cancer cell studiesJasmina Stojkovska^{1,2}, Milena Milivojević³, Milena Stevanović^{3,4,5}, Bojana Obradović¹

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Traditionally, anti-cancer drug testing has involved *in vitro* analysis using two-dimensional (2D) cell cultures and *in vivo* animal models. It is well known that 2D cell cultures have severe limitations such as a loss of tissue-specific architecture and extracellular matrix (ECM), mechanical and biochemical signals, and cell-cell communication, while animal models, apart from being expensive and raising ethical concerns, often produce misleading results due to intrinsic interspecies differences. In order to improve models for drug testing some of the approaches include immobilization of cells in an artificial ECM as well as *in vitro* cultivation under *in vivo* - like conditions. The aim of this work was to develop a 3D model system, based on alginate hydrogels with immobilized cancer cells followed by cultivation in a biomimetic perfusion bioreactor under physiologically relevant conditions. Alginate hydrogels with immobilized cells in forms of microfibers and microbeads were obtained by extrusion techniques. We have examined influence of the applied electrostatic potential (4-7 kV), needle diameter (22 G- 28G), cell density (1×10^6 - 4×10^6 cells/ml of alginate solution) and different cancer cell lines (cervical carcinoma SiHa and CaSki, and embryonal carcinoma NT2/D1) on cell immobilization and viability. The best electrostatic extrusion parameters were 5 kV applied electrostatic potential, 28 G needle and 1×10^6 cells/ml cell density resulting in microbeads (500 μ m in diameter) with immobilized NT2/D1. The best alginate microfibers (500 μ m in diameter) with immobilized SiHa and CaSki were obtained by applying a 25 G needle at 4×10^6 cells/ml. The obtained microbeads and microfibers were cultivated in a perfusion bioreactor at continuous medium flow (interstitial velocities: 15 and 80 μ m/s) in short term 72 h and 10 day studies. SiHa and NT2/D1 cells stayed viable and metabolically active displaying compatibility with the developed 3D system. The overall results have shown potentials of the perfusion bioreactor in conjunction with alginate hydrogels as cell carriers for long-term anti-cancer drug screening

P.S.E.2.

From wood to bone: how to convert wood structures into biomimetic hydroxyapatite scaffolds

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The living organism found in the nature (for example: plants, trees, animal bones) developed an optimal structure against a specific set of mechanical stresses and living conditions. Copying these structures or using them as a bio-template during the production of artificial materials (e.g.: bioceramics, bioactive glass-ceramics) can result improvement of certain properties of these materials.

The three-dimensional, highly oriented pore channel anatomy of oak, pine and bamboo were used as a template to produce biomorphous hydroxyapatite ceramics designed for bone regeneration scaffolds. The parallel hollow tubes and channel-like porous areas makes wood an elective material to be used as a template in preparation of a new bone substitute characterized by a biomimetic hierarchical structure.

The aim of the present work is to obtain a new biomimetic hydroxyapatite bone scaffold having highly organized micro- and macro-porosity. The honeycomb like microstructures of elongated hollow tubes may well be used for infiltration of liquid reactants into the template. For this aim a chemical process has been investigated starting from natural wood and implying a multi-step procedure: In the transformation process natural wood was pyrolysed to obtain biocarbon templates which were infiltrated with hydroxyapatite gel. Heat treatment in air atmosphere caused oxidation of the carbon skeleton and sintering of the hydroxyapatite. SEM analysis confirmed detailed replication of wood anatomy. Porosity of the samples showed a multimodal pore size. The phase composition was determined by XRD revealing hydroxyapatite as the dominant phase. The porosity structure of these scaffolds is similar to the anatomy of cortical bone with porosity of 55-70%. Thus, mimicking the anatomy of these plants offers an interesting potential for regeneration of cortical bone tissue.

P.S.E.3.

Functionalization and biomimetics of insect photonic structures

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A large number of technological achievements are inspired by nature. Many sophisticated structures from nature have prompted scientists and engineers to use them in natural form or imitate them, for numerous applications.

Insects, as one of the most numerous groups of organisms, living in most various environmental conditions, have developed different adaptations. Many of these, man has artificially imitated for solving everyday problems. Structural colouration (photonic structures) in numerous insect taxa attracts much research interest due to the great potential for different applications. Such colors can be of particular importance for the future color industry and related ones, because they do not fade and do not harm the environment. The reproduction of structural color has inspired biomimeticists to develop various optical coatings, films, cosmetics, textiles, and anti-counterfeiting devices.

We examined and demonstrated potential biomimetic and other technological applications of some of these structures. The strong convergence of biology, physics, chemistry and materials science at the nanoscale will likely affect many of the ways we see and understand the world, and the ways we produce objects.

P.S.E.4.

Evaluation of colour modifications and surface morphology of dental composites

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Objectives: This study evaluates colour modifications and surface morphology of dental composites (P11, P21, Gradia and Premise), after 7 days immersed in coffee and bleached with natural bleaching gel G30®.

Materials and Methods: Each type of composite was prepared in Teflon moulds (1 × 1.5 mm), and was further divided into two groups [n = 5 controls were placed in artificial saliva and the other group of n = 5 were placed in coffee], for 7 days, and afterwards bleached with experimental gel. The measurements were performed with a UV-Vis spectrophotometer (Jasco) and from the reflection spectrum were determined the colour coordinates (Δa^* , Δb^* , ΔL^*) and the colour differences ($\Delta E_{a,b}$), as well as after immersion in solutions and also after bleaching. Two techniques of investigation were used: AFM (NTEGRA Spectra (NT-MDT)), in order to study the surface roughness (Ra) and SEM (Inspect F-FEI), to observe the effect of bleaching agents on the surface of the composites.

Results: All nanocomposite samples immersed in coffee showed significant coloration compared to baseline values ($P < 0.05$). Discoloration in samples immersed in artificial saliva was not significant compared to baseline ($P > 0.05$). ΔE values obtained from the UV-Vis spectra, were significantly different to all four types of nanocomposite stored in coffee ($P < 0.05$); while no significant difference was observed in those stored in artificial saliva ($P > 0.05$). No changes were observed on the composite surface for the experimental natural bleaching gel G30®.

Conclusions: The surface morphology of initial samples, before whitening, offers an important reference point for the correct and accurate assessment of effects induced by these treatments.

P.S.E.5.

The morphology studies of different nanohybrid dental composites

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The purpose of this study is to investigate the morphology of experimental nanohybrid dental composites with nanoparticles and bioglasses, for improving the surface properties, by determining the topography of the surface.

Materials used in our study were four experimental nanohybrid dental composites with bioglasses, colloidal silica and nanoparticles as filler in different percent dispersed in an organic matrix consisting of Bis-GMA/TEGDMA. As a reference material, we used commercial nanohybrid dental composite Herculite XRV Ultra (Kerr Company, Italy). The bioglasses and nanoparticles were added for improving the biocompatibility and surface properties of the experimental composites. Cylindrical specimens (10 mm x 1 mm) were cured with a Woodpecker LED Lamp for 160 s in a teflon mold on which was applied gently to compress a flat glass piece.

The morphology of nanohybrid dental composites surfaces were studied by scanning electron microscopy (SEM- Inspect S, FEI Company) and the topography by atomic force microscopy (AFM- STM: JSPM 4210 Equipment).

From SEM and AFM images (topographic and SEM images) emphasized a relatively uniform structure of the material, in which the filler particles are fixed in the polymer matrix for all experimental investigated composites. The commercial composite present a uniform structure. SEM images highlights the nanometric size of particles from the compoition.

In conclusion, from both the images of electron microscopy (SEM) and the images of atomic force microscopy (AFM), one can observe the homogeneity of the material and the uniform distribution of the nanohybrid filler in the organic matrix.

P.S.E.6.

The identification of branched-chain amino acids and the testing of the antibacterial effect of whey and soy protein powders

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Objectives: the main objective of this study is the determination of Branched-Chain Amino Acids (BCAA) from whey and soy protein isolates and hydrolysates and the testing of their antibacterial effect.

Materials and methods: five types of solid powders of whey and soy protein concentrates have been tested: CWP – lyophilized whey concentrate; BWP – whey byo powder; IWP – Whey Protein Isolate, ISP – Soy Protein Isolate and SPH – soy protein hydrolysates. The determination of branched-chain amino acids from the whey and soy protein concentrates and hydrolysates have been made by Overpressured Layer Chromatography OPLC technique. The antimicrobial capacity of whey and whey protein isolates have been tested by disk diffusion susceptibility (disk method). The tested microorganisms in this study were *Escherichia coli* ATCC 25922 and *Staphylococcus aureus* ATCC 25923.

Results: Valine, isoleucine, and leucine (BCCA) have been quantitatively determined by OPLC. The tests have been made in the case of soy proteins both before and after acidic hydrolysis in order to evaluate the degree of enzymatic hydrolysis. The test applied on as-prepared samples of soy proteins subjected to enzymatic hydrolysis revealed no BCCA into the sample conducting to the conclusion that applying enzymatic hydrolysis the process conducted to peptides not to amino-acids. If the samples were subjected prior to OPLC analysis to a process of acidic hydrolysis, the lowest content of BCCA (valine+isoleucine+leucine) has been identified in BWP powder (2.324 g/100 g), while the highest quantity of BCCA has been determined in SPH (29.56 g/100 g). The diameter of bacterial inhibition zone is higher in the case of CWP (19 mm) and BWP (20 mm) on *Escherichia coli*, while in the case of *Staphylococcus aureus*, the inhibition zone was of 11 mm for IWP and 18 mm for ISP.

P.S.E.7.

Comparison of the carbon content in various biomasses based on calorimetric tests

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The conversion of biomass resources into useful energy service products can be undertaken using a wide range of technological pathways. Renewable energy technologies can help countries meet their policy goals for secure, reliable and affordable energy to expand electricity access and promote development. The development of a biomass-to-energy requires careful preparation, and research will help project developers and investors prepare successful projects, adopting industry best practices in the development, construction, operation, and financing of biomass-to-energy projects. Aim of this study was to analyze available biomasses, in order to obtain low-carbon energy materials. In this study, the elementary chemical analysis was performed for various raw biomass feedstock, as well as their carbonized products. The special attention was given to carbon, oxygen and hydrogen contents analysis in biomass assessments and their application for thermo-chemical conversion. For utilization and valorization of studied biomasses and processes such as gasification, pyrolysis and combustion, the additional characterization techniques were applied: Scanning electron microscope (SEM), Fourier-transform infrared (FTIR) spectroscopy and X-ray diffraction (XRD).

P.S.E.8.

Hybrid bio-nanoentities with potential applications in biomedical field

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Hybrid entities based on biogenic nanosilver (bio-AgNPs) chitosan, bioinspired membranes labelled with chlorophyll *a* were prepared by “green” approach. The new silver nanoparticles were eco-synthesized from different vegetal sources. In order to get deep inside about the structure of the bio-AgNPs alone, and incorporated into the assemblies with liposomes and chitosan, and also about the interaction between the components of the biohybrids, spectral methods have been used: UV-Vis absorption and emission spectroscopy. The internal structural of the bio-AgNPs in presence of liposomes and chitosan has been studied by Small-angle neutron scattering, Small-angle X-ray scattering, and X-ray diffraction at the nanoscale and Infrared spectroscopy (FT-IR) at the molecular scale. The size and morphology of the biohybrid systems were studied by AFM and SEM analysis. The bioperformances are closely related to the structure of the biohybrids. Thus, the obtained biohybrid entities exhibited: good antioxidant properties (up to 98.5%, *in vitro* tested through chemiluminescence method) and good antibacterial activity against the pathogenic bacteria: *E. faecalis*, *Escherichia coli* ATCC 8738 and *Staphylococcus aureus* ATTC 2592. The obtained bio-based hybrids could be used in biomedical field, as antioxidant and biocide materials.

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P.S.F.1.

Sintering heating and cooling rates as a method of modifying electrical properties of BiFeO_3 ceramics

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Bismut ferrite powder was prepared by sol-gel method. It was calcined at 600 °C and then milled in order to break agglomerates and eventually obtain ceramic samples of high density. Such way treated powders were pressed uniaxially under 196 MPa and sintered at 800 °C. Conventionally sintered samples were heated by the rate of 10 °C/min and furnace cooled. Other samples were inserted into preheated oven and/or taken out from the hot oven directly to air or water at room temperature. Influence of heating and cooling rates on structure, microstructure and electrical properties were studied. Reducing the processing time in temperature interval between 447 °C and 767 °C prevents formation of secondary phases, but the effect on phase composition is not large. It is significantly easier to notice the effect on electrical properties.

P.S.F.2.

Nickel ferrite/zinc ferrite nanopowder with core/shell structure: magnetic properties and sinterability

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Nickel ferrite/zinc ferrite nanocomposite powder with core/shell structure was synthesised using co-precipitation and hydrothermal synthesis in a two-step procedure. Core particles of NiFe_2O_4 have size about 100 nm while shell ZnFe_2O_4 particles are in the range of few nanometres. As-obtained powders were well crystalline with crystallites at the nanometre scale. XRD and Raman showed single spinel phases. However, they could not confirm phase separation due to the structural similarity between nickel and zinc ferrite. On the other hand, core/shell structure was confirmed by TEM/EDS. There was a clear distinction between different ferrite phases at the core/shell boundary. Magnetic properties were significantly influenced by the synthesis procedure. Separate ferrite particles were paramagnetic. However, after mixing and assembling of the core/shell structure powders became superparamagnetic with very thin hysteresis loop. Sinterability of the nanopowder was examined at different temperatures to obtain high density ceramics. Densities were measured both geometrically and by Archimedes' method and showed values above 95% TD.

P.S.F.3.

Sintering of scaffolds based on doped hydroxyapatite powders

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Hydroxyapatite powders, pure (HAp) and doped with Si^{4+} , Ag^+ , Cu^{2+} and Zn^{2+} ions (Si-HAp, Ag-HAp, Cu-HAp, AgCuSi-HAp and AgZnSi-HAp) have been prepared by hydrothermal method. The powders were calcinated at 1100 and 1150 °C giving as a result the powders suitable for making the scaffolds by the replica foam technic. The obtained scaffolds were sintered at 1300 and 1400 °C and then the fresh made scaffolds were sinked in simulated body fluid (SBF) for 14 days. After this period, the scaffolds were characterized by field emission scanning electron microscopy, Fourier transform infrared spectroscopy and powder X-ray diffraction. The analyses confirmed the presence of new, well developed HAp crystals on the surface of scaffolds after incubation in SBF as a proof of their excellent bioactivity.

The scaffolds obtained by replica foam technic did not exhibit good mechanical properties so they should be improved by impregnation with an additional amount of HAp powders. In addition, the scaffolds made of powders doped with three metal ions showed better results during mechanical testing. The temperature regime of the calcination of powders as well as the sintering of scaffolds is important for good properties of those materials, so finding the optimal temperature regime raises a major challenge.

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P.S.F.4.

Two-step sintered monophasic HAp dental inserts as materials for dentin replacement

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Hydroxyapatite (HAp) as a logical dentin substitute is for numerous reasons a favorable material for processing of dental inserts. The application of sintered dental HAp inserts in the central part of cavities, due to similar mechanical properties to human dentin, can result in the reducing amount of composite dental filling material and potentially reduce polymerization shrinkage. The aim of this study was to investigate the influence of different clinical protocols on the shear bond strength (SBS) between two-step sintered (TSS) HAp inserts and different restorative composites. Starting from nano particles of HAp, TSS at temperatures lower than 1000 °C resulted in monophasic very tough HAp inserts, with fracture toughness close to the values for human dentin. SBS values indicated that resin-based composites could be strongly bonded to TSS HAp inserts, in the case of “self-etch” and “total-etch” clinical protocols. Mechanical properties of TSS inserts and SBS values indicated the possibility of their usage as material for dentin replacement.

P.S.F.5.

Surface-selective laser sintering of ultrafine polymer powders. A new approach to high resolution three-dimensional printing

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The process of a high spatial resolution (ca. 30 μm) three-dimensional (3D) printing with ultrafine polymer powders consisted from spherical polymethylmethacrylates (PMMA) microparticles (mean diameters - 0.5 to 3 μm) based on surface-selective laser sintering (SSLS) has been developed. Initial samples of ultrafine PMMA powders with a given microparticles distribution in sizes have been produced by dispersion polymerization in supercritical carbon dioxide. Experimental fine mechanical system to form homogeneous thin (ca. 20 μm) layers of PMMA powders has been developed. Laser beam delivering optical system based on X-Y galvanoscanner and focusing microobjective has been developed for guiding and scanning laser radiation at a wavelength of 405 nm along the working surface of the polymer powder layers. As a results of both single PMMA layer-by-layer formation and SSLS parameters optimization, computer-controlled PMMA 3D structures with a spatial resolution less then 30 μm were fabricated and tested.

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P.S.F.6.

Influence of 3D-printing additive to freeze casting structureYueh-Ying Chou¹, Po-Yu Chen¹, Vojislav V. Mitić^{2,3}, Goran Lazović⁴¹National Tsing Hua University, Taiwan; ²Institute Technical Sciences of SASA, Belgrade, Serbia; ³Faculty of Electronic Engineering University Nis, Serbia; ⁴Faculty of Mechanical Engineering University of Belgrade, Serbia

Cellular design inspired by nature has the ability to decrease body weight while maintaining the same function. Some studies have managed to mimic those structures through several artificial processes and manufactured into functional materials. According to some literature, freeze casting can form the shape of dendrites and remain a foam structure after ice sublimation. Ice nucleation became more heterogeneous with the aid of printing materials during freeze casting. This procedure can even improve the issue of crack formation. In this paper, we studied the mechanical properties of Hydroxyapatite scaffold which is a type of bio-ceramic. We also analyzed the porosity by fractal nature characterization, and successfully reconstructed pore shape, which is important for predicting ceramic morphology. After compression characterization, we found that higher solid loading and lower printing pin diameter have better strength, which can be used for further design.

P.S.F.7.

Resintering effect on high gamma phase content cemented carbideMarco Mendez, Luis Garcia

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Abstract: Mechanical properties are the most important characteristics for cemented carbides. The control of particle sintered grain size is crucial for obtaining that properties. High gamma phase cemented carbides can contain between 10 to 20% vol of cubic carbides of TaC, NbC and TiC. Resintering is needed in some cases to adjust geometrical distortions of production pieces. Therefore, the mechanical properties can be compromised due to this rework. In some cases, the final product can be out of the specifications for the appropriate field performance. We determined experimentally the grain growth and properties after each several resintering processes. The results indicate that the total carbon is not affected but that the hardness and toughness of the material is diminished with each rework. The fall in hardness is noticed and an inverted relation with toughness was found until the end of the experiment where we got a toughness decrease.

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