TWENTY-THIRD ANNUAL CONFERENCE
YUCOMAT 2022
&
TWELFTH WORLD ROUND TABLE CONFERENCE ON SINTERING
XII WRTCS

Hunguest Hotel Sun Resort, Herceg Novi, Montenegro
August 29 - September 2, 2022

Program
and
the Book of Abstracts

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

Endorsed by:
Federation of European Material Societies

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WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA & IISS

Dear Colleagues, Ladies, and Gentlemen,

It is my great pleasure to greet you on behalf of the organizers of the Materials Research Society of Serbia (MRS-Serbia) and the International Institute for the Science of Sintering (IISS) and welcome you to the 23rd YUCOMAT and the 12th World Round Table Conference on Sintering (WRTCS). I wish for the rewarding program of the two parallel conferences, a plenty of pleasant conversations with other participants, and wonderful walks in this beautiful city where we have enjoyed the hospitality of our hosts for many years now.

In the long history of organization of YUCOMAT and WRTCS, the last three years may have been the most dramatic. They have entirely changed everything we know about the organization of our special "Herceg Novi Gordon Research Conferences" with great plenary speakers and 80% of foreign participants. First, we postponed YUCOMAT 2020 to 2021 at the last moment due to the COVID-19 pandemic, when it became obvious that proceeding with it would be risky for everyone. Last year we held YUCOMAT 2021 with a smaller number of plenary sessions and about a hundred participants, full of hope that we were finally free of COVID, which would make our lives easier, just as it was before the pandemic. And indeed, by the end of 2021, we had 25 confirmed plenary speakers for YUCOMAT and 10 for WRTCS.

However, things suddenly got complicated. Not only did we not get rid of COVID, but another global threat emerged with the war in Ukraine. Since March we have been overwhelmed with a series of cancellations of plenary sessions for both Conferences, and we have also experienced a smaller number of applications for oral and poster presentations than the anticipated. The feeling of uncertainty is ever-present. Having learnt from the last year’s experience, I am afraid that we would not know the real situation before the conference starts to take place.

The Program includes 13 plenary speakers for the YUCOMAT Conference, 3 of which will have an online presentation, and 7 for the WRTCS. The number of oral and poster presentations is about 150, of which 47 is from Serbia, 31 from Ukraine, 17 from the Czech Republic, 11 from Poland, 8 from South Korea, 6 from Turkey, 4 from Montenegro, 3 from Latvia and 3 from Slovenia, whereas 9 more countries are represented by 1 or 2 presenters each. Compared to the years prior to 2021, when most of the researchers came from the USA, the European Union, and the Far East, the structure of the participants is similar to the last year, when most participants came from Serbia, the Czech Republic, and Poland.

This year's winner of the MRS-Serbia Award for Lasting and Outstanding Contribution to Materials Science and Engineering is Richard W. Siegel, Rensselaer Polytechnic Institute Professor, Member of the International Advisory Board of our Society, and a plenary speaker at many YUCOMAT Conferences. He is a scientist and innovator with an enormous contribution to Materials Science and Engineering, and the complete nomination can be found in the Program and the Book of Abstracts. Professor Siegel is here and he will present his lecture to us a little later.

One of the important activities of our Society, ever since its establishment, has been the encouragement of young researchers through the competition for the best doctoral thesis between the two Conferences, and the best oral and poster presentations. The total number of winners so far is close to 100, with an almost equal number of domestic and foreign award winners (https://www.mrs-serbia.org.rs/index.php/about-us-m/mrs-serbia-past-present-and-future-1995-2020). As of 2021, MRS-Singapore joined us in this activity, and now they also financially support 10 award winners. At this Opening Ceremony, immediately after this speech, last year's winners will receive a diploma and a small compensation. At this year's Conference, we have 47 young researchers, 31 competing for the best poster presentations and 16 for the best oral presentations. They will receive 10 awards in total and the winners will be announced at the Closing of the Conference on Friday.

It is my great pleasure to tell you that after fifteen years of inactivity, we have renewed the work of the International Institute for Sintering Science (https://www.iiss-sci.org/index.php). In 2019, together with YUCOMAT, we organized the 11th WRTCS and that was when we elected fifteen new active IISS members. This year, we have elected approximately thirty new members, including the full, the corresponding, and the honorary. From the time IISS was formed, in 1969, until now, a total of more than 200 distinguished "sinterers" were selected, which makes it a kind of an Academy. The total number of active members is currently more than 100, which gives us a hope and justifies our expectation of return to the old paths of glory. At the Managing Board Meeting on Tuesday, August 30, we will discuss how to make this happen. All suggestions are welcome.

Many participants from all over the world paraded through this and other halls within the YUCOMAT and the WRTCS conferences. During the 25 years of existence of MRS-Serbia, 4,200 lectures were held by authors from around 60 countries, of which more than 400 were plenary. The first Sintering Conference was held in 1969 at this very building, and despite the fifteen-year long hiatus, more than 2500 lectures were held in total, be it here, in Herceg-Novi, the cities of the former Yugoslavia or across Europe, North America, Far East, *etc*. The First Yugoslav-Ukrainian school (conference) was held in this hall on powder metallurgy in 1966, which, with the input of German and USA colleagues, formed the nucleus for the formation of IISS in 1969. At that time, researchers like I. N. Francevich, I. M. Fedorchenko, Ya. E. Geguzin, V. V. Skorohod, P. S. Kisliy, V. A. Lavrenko and others wrote bright pages of the sintering history. Many of their followers in Ukraine and abroad still do it.

To reduce the strained relations that might have arisen between Russian scientists and the international research community, immediately after the invasion of Ukraine, the Ministry of Science and Higher Education of the Russian Federation made a decision (March 21, 2022) that Russian scientists would not participate at international conferences in 2022. On the other side, in these difficult moments for our colleagues in Ukraine, about thirty of them will be with us, some here in the hall, some with online lectures. I want to take a moment and personally thank Drexel University, AFOSR, Office in London, and MRS-Serbia for the support given to our Ukrainian colleagues.

Finally, I wish us all a pleasant stay in Herceg-Novi, another successful and memorable conference, and of course, a safe journey home.

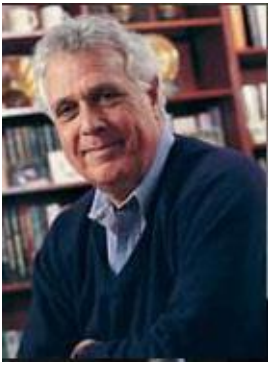
Sincerely Yours,

Dragan Uskoković

2022 MRS-SERBIA AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

We are pleased to announce that the laureate of the 2022 **MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering** is

Prof. Dr. Richard W. Siegel



He is awarded for his achievements in the materials science and nano-technology- science and innovation.

This is the decision of the MRS-Serbia Executive Board:
The Executive Board of the MRS- Serbia Presidency, at their online meeting on 15. 02. 2022, considered the submitted nomination for the MRS-Serbia's 2022 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering. It is concluded that the procedure was conducted in accordance with the Awarding Rulebook, that the Call was announced on the MRS- Serbia's website on December 31st, 2021, and that in the stipulated period of 45 days two candidates were submitted:

- **Prof. Dr. Richard W. Siegel**
- **Prof. Dr. Knut Urban**

Having received the opinion from the Expert Committee members: Prof. Dr. Dragan Uskoković (President of MRS- Serbia), Prof. Yury Gogotsi (Chair of YUCOMAT Conferences International Advisory Board and as 2021 Laureate), Prof. Robert Sinclair (Honorary Chair of YUCOMAT Conferences International Advisory Board and as 2020 Laureate), Prof. Dejan Raković (Vice-President of MRS-Serbia), Dr. Slobodan Milonjić (President of the Council and Member of the Presidency of MRS-Serbia), Prof. Dr. Nenad Ignjatović (Member of the Presidency and Secretary General of MRS-Serbia) and Prof. Dr. Ivan Bozovic as 2015 Laureate, Prof. Dr. Gordana Vunjak- Novaković as 2016 Laureate, Prof. Dr. Velimir Radmilović as 2017 Laureate, Prof. Dr. László Forró as 2018 Laureate and Prof. Danilo Suvorov as 2019 Laureate, the Executive Board of the MRS-Serbia Presidency took the decision that Prof. Dr. Richard W. Siegel should be granted MRS-Serbia's 2022 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering while Prof. Dr. Knut Urban should be Laureate of 2023 MRS- Serbia Award. Prof. Dr. Richard W. Siegel was strongly supported by Prof. Dr. Dragan Uskoković, Dr. Slobodan Milonjic, Prof. Dr. Velimir Radmilović, Prof. Dejan Raković, Prof. Dr. Nenad Ignjatović, Prof. Dr. Đorđe Janaćković and Prof. Dr. Petar Uskoković.

Prof. Dr. Richard W. Siegel's invited plenary lecture will be presented during the Opening Ceremony of the 23rd MRS-Serbia Annual Conference YUCOMAT 2022, starting at 9.00 a.m. on Monday, August 29, 2022.

President of MRS-Serbia, Prof. Dr. Dragan Uskoković
Vice-President of MRS-Serbia, Prof. Dr. Velimir Radmilović
Vice-President of MRS-Serbia, Prof. Dr. Dejan Raković
Vice-President of MRS-Serbia, Dr. Smilja Marković
General Secretary of MRS-Serbia, Prof. Dr. Nenad Ignjatović

MATERIALS RESEARCH SOCIETY OF SERBIA

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President: Dragan Uskoković
Vice-presidents: Velimir Radmilović, Dejan Raković, Smilja Marković
General Secretary: Nenad Ignjatović
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YUCOMAT 2022

Conference Organising Committee
Chairpersons: Đorđe Veljović, Zoran Jovanović
Members: Branko Matović, Irena Nikolić, Bojana Obradović, Vuk Radmilović, Veljko Đokić, Ljiljana Damnjanović, Sonja Jovanović, Aleksandar Dekanski, Mira Vukčević, Željko Radovanović
Conference Managers: Ivana Kovačević, Dušana Nedović, Jasmina Jevtić

Conference Technical Committee
Ivana Dinić, Željko Mravik, Vukašin Ugrinović, Tamara Matić, Marija Milivojević, Milica Stefanović, Ivana Banićević, Marija Stevanović, Jelena Petrović, Anđela Radisavljević, Nemanja Barać, Marko Jelić

HISTORY

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).

INTERNATIONAL INSTITUTE FOR THE SCIENCE OF SINTERING

Managing Board

President:	Prof. Danilo Suvorov
President of Managing Board:	Prof. Dragoljub P. Uskoković
Members of Managing Board:	Prof. Rajendra Bordia, Prof. Suk-Joong L. Kang, Prof. Bernd Kieback, Prof. Zoran S. Nikolić, Prof. Eugen A. Olevsky, Prof. Andrey B. Ragulya, Prof. Masahiro Yoshimura
Conference Local (Serbia) Co- chair:	Biljana Stojanović, Đorđe Janaćković

The International Institute for the Science of Sintering (IISS https://www.iiss-sci.org) was originally established in 1968 as the International Team of Study of Sintering, based in Belgrade, Yugoslavia (today the Republic of Serbia) at the Vinča Institute of Nuclear Science. The founding assembly was held next year in Herceg Novi, and it brought about one hundred scientists from different parts of the world. This was an open symposium where all the founders gave plenary lectures on their most up-to-date research. The team decided to organize this conference at the same place every other year. After the first one, the interest grew rapidly in the world, so by 1973 many new members joined. The International Team for the Study of Sintering soon became the International Institute for the Science of Sintering. At the initiative of the President of the Serbian Academy of Science and Arts (SASA), Pavle Savić, the Institute received the patronage of SASA and eminent institutions from the member countries. At that time, the Institute played an enormous role in bringing scientists from all over the world closer together. This was especially important during the Cold War when Yugoslavia was the only place where scientists from the East and from the West could meet. The 11th conference was held in 2019 in Herceg Novi, Montenegro (https://www.mrs-serbia.org.rs/files/50.pdf) in the same hotel resort where the first conference was organized more than 50 years ago. It re-established the activity of the Institute and marked the new beginning of new series of famous Yugoslav Sintering Conferences.

A significant rejuvenation of IISS membership was achieved during the previous XI WRTCS, 2019 in Herceg Novi, and a major revival during this year 2022. Due to intense work of the IISS members, despite the many challenges we faced due to the COVID pandemic, more than thirty reputable scientists were elected. In this relatively short period, the IISS Composes close to 100 active members now, which confirms and justifies our expectations about the restoration of the Institute. All of us are now certain we’ll reinstate it to its full glory of the 1980 and the 1990s of the last century.

XII WRTCS

Conference Organising Committee

Chairpersons: Đorđe Veljović, Zoran Jovanović

Members: Branko Matović, Irena Nikolić, Bojana Obradović, Vuk Radmilović, Veljko Đokić, Ljiljana Damnjanović, Sonja Jovanović, Aleksandar Dekanski, Mira Vukčević, Željko Radovanović

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GENERAL INFORMATION

DATE AND VENUE: The joint event YUCOMAT 2022 & XII WRTCS conferences will be held on August 29 - September 2, 2022, at the Hunguest Hotel Sun Resort, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, August 29th, at 09.00 and end on Friday, September 2nd, 2022, at 12.30.

REGISTRATION: Registration, registration fee payment, conference materials distribution, etc, will take place at the conference desk (Conference Secretariat) open on Sunday, August 28, and Monday, August 29, from 8.00 to 19.00, on Tuesday, Wednesday and Thursday 8.00-12.00 and 19.00-20.00, and on Friday from 8.00 to 12.00. At registration, the participants are requested to submit a proof of their advance registration fee payment.

VIRTUAL PRESENTATIONS: The abstracts of the Virtual Presentations are within the abstracts of the Plenary, Oral and Poster Sections in this book. Lectures are located on the YUCOMAT 2022 Conference site: *https://www.mrs-serbia.org.rs/index.php/virtual-presentation* from August 23, 2022, to 7 days after the deadline for the end of the Conference (September 10, 2022).
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INSTRUCTION FOR AUTHORS: The conference will feature Plenary Sessions, Oral Sessions, Poster Sessions, Virtual Offline Session. 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 the start of session. 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 from Tuesday to Wednesday.

CONFERENCE AWARDS: Joint Award by MRS-Singapore and MRS-Serbia at the YUCOMAT 2022 Conference. Sponsorship of the ten Awards in the financial amount by the MRS-Singapore, to the authors not older than 35 for the best: Five Oral presentation and Five Posters presentation. Awarded authors will be announced at the Closing Ceremony of the Conference. Each award consists of a financial amount honorarium, diploma, meeting registration fee to attend the next YUCOMAT 2023 Conference, and a one-year MRS Serbia membership.

ADDITIONAL ACTIVITIES: Traditional Cocktail Party on Monday evening and excursion on Thursday afternoon (boat trip around Boka Kotorska Bay) will be organized again.

GENERAL YUCOMAT 2022 & XII WRTCS CONFERENCE PROGRAM

Sunday, August 28, 2022

08.00-19.00 **Registration**

Monday, August 29, 2022

08.00-19.00 **Registration**

09.00-09.30 **OPENING CEREMONY,** Main Conference Hall

Welcome Speech - **Dragan Uskoković**, president of IISS and MRS-Serbia
Welcome Address - **Yury Gogotsi**, Chair of International Advisory Board
Presentation of the YUCOMAT 2021 Awards for young authors of the best oral and poster presentation

09.30-10.15 The Laureate of the 2022 MRS-Serbia, Award for a Lasting and Outstanding Contribution to Materials Science and Engineering, **Richard W. Siegel**

10.45-13.15 **First YUCOMAT Plenary Session**, Main Conference Hall

13.15 **Photo Session**

15.00-18.45 **Second YUCOMAT Plenary Session** , Main Conference Hall

19.30-21.30 **Cocktail Party**

Tuesday, August 30, 2022

08.30-10.00 **First YUCOMAT Poster Session,** National Restaurant Jadranka Terrace
Competition for the best Oral presentation of young researchers

10.30-14.00 **First WRTCS Plenary Session**

15.00-19.15 **First YUCOMAT Oral Session, Main Conference Hall**
Competition for the best YUCOMAT Oral presentation of young researchers

Wednesday, August 31, 2022

08.30-10.00 **Second YUCOMAT Poster Session**, National Restaurant Jadranka Terrace

10.30-12.00 **Third YUCOMAT Plenary Session**, Main Conference Hall

12.30-14.00 **Fourth YUCOMAT PLENARY** Virtual Session

Thursday, September 1, 2022

08.30-09.45 **Third YUCOMAT Poster Session**, National Restaurant Jadranka Terrace

10.00-12.45 **Second WRTCS Plenary Session,** Main Conference Hall

14.00-19.00 **Boat-trip around Boka Kotorska Bay**

Friday, September 2, 2022

08.30-11.15 **Second YUCOMAT Oral Session**, Main Conference Hall

08.30-11.45 **Third YUCOMAT Oral Session**, Small Conference Hall

12.00 **Awards and Closing of the Conference**

12.30 **Cocktail and Greetings for Goodbye**

SCIENTIFIC PROGRAM

Sunday, August 28, 2022

08^{00} - 19^{00} Registration

Monday, August 29, 2022

OPENING CEREMONY, Main Conference Hall

09.00-09.30 Welcome Speech **- Dragan Uskoković**, president of IISS and MRS-Serbia,
Welcome Address - **Yury Gogotsi**, Chair of International Advisory Board
Presentation of YUCOMAT 2021 Awards for young authors of the best oral and poster presentation

09.30-10.15 **MRS-Serbia 2022 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering**
Richard W. Siegel
Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, New York, USA
Looking Back, Moving Forward: On safari in materials with gun and camera

10.15-10.45 **Break**

FIRST YUCOMAT PLENARY SESSION, Main Conference Hall

Session I: 10.45 -13.15
Chairpersons: Sir Andre K. Geim, *Nobel Prize Winner*, Pulickel M. Ajayan

10.45-11.30 **Y.PL.S.I.1.**
Two-dimensional emptiness and its unique properties
Sir Andre K. Geim, *Nobel Prize Winner in Physics*
University of Manchester, United Kingdom

11.30-12.15 **Y.PL.S.I.2.**
Materials science with 2D atomic layers
Pulickel M. Ajayan
Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA 77005

12.15-12.45 **Y.PL.S.I.3.**
Cluster-assembled materials
Horst Hahn, Gleb Iankevich, Ramin Shadkam
Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Germany

12.45-13.15 **Y.PL.S.I.4.**
Probing structure and dynamic behaviors of topological polar solitons by electron microscopy
Xiaoqing Pan
Department of Materials Science and Engineering, Department of Physics and Astronomy, Irvine Materials Research Institute (IMRI), University of California, Irvine, CA 92697, USA

13.15-13.30 **Photo session**

13.30-15.00 **Break**

SECOND YUCOMAT PLENARY SESSION Main Conference Hall

Session I: 15.00-18.45
Chairpersons: Robert Sinclair, Yury Gogotsi, John A. Rogers

15.00-15.45 **Y.PL.S.II.1.**
Two-dimensional carbides and nitrides pave the road to future technologies
Yury Gogotsi
A.J. Drexel Nanomaterials Institute, and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA

15.45-16.30 **Y.PL.S.II.2.**
Advanced materials for health monitoring and haptic interactions
John A. Rogers
Northwestern University, Evanston, IL, USA

16.30-17.00 **Break**

17.00-17.30 **Y.PL.S.II.3.**
Correlative imaging of mineral deposits in brain tissue of Alzheimer's disease patients: application to the valence state of iron deposits by STEM-EELS
Robert Sinclair[1], Yitian Zeng[1], Philip S. Digiacomo[2], Michael M. Zeineh[3]
Departments of [1]Materials Science and Engineering, [2]Bioengineering and [3]Radiology, Stanford University, Stanford, CA 94305, USA

17.30-18.00 **Y.PL.S.II.4.**
Advances in engineering novel materials for nanomedicine
Vladimir Torchilin
Center for Pharmaceutical Biotechnology and Nanomedicine, Northeastern University, Boston, MA 02115, USA

18.00-18.30 **Y.PL.S.II.5.**
SARS-CoV-2: Molecular interaction specifics viewed through the prism of nanotechnologies
Vuk Uskoković
TardigradeNano LLC, Irvine, CA 92604, USA and Department of Mechanical Engineering, San Diego State University, San Diego, CA, USA

18.30-18.45 **Y.PL.S.II.6.**
Air force office of scientific research grant funding opportunities
David Swanson
U.S. Air Force Office of Scientific Research, European Office of Aerospace Research and Development

19.30-21.30 **Cocktail Party**

Tuesday, August 30, 2022

First YUCOMAT Poster Session, National Restaurant Jadranka Terrace
Competition for the best Poster Presentation of young researchers

Session I: 08.30-10.00
Chairpersons: Bojana Obradović and Zoran Jovanović

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

P.S.I.A.1.
Silica-based organo-inorganic hybrid materials with carboxyl groups for water purification
Viktoriia Kyshkarova[1,2], Zbigniew Wzorek[3], Anna K. Nowak[3], Inna Melnyk[1]
[1]Institute of Geotechnics, Slovak Academy of Sciences, Košice, Slovakia; [2]Technical University of Košice, Faculty of Materials, Metallurgy and Recycling, Košice, Slovakia, [3]Cracow University of Technology, Krakow, Poland

P.S.I.A.2.
Mg/Fe layered double hydroxides-based adsorbents for removal of inorganic toxicants commonly found in aquatic environments
Tetiana Hubetska, Victor Demchenko, Natalia Kobylinska
A.V. Dymansky Institute of Colloid and Water Chemistry NAS of Ukraine, Kyiv, Ukraine

P.S.I.A.3.
Supercritical CO_2 assisted deposition of $MAPbBr_3$ perovskite onto TiO_2 nanotubes
Milica Stefanović[1], Ivana Lukić[2], Jelena Vujančević[3], Rada Petrović[2] and Đorđe Janaćković[2]
[1]Innovation Center of Faculty of Technology and Metallurgy, Ltd, Belgrade, Serbia, [2]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, [3]Institute of Technical Sciences of SASA, 11000, Belgrade, Serbia

YUCOMAT SYMPOSIUM B:
ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

P.S.I.B.1.
Crystal structure prediction and investigation of mechanical properties of the SiB_6 compound through ab initio calculations
Tamara Škundrić[1,2], Dejan Zagorac[1,2], Aleksandra Zarubica[3], Jelena Zagorac[1,2], Milan Pejić[1,2], Dušica Jovanović [2,3], Peter Tatarko[4], Branko Matović[1,2]
[1]Materials Science Laboratory, Institute of Nuclear Sciences "Vinča", University of Belgrade, Belgrade, Serbia, [2]Center for synthesis, processing and characterization of materials for application in the extreme conditions "CextremeLab", Belgrade, Serbia, [3]Department of Chemistry, Faculty of Sciences and Mathematics, University of Niš, Niš, Serbia, [4]Institute of Inorganic Chemistry, Slovak Academy of Sciences, 845 36 Bratislava, Slovakia

P.S.I.B.2.
The influence of high-temperature annealing on the evolution of precipitates in Inconel 625 superalloy additively manufactured by laser powder bed fusion
Sylwia Staroń, Kewin Gola, Beata Dubiel
AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Al. A. Mickiewicza 30, 30-059 Kraków, Poland

P.S.I.B.3.

The kinetics of γ'' and δ phase precipitation during the high temperature annealing of Inconel 625 additively manufactured by laser powder bed fusion

Hubert Pasiowiec, Beata Dubiel, Kewin Gola
AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Al. A. Mickiewicza 30, 30-059 Kraków, Poland

P.S.I.B.4.

Cellulose nanocrystals with different surface functionalities as outstanding scaffolds for supercapacitor materials

Gordana Backović, Wim Thielemans
Sustainable Materials Lab, Department of Chemical Engineering, KU Leuven, campus Kulak Kortrijk, Etienne Sabbelaan 53, 8500 Kortrijk, Belgium

P.S.I.B.5.

A hierarchically porous all-polysaccharide composite anode for an asymmetric supercapacitor

Julien Lemieux, Wim Thielemans
Sustainable Materials Lab, Department of Chemical Engineering, KU Leuven, campus Kulak Kortrijk, Etienne Sabbelaan 53, 8500 Kortrijk, Belgium

P.S.I.B.6.

Aqueous multivalent-ion chemistry of vanadium oxides: Novelties and Challenges

Milica J. Vujković
University of Belgrade-Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

P.S.I.B.7.

pH-triggered sol-gel synthesis of $Na_4Fe_3(PO_4)_2P_2O_7$ cathode material

Aleksandra Gezović[1], Miloš Milović[2], Danica Bajuk-Bogdanović[3], Veselinka Grudić[1], Slavko Mentus[3,4], Milica Vujković[3]
[1]University of Montenegro, Faculty of Metallurgy and Technology, Cetinjski put bb, Podgorica, Montenegro, [2]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Knez Mihajlova 35/IV, 11158 Belgrade, Serbia, [3]University of Belgrade, Faculty of Physical Chemistry, Studentski Trg 12–16, Belgrade, Serbia, [4]Serbian Academy of Sciences and Arts, Knez Mihajlova 35, Belgrade, Serbia

P.S.I.B.8.

Experimental evaluation of mechanical anisotropic material behaviour of carbon reinforced PET-G material

Milan Janković[1], A. Petrović[1], V. Lojpur[2], S. Dikić[3], M. Miloš[1], I. Balać[1]
[1]Faculty of Mechanical Engineering, University of Belgrade, Kraljice Marije 16, 11000 Belgrade, Serbia, [2]Vinča Institute of Nuclear Sciences, University of Belgrade, Mike Pertovića Alasa 12-14, Vinča, 11000 Belgrade, Serbia, [3]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia

P.S.I.B.9.

Fluidising low temperature thermochemical energy storage materials: degredation and damage assesment

Louis F. Marie, Tadhg S. O'Donovan
Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom

YUCOMAT SYMPOSIUM C: **NANOSTRUCTURED MATERIALS**

P.S.I.C.1.

Investigation of 3D printing and thermomechanical properties of free-radical resin filled with TiO_2 nanoparticles

Juraj Svatík, Martina Korčušková, Martina Štaffová, Veronika Sevriugina, František Ondreáš, Petr Lepcio
Central European Institute of Technology, Brno University of Technology, Purkyňova 656/123, 61200 Brno, Czech Republic

P.S.I.C.2.

Thiacarbocyanine dye TCC: features of J-aggregation in aqueous solutions and polymer films

Polina Pisklova[1,2], Iryna Ropakova[1], Svitlana Yefimova[1], Alexander Sorokin[1]
[1]Institute for Scintillation Materials of NAS of Ukraine, Kharkiv, Ukraine, [2]Institute of Physics, University of Rostock, Rostock, Germany

P.S.I.C.3.

Influence of physical cross-linking by montmorillonite on structure and thermostability of hydrogel composites based on polyacrylamide

Olena Siryk[1], Katarzyna Szewczuk-Karpisz[2], Olena Goncharuk[1], Yurii Samchenko[1], Dariusz Sternik[3]
[1]Ovcharenko Institute of Biocolloidal Chemistry National Academy of Sciences of Ukraine, Akademika Vernadskogo Blvd. 42, 03680, Kyiv, Ukraine, [2]Institute of Agrophysics, Polish Academy of Sciences, Doświadczalna 4, 20-290 Lublin, Poland, [3]Maria Curie-Sklodowska University, M.C. Sklodowska Sq.3, 20031 Lublin, Poland

P.S.I.C.4.

Effect of polymer molecular weight on thermal and surface structural characteristics of MWCNTs/PDMS nanocomposites

Iryna Sulym[1], Mykola Borysenko[1], Yuriy Sementsov[1], Dariusz Sternik[2], Anna Derylo-Marczewska[2]
[1]Chuiko Institute of Surface Chemistry of NASU, 17 General Naumov Str., 03164 Kyiv, Ukraine, [2]Maria Curie-Skłodowska University, pl. Maria Curie-Skłodowskiej 3, 20-031 Lublin, Poland

YUCOMAT SYMPOSIUM D: **ECO-MATERIALS AND ECO-TECHNOLOGIES**

P.S.I.D.1.

Waterborne polyurethanes based on poly(dimethylsiloxane)

Ivan Stefanović[1], Jasna Džunuzović[1], Enis Džunuzović[2], Carla Marega[3]
[1]Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia, [3]Department of Chemical Sciences, University of Padova, via Marzolo 1, 35131 Padova, Italy

P.S.I.D.2.

Structural characterization of geopolymers with the addition of egg shell

Sanja Knežević[1], Marija Ivanović[1], Miljana Mirković[1], Ljiljana Kljajević[1], Miloš Nenadović[2], Vladimir Pavlović[3], Snežana Nenadović[1]

[1]Department Department of Materials, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia,University of Belgrade, Mike Petrovića Alasa 12-14, Vinča, 11000 Belgrade, Serbia, [2]Department of Atomics Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, Mike Petrovića Alasa 12-14, Vinča, 11000 Belgrade, Serbia, [3]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, University of Belgrade, Belgrade, Serbia

P.S.I.D.3.

Sequential extractions and leaching tests as methods for characterization of mine tailings for the purpose of their probable application in eco-friendly geopolymers

Lyudmila Angelova, Darya Ilieva, Temenuzhka Radoykova, Andriana Surleva

University of Chemical technology and Metallurgy,8 „St. Kl. Ohridski” blvd., 1756 Sofia, Bulgaria

P.S.I.D.4.

Obtaining and characterising Cu-infused antimicrobial films formed from regenerated cellulose-$CaCO_3$ composite

Aleksandra Ivanovska[1], Nemanja Barac[1], Vesna Radojević[2], Petar Uskoković[2], Đorđe Janacković[1,2], Ernest Barcelo[3,4], Patrick Gane[2,4], Mirjana Kostic[1]

[1]University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy in Belgrade Ltd., Karnegijeva 4, 11000 Belgrade, Serbia, [2]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia, [3]Omya International AG, Baslerstrasse 42, 4665 Oftringen, Switzerland, [4]Aalto University, Department of Bioproducts and Biosystems, School of Chemical Engineering, 00076 Aalto, Helsinki, Finland

P.S.I.D.5.

Comparative study of biomass-derived carbon interfacial processes in Aluminum-based and conventional acidic electrolyte

Jana Mišurović[1], Aleksandra Gezović[1], Jugoslav Krstić[2], Branislav Milovanović[3], Veselinka Grudić[1], Slavko Mentus[3], Milica Vujković[3]

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YUCOMAT SYMPOSIUM E:
BIOMATERIALS

P.S.I.E.1.

Laser-induced chemical and mophological changes of the titanium alloy surface under different irradiation parameters

Slađana Laketić[1], Marko Rakin[2], Miloš Momčilović[1], Jovan Ciganović[1], Đorđe Veljović[2], Ivana Cvijović-Alagić[1]

[1]Institute of Nuclear Sciences „Vinča“, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia; [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia

P.S.I.E.2.

Search for "needles" of hydroxyapatite in the "haystack" of ovarian cancer

Ruslana Chyzhma, Roman Moskalenko
Sumy State University, Sumy, Ukraine

P.S.I.E.3.

The role of oxalate nanocrystalline for the differential diagnostics of the breast pathology

Olena Kolomiiets[1], Artem Piddubnyi[1,2], Serhey Danilchenko[3], Roman Moskalenko ,[2]
[1]Department of Pathology, Sumy State University, Sumy, Ukraine, [2]Ukrainian-Swedish Research center SUMEYA, Sumy State University, Sumy, Ukraine, 3 Institute of Applied Physics, NAS of Ukraine, Sumy, Ukraine

P.S.I.E.4.

Optimisation of a 3D in vitro model for osteosarcoma cell cultivation

Ivana Banićević[1], Jelena Petrović[2], Milena Milivojević[3], Milena Stevanović[3,4,5], Radmila Janković[6], Jasmina Stojkovska[1,2], Bojana Obradović[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, [3]University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia, [4]University of Belgrade, Faculty of Biology, Belgrade, Serbia, [5]Serbian Academy of Sciences and Arts, Belgrade, Serbia, [6]University of Belgrade, School of Medicine, Belgrade, Serbia

P.S.I.E.5.

Development of a 3D in vitro model based on alginate microfibers with immobilized cancer cells for cancer research and anticancer drug testing

Jelena Petrović[1,2], Ivana Banicević[1], Jasmina Stojkovska[1,2], Miodrag Dragoj[3], Milica Pešić[3], Milena Milivojević[4], Milena Stevanović[4,5,6], Bojana Obradović[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia; [3]University of Belgrade, Institute for Biological Research "Sinisa Stanković" - National Institute of the Republic of Serbia, Belgrade, Serbia, [4]University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia, [5]University of Belgrade, Faculty of Biology, Belgrade, Serbia, [6]Serbian Academy of Sciences and Arts, Belgrade, Serbia

P.S.I.E.6.

PCL-MXene composite electrospun membrane for nerve regeneration: structural and biological assessment

Kateryna Diedkova[1], Yevhen Samokhin[1], Veronika Zahorodna[2], Ivan Baginskiy[2], Vitalii Balitskyi[2], Oleksiy Gogotsi[2], Viktoriia Korniienko[1]
[1]Sumy State University, 31 Sanatorna St, Sumy 40007, Ukraine, [3]Materials Research Centre, 3 Krzhizhanovskogo St, Kyiv 03680, Ukraine

P.S.I.E.7.

3D printed calcium phosphate cement scaffolds loaded with liposomal antibacterial enzymes for the prevention of osteomyelitis

Zuzana Kadlecová, Kristýna Hlináková, Lucy Vojtová
Central European Research Institute, Brno University of Technology

P.S.I.E.8.
Hydrogel dressings for phage therapy of chronic wounds
E. Černá[1], L. Vacek[2], F. Růžička[2], B. Lipový[3], M. Benešík[4], T. Botka[4], R. Pantůček[4],L. Vojtová[1]
[1]Central European Institute of Technology, Brno University of Technology, Brno, Czech Republic; [2]Department of Microbiology, St. Anne's University Hospital Brno and Faculty of Medicine, Masaryk University, Brno, Czech Republic; [3]Department of Burns and Plastic Surgery, University Hospital Brno and Facultyof medicine, Masaryk University, Brno, Czech Republic; [4]Section of Genetics and Molecular Biology, Faculty of Science, Masaryk University, Brno, Czech Republic

P.S.I.E.9.
Biomechanical DMA characterization of calcium and barium alginate hydrogel scaffolds
Alexandra Zühlke[1], Ivana Banićević[2], Bojana Obradović[2], Michael Gasik[1]
[1]Aalto University Foundation, Espoo, Finland. [2]University of Belgrade, Belgrade, Serbia

P.S.I.E.10.
Hydroxyl radical scavenging activity of titanium oxide nanocrystals
Pavel Maksimchuk[1], Kateryna Hubenko[1], Vladyslav Seminko[1], Andrey Onishchenko[2], Iryna Bespalova[1], Anatolii Onishchenko[3], Volodymyr Prokopiuk[3], Anton Tkachenko[3], Svetlana Yefimova[1]
[1]Department of Nanostructured Materials, Institute for Scintillation Materials NAS of Ukraine, Kharkiv, Ukraine, [2]Department of Physics, Kharkiv National University of Radio Electronics, Kharkiv, Ukraine, [3]Research Institute of Experimental and Clinical Medicine, Kharkiv National Medical University, Kharkiv, Ukraine

P.S.I.E.11* Magnesium alloy with yttrium, gadolinium and calcium alloying elements designed for aviation applications
Jitka Strásk á[1], Stanislav Šašek[1], Peter Minárik[1], Robert Král[1], Jozef Veselý[1], Jiří Kubásek[2]
[1]Charles University, Faculty of Mathematics and Physics, Department of Physics of Materials, Ke Karlovu 5, 121 16 Praha, Czech Republic, [2]University of Chemistry and Technology, Faculty of Chemical Technology, Department of Metals and Corrosion Engineering, Technická 5, 166 28 Praha, Czech Republic

P.S.I.E.12* Resonance ultrasound spectroscopy measurements of elastic modulus of biomedical Ti-based alloys prepared by SPS
Josef Stráský[a], Jiří Kozlík[a], Dalibor Preisler[a], Hanuš Seiner[b], Michaela Janovská[b], Martin Koller[b], Miloš Janeček[a]
[a]Department of Physics of Materials, Faculty of Mathematics and Physics, Charles University, Czechia, [b]Institute of Thermomechanics, Czech Academy of Sciences, Czechia

***They do not participate in the Competition for the best Poster Performance of young researchers**

10.00-10.30 **Break**

First WRTCS Plenary Session, Main Conference Hall

Session I: 10.30-14.00
Chairpersons: Eugene A. Olevsky, Suk-Joong L. Kang

10.30-11.00 **W.PL.S.I.1**
Sintering assisted additive manufacturing
Eugene A. Olevsky
San Diego State University

11.00-11.30 **W.PL.S.I.2.**
Challenges and opportunities for machine learning approaches for sintering and microstructure development
Rajendra Bordia, Fei Peng
Materials Science and Engineering, Clemson University,Clemson, SC 29634 USE

11.30-12.00 **W.PL.S.I.3.**
Electric field assisted sintering of oxide ceramics: fields matter!
Olivier Guillon
Institute of Energy and Climate Research: Materials Synthesis and Processing Forschungszentrum Jülich GmbH & RWTH Aachen University, Germany

12.00-12.30 **Break**

12.30-13.00 **W.PL.S.I.4.**
Enhancing powder metallurgy processing using advanced microstructural characterization and physical metallurgy
Hamish L. Fraser
Center for the Accelerated Maturation of Materials, Department of Materials Science and Engineering, The Ohio State University, Columbus OH, USA

13.00-13.30 **W.PL.S.I.5.**
The role of sintering in process design for aerosol synthesis of nanostructured materials
Sotiris E. Pratsinis
Particle Technology Laboratory, Institute of Process Engineering, Swiss Federal Institute of Technology (ETH Zurich), CH-8092 Zurich, Switzerland

13.30-14.00 **W.PL.S.I.6.**
Grain growth: the mixed control mechanism of atom transport
Suk-Joong L. Kang
KAIST, Daejeon, Korea

14.00-15.00 **Break**

First YUCOMAT Oral Session, Main Conference Hall
Competition for the best Oral Presentation of young researchers

Session I: 15.00-19.15
Chairpersons: Snežana Lazić, Vuk Radmilović

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

15.00-15.15 **O.S.I.A.1.**
Characterization of thin films obtained using pulsed laser deposition technique
Agnieszka Radziszewska, Kazimierz Kowalski, Tomasz Moskalewicz
AGH University of Science and Technology, Krakow, Poland

15.15-15.30 **O.S.I.A.2.**
Selective laser melting technology of hot work tool steel influenced by remelting method without preheating of the base plate
K. Fryzowicz, R. Dziurka, R. Bardo, P. Bała
AGH Univeristy of Science and Technology, Cracow, Poland

15.30-15.45 **O.S.I.A.3.**
Effect of sodium on phase transformation of gamma-alumina
Darya Farrokhnemoun
Materials Science and Nanoengineering, Sabanci University, Orta Mahalle, Tuzla, Istanbul, 34956, Turkey

15.45-16.00 **O.S.I.A.4.**
Densification and microstructural evolution of Na-doped alphaalumina
Shahrzad Sajjadivand, Mehmet Ali Gülgün
Sabanci University, Tuzla, Istanbul, 34956, Turkey

YUCOMAT SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

16.00-16.15 **O.S.I.B.1.**
Graphene supported PdAu nanoparticles as catalyst for hydrogen evolution reaction
Lazar Rakočević[1],Irina Srejić[1],Aleksandar Maksić[1],Jelena Golubović[2],Svetlana Štrbac[2]
[1]INS Vinca, Department of Atomic Physics, University of Belgrade, Mike Alasa 12-14, 11001 Belgrade, Serbia, [2]Institute of Chemistry, Technology and Metallurgy, Department of Electrochemistry, University of Belgrade, Njegoseva 12, 11000 Belgrade, Serbia

16.15-16.30 **O.S.I.B.2.**
Metal-ceramic composites based on reinforced ceramics
Ievgen Solodkyi, Sergii Teslia, Iurii Bogomol, Petro Loboda
Igor Sikorsky Kyiv Polytechnic Institute, 35 Politechnichna Str., Kyiv, 03056, Ukraine

16.30-16.45 **O.S.I.B.3.**
Suspension plasma spraying of $BaTiO_3$ and $BaTiO_3/ZrO_2$
Vojtech Marak[1], Daniel Drdlik[1,2], Dapeng Zhou[3], Robert Vaßen[3]
[1]CEITEC BUT, Brno University of Technology, Purkynova 123, 612 00 Brno, Czech Republic, [2]Faculty of Mechanical Engineering, Brno University of Technology, Technicka 2, 616 69 Brno, Czech Republic, [3]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research IEK-1, 524 25 Jülich, Germany

16.45-17.00 **O.S.I.B.4.**
Investigation of the dynamics of deformation mechanisms in Mg-Gd alloys
Andrea Szabóová[1], Kristián Máthis[1], Daria Drozdenko[1], Michal Knapek[1], Gergely Farkas[2], Gergely Németh[2], Petr Harcuba[1]
[1]Department of Physics of Materials, Faculty of Mathematics and Physics, Charles University, 121 16 Prague 2, Ke Karlovu 5, Czech Republic, [2]Nuclear Physics Institute, Czech Academy of Sciences, 250 68 Řež, Husinec - Řež, čp. 130, Czech Republic

17.00-17.15 **O.S.I.B.5.**
Investigations of pressed and sintered components using 17-4PH powder collected in the chamber of an SLM printer
Mohammed Qasim Kareem, Tamás Mikó, Gréta Gergely, Zoltán Gácsi
Institute of Physical Metallurgy, Metalforming and Nanotechnology, University of Miskolc, Hungary

17.15-17.45 **Break**

YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS

17.45-18.00 **O.S.1.C.1.**

Electrochemically-grown Cu_2O nanocubes favorably electroreduce CO_2 to methane: What triggers the activity?

S. Popović[1,2], M. A. Nazrulla[1], N. Hodnik[1,2]

[1]Department of Materials Chemistry, National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia, [2]University of Nova Gorica, Vipavska 13, 5000 Nova Gorica, Slovenia

18.00-18.15 **O.S.1.C.2.**

N-Heterocyclic carbenes - the design concept for densely packed and thermally ultra-stable aromatic self-assembled monolayers

Mateusz Wróbel,[1] Daria M. Cegiełka,[1] Andika Asyuda,[2] Krzysztof Kozieł,[3] Michael Zharnikov[2] and Piotr Cyganik[1]

[1]Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Krakow, Poland, [2]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany, [3]Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Poland

18.15-18.30 **O.S.1.C.3.**

Probing improper ferroelectricity in oxygen-deficient $YMnO_3$ ultrathin films

Alexander Vogel[1,2], Alicia Ruiz-Caridad[1], Johanna Nordlander[2,3], Morgan Trassin[2], Marta D. Rossell[1]

[1]Electron Microscopy Center, Empa, Swiss Federal Laboratories for Material Science and Technology, Dübendorf, Switzerland, [2]Department of Materials, Eidgenössische Technische Hochschule Zürich, Zürich, Switzerland, [3]Department of Physics, Harvard University, Cambridge, MA, United States of America

YUCOMAT SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

18.30-18.45 **O.S.1.D.1.**

Effect of metakaolin and lime on strength development of blended cement paste

Kosar Hassannezhad, Yasemin Akyol, Mehmet Can Dursun, Cleva Ow-Yang, Mehmet Ali Gulgun

Sabanci University, Istanbul, Turkey

YUCOMAT SYMPOSIUM E: BIOMATERIALS

18.45-19.00 **O.S.I.E.1.**

Nanoparticles in our brains

Anastasiia Denysenko, Roman Moskalenko

Department of Pathology, Sumy State University, Sumy, Ukraine

19.00-19.15 **O.S.I.E.2.**

Sintering of biodegradable Mg-Y and Mg-Nd magnesium alloys fabricated for medical applications

[1]Mária Zemková, [2]František Lukáč, [2]Zdeněk Dlabáček, [1]Robert Král, [1]Peter Minárik
[1]Charles University, Prague, Czech Republic, [2]Institute of Plasma Physics, Czech Academy of Science, Prague, Czech Republic

Wednesday, August 31, 2022

Second YUCOMAT Poster Session, National Restaurant Jadranka Terrace

Session I: 08.30-10.00
Chairperson: Đorđe Veljović, Sonja Jovanović

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

P.S.II.A.1.
Synthesis and characterization of glass-ceramic-metal composite materials obtained by sintering
Vladimir Pavkov[1], Gordana Bakić[2], Vesna Maksimović[1], Dušan Bučevac[1], Marija Prekajski Đorđević[1], Branko Matović[1]
[1]Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, [2]Faculty of Mechanical Engineering, University of Belgrade, Serbia

P.S.II.A.2.
Positronics science in the contemporary nanocomposites engineering: towards guided functionality of PVP-nanosized glassy arsenoselenides
Oleh Shpotyuk[1,2], Adam Ingram[3], Yaroslav Shpotyuk[4,5], Jacek Filipecki[1]
[1]O.G.Vlokh Institute of Physical Optics, Lviv, Ukraine, [2]Jan Dlugosz University in Czestochowa, Czestochowa, Poland, [3] Opole University of Technology, Opole, Poland, [4]University of Rzeszow, Rzeszow, Poland, [5]Ivan Franko National University of Lviv, Lviv, Ukraine

P.S.II.A.3.
Novel technology for production of nanopowders by electroerosion dispersion method
Gennadii Kochetov, Mykola Monastyrov, Tetiana Prikhna, Dmytro Samchenko
Kyiv National University of Construction and Architecture, Kyiv, Ukraine

P.S.II.A.4.
New directions of arylamines oxidation with H_2O_2: polymerization of aniline in the presence of para-aminodiphenylamine
Jana Mišurović[1], Gordana Ćirić-Marjanović[2]
[1]University of Montenegro-Faculty of Metallurgy and Technology, Cetinjski put bb. 81000 Podgorica, Montenegro, [2]University of Belgrade-Faculty of Physical Chemistry, Studentski Trg 12–16, 11158 Belgrade, Serbia

P.S.II.A.5.
Laser processing structure optimization of the metal materials created using additive technologies
I. Galstian, Y. Len, M. Shevchenko, O. Gerasimov, S. Mulenko, I. Sydorchenko, M. Yakymchuk, D. Savvakin, M. Rud, S. Smolnik
G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine

YUCOMAT SYMPOSIUM B:
ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

P.S.II.B.1.
Reduced mobility for H3 + in n-Butanol gas

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

P.S.II.B.2.
Intrinsic magnetic properties of the $RFe_{11}Ti$ (R = Y, Gd and Pr) by Zr, Co and C doping

Diana Benea, Razvan Hirian, Simona Gutoiu[1] and Viorel Pop
Babes-Bolyai University, Cluj-Napoca, Romania,[1]INCDTIM Cluj-Napoca, Romania

P.S.II.B.3.
Lanthanides-doped tellurite glasses: A new screen material candidate for volumetric 3D display applications

Naji Vahedigharehchopogh, Orhan Kıbrıslı, Miray Çelikbilek Ersundu, Ali Erçin Ersundu
Yildiz Technical University, Faculty of Chemical and Metallurgical Engineering, Department of Metallurgical and Materials Engineering, Glass Research and Development Laboratory, Istanbul, 34220, Turkey

P.S.II.B.4.
Phosphorescence decay kinetics of the Becquerel type in YAP:Mn

Sergii Ubizskii[1], Oleh Buryy[1], Volodymyr Degoda[2], Halyna Podust[2]
[1]Lviv Polytechnic National University, Lviv, Ukraine, [2]Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

P.S.II.B.5.
Organic and Perovskite Solar Cells-Which Wet Will Win the Bet?

Vuk V. Radmilović[1], Yi Hou[2], Fei Guo[2], Christoph J. Brabec[2], Erdmann Spiecker[3], Velimir R. Radmilović[4]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Serbia; [2]Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander-University Erlangen-Nuremberg, Germany; [3]Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich –Alexander-University of Erlangen-Nuremberg, Germany; [4] Serbian Academy of Sciences and Arts, Belgrade, Serbia

P.S.II.B.6.
Synthesis and properties of stable nitrogen-doped MWCNTs for thermoelectric applications

Mikhail V. Katkov[1], Krisjanis Buks[1], Jana Andzane[2], Anatolijs Šarakovskis[3], Krišjānis Šmits[3] and Donats Erts[2]
[1]D Strong Ltd, Instituta str. 36-17, Ulbroka, Latvia, LV-2130, [2]Institute of Chemical Physics, Faculty of Chemistry, University of Latvia, Raina blvd. 19, Riga, Latvia, LV-1586, [3]Institute of Solid State Physics, University of Latvia, Kengaragastr. 8, Riga, Latvia, LV-1063

P.S.II.B.7.

Fabrication and characterization of high entropy pyrochlore ceramics

Branko Matović[1], Dejan Zagorac[1], Ivana Cvijović-Alagić[1], Jelena Zagorac[1], Svetlana Butulija[1], Jelena Erčić[1], Ondrej Hanzel[2], Richard Sedlák[3], Maksym Lisnichuk[4], Peter Tatarko[2]

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P.S.II.B.8.

Discrimination of the exhaled compound of lung cancer patients and healthy subjects by a biosensor based on essential 20 amino acids.

Gyeong-Ha Bak[1], Eun Jung-Choi[2], Thanh Mien Nguyen[1],Minsu Jang[1], Jung-Geun Lee[3], Nayeoung Kim[2], Yeong Ju Lee[2], Jin-Woo Oh[1,2 3]

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P.S.II.B.9.

Three-dimensional plasmonic nanoclusters for high sensitivity SERS platform development

Minsu Jang[1], Gyeong-Ha Bak[1], Thanh Mien Nguyen[1], Jung-Geun Lee[2], Nayeoung Kim[3], Yeong Ju Lee[3], Eun-Jung Choi[3], Jin-Woo Oh[1,2,3]

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P.S.II.B.10.

Dielectric properties of polyvinyl alcohol composites with improved ionic conductivity

T. A. Filip[1,2], C. Hamciuc[3], T. Vlad-Bubulac[3], I. Turcan[1,2], M. Olariu[1,2]

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P.S.II.B.11.

Synthesis and characterization of iridium oxide based films

Ljiljana Gajić-Krstajić, Mila Krstajić Pajić[1], Piotr Zabinski[2], Vladimir Jović[3], Uroš Lacnjevac[3], Nevenka R. Elezović[3]

Institute of Technical Sciences of the Serbian Academy of Science and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia, [1]University of Belgrade Faculty of Technology and metallurgy, 11000 Belgrade, [2]AGH University of Science and Technology, Faculty of Non-Ferrous Metals, Al. Mickiewicza 30, 30-059 Krakow, Poland, [3]University of Belgrade Institute for Multidisciplinary Research, 11030 Belgrade, Kneza Viseslava 1, Serbia

P.S.II.B.12.

3D printed auxetic structures with enhanced energy absorption

Martina Šťaffová, Petr Lepcio, Juraj Svatík, Martina Korčušková, František Ondreáš

Central European Institute of Technology, Brno, University of Technology, Purkynova 656/123, Brno 612 00, Czech Republic

P.S.II.B.13.

Effect of molten salts and high temperatures on the corrosion resistance of materials

Jana Rejková, Marie Kudrnová

Department of Power Engineering, University of Chemistry and Technology, Prague, Czech Republic

P.S.II.B.14.

Surface characterization of chromium nickel alloys in molten salts using x-ray photoelectron spectroscopy (XPS)

Marie Kudrnová[1,2], Jana Rejková[1], Hana Juklíčková[1]

[1]University of Chemistry and Technology, Department of Power Engineering[1], Central Laboratories[2], Technická 5, Prague 6, 16628, Czech Republic

P.S.II.B.15.

Selection of container materials for deep repositories of radioactive waste in connection with microbial corrosion

Jana Rejková, Hana Juklíčková

Department of Power Engineering, University of Chemistry and Technology, Prague, Czech Republic

YUCOMAT SYMPOSIUM C:
NANOSTRUCTURED MATERIALS

P.S.II.C.1.

Photocatalytic activity of g- and n-C_3N_4 in phodegradation of textile dye Acid Orange 7

Nadica Abazović, Tatjana Savić and Mirjana Čomor

Vinča Institute of Nuclear Sciences, University of Belgrade, National Institute of the Republic of Serbia

P.S.II.C.2.

Band gap engineering in novel fluorite-type rare earth high-entropy oxides (RE-HEOs) with computational and experimental validation for photocatalytic water splitting applications

Igor Đerđ, Dalibor Tatar, Jelena Kojčinović, Srijita Nundy[1], Habib Ullah[1], Aritra Ghosh[1], Tapas K. Mallick[1], Asif Ali Tahir[1], Rafael Meinusch [2], Bernd Smarsly[2]

Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, HR-31000 Osijek, Croatia, [1] Environment and Sustainability Institute, University of Exeter, Penryn TR10 9FE, United Kingdom, [2] Institute of Physical Chemistry and Center of Materials Research, Justus Liebig University, Heinrich-Buff-Ring 17, D-35392 Giessen, Germany

P.S.II.C.3.

Influence of different synthesis methods on morphological and optical properties of the rare earth doped fluorides

Ivana Dinić[1], Marina Vuković[2], Maria Eugenia Rabanal[3], Lidija Mancic[1]

[1]Institute of Technical Sciences of Serbian Academy of Sciences and Arts, Belgrade, Serbia, [2]Innovative Centre, Faculty of Chemistry, University of Belgrade, Serbia, [3]Materials Science and Engineering Department and IAAB, Universidad Carlos III de Madrid, Leganes, Madrid, Spain

P.S.II.C.4.

Possibilities of application of green's function methods to research of nanoscopic crystal structures

Jovan P. Šetrajčić[1], Siniša M. Vučenović[2], Dušan I. Ilić[3], Stevo K. Jaćimovski[4]

[1]Academy of Sciences and Arts of Republic of Srpska, Banja Luka, Republic of Srpska, Bosnia and Herzegovina, [2]University of Banja Luka, Faculty of Natural Sciences and Mathematics, Banja Luka, Republic of Srpska, Bosnia and Herzegovina, [3]University of Novi Sad, Faculty of Technical Sciences, Novi Sad, Vojvodina - Serbia, [4]University of Criminal Investigation and Police Studies, Zemun-Belgrade, Serbia

P.S.II.C.5.

Characterization of magnetron sputtered Ti-Al-N thin films

Kwang Ho Kim and Kyung Mox Cho

GFHIM, School of Materials Science and Engineering, Pusan National University, Busan, 46241 Korea

P.S.II.C.6.

Characterization of adsorption site heterogeneity in gas sensors based on LPE graphene by using sensor noise analysis

Stevan Andrić, Ivana Jokić, Miloš Frantlović, Katarina Radulović,Marko Spasenović

University of Belgrade, Institute of Chemistry, Technology and Metallurgy-National Institute of the Republic of Serbia, 11000 Belgrade, Serbia

P.S.II.C.7.

Impact of TiO_2 nanoparticles on the kinetics of free-radical and cationic photopolymerization in Vat 3D printing

Martina Korčušková, Juraj Svatík, Veronika Sevriugina, Martina Štaffová, František Ondreáš, Petr Lepcio

Brno University of Technology, Central European Institute of Technology, Purkyňova 656/123, Brno, 612 00, Czech Republic

P.S.II.C.8.

Study of influence of Mn dopant on dielectric response of $SrTiO_3$ ceramics

J. Živojinović[1], D. Kosanović[1], V. P. Pavlović[2], N. Tadić[3], V. B. Pavlović[4]

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P.S.II.C.9.

Physicochemical properties of copper-doped bismuth vanadate nanoparticles

Marko Jelić[1], Igor Pašti[2], Bojana Nedić Vasiljević[2], Jelena Erčić[3], Danica Bajuk-Bogdanović[2], Zoran Jovanović[1], Sonja Jovanović[1]

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P.S.II.C.10.
The effect of heat treatment and pulsed laser treatment on the morphology of Au and Ag nanoparticles and nanowires

B. Polyakov[1], E. Butanovs[1], S. Oras[2], V. Zadin[2], S. Vlassov[2]
[1]Institute of Solid State Physics, University of Latvia, Kengaraga street 8, LV-1063 Riga, Latvia, [2]Institute of Physics, University of Tartu, W. Ostwaldi tn 1, 50412, Tartu, Estonia

P.S.II.C.11.
Structural chemistry, electrical and x-ray spectroscopic properties of the ternary Ce-Ni-P compounds

Ivan Shcherba[1], Vitaliy Denys[1], Volodymyr Babizhetskyy [1], Viktor Antonov[2], Dragan Usković[3], Henryk Noga[4], Bohdan Jatsyk[5]
[1]Ivan Franko National University of Lviv, Ukraine, [2]Institute of Physics of Metals, NASU, Kyiv, Ukraine, [3]Institute of Technical Sciences of the SASA, Belgrade, Serbia, [4]Institute of Technology, the Pedagogical University of Cracow, Cracow, Poland, [5]Lviv National University of Veterinary Medicine and Biotechnologies, Lviv, Ukraine

10.00-10.30 **Break**

Third YUCOMAT Plenary Session, Main Conference Hall

Session I: 10.30-11.45
Chairperson: Kwang Ho Kim, Peter Rogl

10.30-11.00 **Y.PL.S.III.1.**
Hard films for industrial applications: design-synthesis-evaluation

Kwang Ho Kim
Global Frontier R&D Center for Hybrid Interface based future Materials, School of Materials Science and Engineering, Pusan National University, Busan 46241, Korea

11.00-11.30 **Y.PL.S.III.2.**
Structure and properties of the compounds TZnSb, T = Ti, V, Cr

P.F. Rogl[1], R. Podloucky[1], G. Rogl[1], H. Michor[2], X. Yan[2], V. Bursikova[3], P.Broz[4], J. Bursik[5], R. Vaclavik[3], Z. Abbasi[6], E. Schafler[6], G. Giester[7]
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11.30-11.45 **Y.PL.S.III.3.**
Electrical resistivity and thermal expansion (4.2-820 K) of nanostructured skutterudites after severe plastic deformation

Gerda Rogl[1,2], Viktor Soprunyuk[2] and Peter Rogl[1]
[1]Institute of Materials Chemistry, Universität Wien, A-1090 Wien, Austria; [2] Physics of Nanostructured Materials, Universität Wien, A-1090 Wien, Austria

11.45-12.30 **Break**

Fourth YUCOMAT Plenary Session, Main Conference Hall

Session I: 12.30-14.00
Chairperson: Đorđe Janaćković, Petar Uskoković

12.30-13.00 **Y.PL.S.IV.1. virtual**
The fundamental science and technology applications of triboelectric nanogenerators
Zhong Lin Wang
Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing, China, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia USA

13.00-13.30 **Y.PL.S.IV.2. virtual**
Carbon dot luminophores
Andrey L. Rogach
Department of Materials Science and Engineering, and Center for Functional Photonics, City University of Hong Kong, Hong Kong SAR

13.30-14.00 **PL.S.IV.3. virtual**
Electron liquid crystals: a Materials science minefield
Ivan Božović
Brookhaven National Laboratory, Upton, NY 11973, USA, Yale University, New Haven, CT 06520, USA

Thursday, September 1, 2022

Third YUCOMAT Poster Session, National Restaurant Jadranka Terrace

Session I: 08.30-09.45
Chairperson: Željko Radovanović, Jelena Vujančević

YUCOMAT SYMPOSIUM C:
NANOSTRUCTURED MATERIALS

P.S.III.C.12.
Electrochemical properties of composites of graphene oxide and cobalt ferrite doped with zink and gallium
Marija Grujičić[1], Željko Mravik[1], Danica Bajuk-Bogdanović[2], Damjan Vengust[3], Zoran Jovanović[1], Ivana Stojković Simatović[2], Sonja Jovanović[1]
[1]Laboratory of Physics,Vinca Institute of Nuclear Sciences-National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [3]Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia

P.S.III.C.13.

Electrochemical charge storage properties of thermally treated and ion-beam irradiated graphene oxide/12-tungstophosphoric acid nanocomposites

Željko Mravik[1], Marko Gloginjić[1], Jelena Rmuš[1], Milica Pejčić[1], Danica Bajuk-Bogdanović[2], Maria Vesna Nikolić[3], Nemanja Gavrilov[2], Zoran Jovanović[1]
[1]Center of Excellence for Hydrogen and Renewable Energy (CONVINCE), Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, P.O. Box 47, 11158, Belgrade, Serbia, [3]Institute for Multidisciplinary Research, University of Belgrade, 1 Kneza Višeslava, 11000 Belgrade, Serbia

P.S.III.C.14.

Mechanochemical synthesis of MgH_2-V nanocomposistes

Z. Sekulić[1], I. Milanović[2], B. Babić[2], M. Prvulović[2], J. Grbović Novaković[2], V. Asanović[3]
[1]Ministry of Capital Investments, The Government of Montenegro, Directorate for Energy and Energy Efficiency, Rimski trg 46, 81 000 Podgorica, Montenegro, [2]Vinča Institute of Nuclear Sciences, National Institute of Republic of Serbia, Centre of Excellence for Renewable and Hydrogen Energy, University of Belgrade, POB 522, 11000 Belgrade, Serbia, [3]Faculty of Metallurgy and Technology, University of Montenegro, Cetinjski put 2, 81000 Podgorica, Montenegro

P.S.III.C.15.

Structural, optical and mechanical characterization of the PMMA- ZrO_2 nanocomposites

Ivan Pešić[1], Miloš Petrović[1], Dragana Pejić[1], Maja S. Rabasović[2], Dragutin Šević[2], Vesna Radojević[1]
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YUCOMAT SYMPOSIUM D:
ECO-MATERIALS AND ECO-TECHNOLOGIES

P.S.III.D.1.

Synthesis and characterization of thermally treated geopolymer composite materials

Miljana Mirković[1], Mira Vukčević[2], Ivana Bošković[2], Snežana Nenadović[1], Ljiljana Kljajević[1], Dunja Đukić[3], Vladimir Pavlović[4]
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P.S.III.D.2.

Photocatalytic activity of N-TiO_2 nanotubes decorated with CdS QD

Jelena Vujančević[1], Anđelika Bjelajac[2], Endre Horváth[3], László Forró[3], Vladimir B. Pavlović[4], Đorđe Janaćković[5]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Innovation Center of Faculty of Technology and Metallurgy, Ltd, Belgrade, Serbia, [3]Ecole Polytechnique Fédérale de Lausanne, Laboratory of Physics of Complex Matter, Lausanne, Switzerland, [4]University of Belgrade, Faculty of Agriculture, Belgarde-Zemun, Serbia, [5]University of Belgarde, Faculty of Technology and Metallurugy, Belgrade, Serbia

P.S.III.D.3.

Study of oil type pollutant adsorption on Vrbas river sediments (Bosnia and Herzegovina)

Sanja Pržulj[1], Gorica Veselinović[2], Marko Ivanišević[1], Slobodan Gnjato[1], Milica Balaban[1], and Branimir Jovančićević[3]
[1]Faculty of Natural Sciences and Mathematics, University of Banja Luka, Mladena Stojanovića 2, 78000 Banja Luka, Bosnia and Herzegovina; [2]Center of Chemistry, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11001 Belgrade, Serbia; [3]University of Belgrade, Faculty of Chemistry, Studentski trg 12-16. 11001 Belgrade, Serbia

P.S.III.D.4.

Evaluation of photocatalytic activity of $Sr_{0.9}La_{0.1}TiO_3$ and $Sr_{0.25}Ca_{0.25}Na_{0.25}Pr_{0.25}TiO_3$ nano-sized ceramic powders for water treatment

Nikola Kanas[1], Aleksandra Jovanoski[2], Vladimir Rajić[3], Annu Sharma[4], Subramshu S. Bhattacharya[4], Stevan Armaković[5,6], Maria Savanović[2,6], Sanja J. Armaković[2,6]
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P.S.III.D.5.

Performance of ternary cement binders containing high volume of fly ash and fluid catalytic cracking catalyst residue

Jelena Rakić[1], Zvezdana Baščarević[1], Rada Petrović[2]
[1]Institute for Multidisciplinary Research, University of Belgrade, Serbia,[2]Faculty of Technology and Metallurgy, University of Belgrade, Serbia

P.S.III.D.6.

Comparative assessment of chemically and 'green' synthesized magnetic nanoparticles and their use for removal of pollutants

Natalia Kobylinska[1], Dmytro Klymchuk[2], Anatolij Shakhovsky[3], Yakiv Ratushnyak[3], Volodymyr Duplij[3], Nadiia Matvieieva[3]
[1]A.V. Dumansky institute of colloidal chemistry and water chemistry NAS of Ukraine, [2]Institute of Botany NAS of Ukraine, Kyiv, Ukraine, [3]Institute of Cell Biology and Genetic Engineering NAS of Ukraine, Kyiv, Ukraine

P.S.III.D.7.

Environmentally friendly hybrid poly(methyl methacrylate)-wood-poly(ethylene terephthalate)-alumina composite material

Anđela N. Radisavljević[1], Marija Vuksanović[2], Aleksandar Grujić[3], Srđan Perišić[1], Vesna Radojević[4]
[1]University of Belgrade, Innovation Centre, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, [2]University of Belgrade, Department of Chemical Dynamics and Permanent Education, „VINČA" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Mike Petrovića Alasa 12-14, 11351 Belgrade, Serbia, [3]University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, Belgrade, Serbia, [4]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia

P.S.III.D.8.

Initial characterization and evaluation of two tailing dumps in Bulgaria for application as precursors for geopolumers

Darya Ilieva, Lyudmila Angelova, Temenuzhka Radoikova, Andriana Surleva
University fo Chemical technology and Metallurgy, 8 „St. Kl. Ohridski" blvd., 1756 Sofia, Bulgaria

YUCOMAT SYMPOSIUM E:
BIOMATERIALS

P.S.III.E.1.

Synthesis, characterization and DFT calculations of Schiff base Co(III) complexes

Milica Savić[1], Mima Jevtović[2], Matija Zlatar[3], Maja Gruden[1], Dragana Mitić[2], Božidar Čobeljić[1], Katarina Anđelković[1]
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P.S.III.E.2.

Osteogenic potential of diluted blood and bone marrow in ectopic osteogenesis

Marija Vukelić-Nikolić[1], Stevo Najman[1], Jelena Živković[1], Jelena Najdanović[1], Sanja Stojanović[1], Vladimir Cvetković[2], Perica Vasiljević[2]
[1]Institute of Biology and Human Genetics, Faculty of Medicine, University of Niš, Serbia,
[2]Department of Biology and Ecology, Faculty of Science and Mathematics, University of Niš, Serbia

P.S.III.E.3.

Novel antimicrobial composites based on calcium- and zinc-alginate hydrogels and activated charcoal

Andrea Osmokrović[1], Ivan Jancic[2], Ivona Janković- Častvan[1], Predrag Petrović[3], Marina Milenković[2], Bojana Obradović[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]University of Belgrade, Faculty of Pharmacy, Belgrade, Serbia, [3]Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia

P.S.III.E.4.

Characterization and drug release of Zn-Al layered double hydroxyde–nifuroxazide composite

Željko Radovanović[1], Lidija Radovanović[1], Đorđe Janaćković[2], Rada Petrović[2]
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P.S.III.E.5.

Bio-mimetic bone-like surface structure of Ti-based implants

Yevheniia Husak[1,2], Pal Terek[3], Sanja Kojić[3], Zoran Bobić[3], Bojan Petrović[4], Sergiy Kyrylenko[1], Maksym Pogorielov[1,5], Wojciech Simka[2]
[1]Sumy State University, 40007 Sumy, Ukraine, [2]Silesian University of Technology, 44-100 Gliwice, Poland, [3]Faculty of Technical Sciences, University of Novi Sad, Novi Sad, Serbia, [4]Faculty of Medicine, University of Novi Sad, Novi Sad, Serbia, [5]University of Latvia, Institute of Atomic Physics and Spectroscopy, LV-1004 Riga, Latvia

P.S.III.E.6.

3D printed scaffold with bisphosphonate for tissue regeneration

Marija N. Jovanović[1], Miloš M. Petrović[1], Anđela N. Radisavljević[2], Dušica B. Stojanović[1], Vesna J. Radojević[1], Svetlana R. Ibrić[3], Petar S. Uskoković[1]
[1]University of Belgrade - Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, [2]University of Belgrade, Innovation Centre, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, [3] University of Belgrade - Faculty of Pharmacy, Department of Pharmaceutical Technology and Cosmetology, Vojvode Stepe 450, 11221 Belgrade, Serbia

P.S.III.E.7.

Processing and characterization of hybrid chitosan (Ch)/polylactic acid (PLA) composite nanofibrous scaffolds for biomedical application

Viktoriia Korniienko[1], Yevhen Samokhin[1], Julia Varava[1], Kateryna Diedkova[1], Bojan Petrović[2], Maksym Pogorielov[1,3]
[1]Biomedical Research Center, Sumy State University, R.-Korsakova, 2, 40007, Sumy, Ukraine, [2]Faculty of Medicine, University of Novi Sad, Novi Sad, Serbia, [3]Institute of Atomic Physics and Spectroscopy, University of Latvia, Jelgavas iela 3, Riga, LV-1004, Latvia

P.S.III.E.8.

Nanostructured surface modification and characterization of titanium based materials for medical application

Dragana R. Barjaktarević, Marko P. Rakin, Đorđe N. Veljović, Bojan I. Međo, Veljko R. Đokić
[1]University of Belgrade, Faculty of Technology and Metallurgy, 11120 Belgrade, Serbia

P.S.III.E.9.

Electrospun poly(ε-caprolactone) nanofiber mats with cefazolin or yarrow extract powder as urinary catheter-coating materials

Anđela N. Radisavljević[1], Marija Jovanović[2], Dušica Stojanović[2], Miloš Petrović[2], Vesna Radojević[2], Petar Uskoković[2], Mirjana Rajilić-Stojanović[2]
[1]University of Belgrade, Innovation Centre, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, [2]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia

P.S.III.E.10.

The effect of liposomal pro-healing protein on the rheological properties of mucoadhesive injectable hydrogel

Veronika Sevriugina[1], Zuzana Kadlecová[1], Lucy Vojtová[1]
[1]Central European Research Institute, Brno University of Technology

P.S.III.E.11.

Encapsulation of bioactive proteins into thermosensitive biodegradable copolymer nanoparticles based on PLGA-PEG-PLGA

Klára Lysáková[1], Monika Obršlíková[2], Zuzana Kadlecová[1], Lucy Vojtová[1]
[1]Brno University of Technology, CEITEC-Central European Institute of Technology, Advanced Biomaterials, Purkyňova 656/123, 612 00 Brno, Czech Republic, [2]Brno University of Technology, Faculty of Chemistry, Purkyňova 464, 612 00 Brno, Czech Republic

P.S.III.E.12.

Composite hydrogels based on gelatin, hydroxypropyl methylcellulose and Mg-doped biphasic calcium phosphate for biomedical applications

Vukasin Ugrinović[1], Veroniki Hristara[2], Maja Marković[1], Predrag Petrović[2], Rada Petrović[2], Đorđe Janćcković[2], Đorđe Veljović[2]
[1]Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

P.S.III.E.13.

Antibiofilm activity of the bioactive ceramic coatings on the 3D printed TC4 scaffold

Marija Milivojević[1], Milena Radunović[2], Marija Stevanović[1], Željko Radovanović[1], Rada Petrović[3], Đorđe Janaćković[3]
[1]Innovation Center of Faculty of Technology and Metallurgy, [2]School of Dental Medicine, University of Belgrade, [3]Faculty of Technology and Metallurgy, University of Belgrade

P.S.III.E.14.

Multicomponent hemostatic dressing may improve bleeding stop and wound regeneration

Katarína Kacvinská[1], Marian Sedlář[1], Radim Dvořák[2], Tomáš Sopuch[3], Lucy Vojtová[1]
[1]Central Eruopean Institute of Technology, Brno Univ. Technol., Brno, CZ; [2]Hemcon Medical Technologies CZ s.r.o., Tišnov, CZ; [3]Holzbecher, spol. s.r.o barevna a bělidlo Zlíč, Česká Skalice-Zlíč, CZ

P.S.III.E.15.

Quantum-informational macrophenomena in biomedicine & holistic psychosomatics: quantum-holographic framework

D. I. Raković
Faculty of Electrical Engineering, University of Belgrade, Serbia

P.S.III.E.16.

Chitosan/tripolyphosphate capsule-forming gelation monitored via light scattering curves: determination of particle forming phases and their effect on physico-chemical and biological parameters

Jana Dorazilova[1,*], Lucy Vojtova[1], Kaja Kasemets[2]
[1]Central European Institute of Technology of Brno University of Technology, Research Group of Advanced Biomaterials, Brno, Czech Republic, [2]National Institute of Chemical Physics and Biophysics, Laboratory of Environmental Toxicology, Estonia.

SYMPOSIUM F:
WRTCS

W.P.S.F.1.

Biodegradable coatings improved mechanical properties and bioactivity of sintered calcium phosphate scaffolds

Đorđe Veljović[1], Vukašin Ugrinović[2], Tamara Matić[2], Julijana Tadić[3], Olivera Dragutinović[1], Teodora Jakovljević[1], Jelena Stanisavljević[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]Innovation Center of the Faculty of Technology and Metallurgy Ltd, Belgrade, Serbia, [3]University of Belgrade, Vinča Institute of Nuclear Sciences, Belgrade, Serbia

W.P.S.F.2.
Composite scaffolds based on magnesium doped hydroxyapatite and mesoporous nanosized bioactive glass
Tamara Matić[1], Zvezdana Baščarević[2], Đorđe Janaćković[3], Đorđe Veljović[3]
[1]Innovation Center of the Faculty of Technology and Metallurgy Ltd, Belgrade, Serbia , [2]University of Belgrade, Institute for multidisciplinary research, Belgrade, Serbia, [3] University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

W.P.S.F.3.
Sinterability study of the zeolite-based porous ceramics for water filter application
Ivan Stijepović, Marija Milanović, Jelena Vukmirović, Andrea Nesterović, Danica Piper, Vladimir V. Srdić
University of Novi Sad, Faculty of Technology Novi Sad, Department of Materials Engineering, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia

W.P.S.F.4.
Influence of aluminium anodizing wastes on Flash sintering of alumina
I. S. Vilarinho, R. Pinho, M. P. Seabra, P. M. Vilarinho, A. M. R. Senos
CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

09.45-10.00 **Break**

Second WRTCS Plenary Session, Main Conference Hall

Session I: 10.00-12.45
Chairperson: Biljana Stojanović, Boris Feigelson

10.00-10.30 **W.PL.S.II.1.**
From nanoparticles to nanocrystalline solids with designed functionalities
Boris N. Feigelson, James A. Wollmershauser, Kevin P Anderson, Benjamin L Greenberg, Alan G Jacobs
U.S. Naval Research Laboratory, 4555 Overlook Ave., SW, Washington, DC 20375, USA

10.30-11.00 **W.PL.S.II.2.**
Studies on the flash sintering of KNN: flash variables, mechanisms and material's properties
Ricardo Serrazina[1], Luis Pereira[2], Paula M. Vilarinho[1], Ana Senos[1]
[1]Department of Materials and Ceramic Engineering, CICECO-Aveiro Materials Institute, University of Aveiro, 3810-193 Campus Santiago, Portugal, [2]CENIMAT-I3N, School of Science and Technology, FCT-NOVA, Universidade NOVA de Lisboa, Campus da Caparica. 2829-516 Caparica, Portugal

11.00-11.30 **W.PL.S.II.3.**
Capsule free hot isostatic pressing as a way towards transparent structural and functional ceramics
Karel Maca, Tomáš Spusta, Katarína Drdlíková, Martin Trunec, Daniel Drdlík, Róbert Klement
Brno University of Technology, Brno, Czech Republic, Funglass Centre of Excellence, Trenčín, Slovakia

11.30-12.00 **Break**

12.00-12.15 **W.PL.S.II.4.**
Additive manufacturing and spark plasma sintering: fabrication of powder components with cooling channels
Elisa Torresani[1], Maricruz Carrillo[1,2], Eugene Olevsky[1,2], Chris Haines[3], Darold Martin[4]
[1]San Diego State University, San Diego, CA, USA, [2]University of California San Diego, CA, USA, [3]US Army DEVCOM - Army Research Laboratory, Aberdeen Proving Ground, MD, USA, [4]US Army DEVCOM-Armaments Center, Picatinny Arsenal, NJ, USA

12.15-12.30 **W.PL.S.II.5. virtual**
Thermal stress and deformation in SiC power chip systems having Ag sintered bonding layers for advanced power conversion
Masaaki Aoki[1/2], Ryousuke Aoki[1], Akihiro Mochizuki[2], Yoshio Murakami[2], Mutsuharu Tsunoda[2], Goro Yoshinari[2], Maurizio Fenech[3], and Nobuhiko Nakano[1]
[1]Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa 223-8521, Japan, [2]MacDermid Alpha Electronics Solutions / MacDermid Performance Solutions Japan, [3]MacDermid Alpha Electronics Solutions / Alpha Assembly Solutions Germany GmbH

12.30-12.45 **W.PL.S.II.6. virtual**
Excellent heat dissipation performance of power device structures having Ag sintered bonding layers
Kazuma Yamashita[1], Masaaki Aoki[1,2], Goro Yoshinari[2], Nobuhiko Nakano[1]
[1]Department of Electronics and Electrical Engineering, Faculty of Science and Technology, MKeio University, Yokohama, Kanagawa 223-8521, Japan, [2]MacDermid Alpha Electronics Solutions / MacDermid Performance Solutions Japan, Hiratsuka, Kanagawa 254-0082, Japan

14.00-19.00 **Boat-trip around Boka Kotorska Bay**

Friday, September 2, 2022

Second YUCOMAT Oral Session, Main Conference Hall

Session I: 08.30-11.15
Chairperson: Tetiana Prikhna, Patrick Gane

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

08.30-08.45 **O.S.II.A.1.**
Influence of brazing conditions on crystallization mechanism and mechanical properties of the TiAlV/TiCuZrPd/TiAlV brazed joints
Anna Sypien
[1]Institute of Metallurgy and Materials Science, Polish Academy of Sciences, Reymonta 25 St. 30-059 Krakow, Poland

08.45-09.00 **O.S.II.A.2.**

Structure integrity of high-entropy alloys (HEA) manufactured by Selective Laser Melting (SLM) using in-situ alloying of elementary powders

R. Bardo, R. Dziurka, P. Bała

AGH University of Science and Technology, A. Mickiewicza 30 Av., 30059 Krakow, Poland

09.00-09.15 **O.S.II.A.3.**

Non-destructive testing of composites using terahertz radiation

Waldemar Swiderski, Martyna Strag, Pawel Hlosta

Military Institute of Armament Technology, Poland

09.15-09.30 **O.S.II.A.4.**

The role of compensation defects in the stabilization of multivalent inorganic systems doped with europium ions

Karol Szczodrowski, Natalia Górecka, Justyna Barzowska, Agata Lazarowska, Marek Grinberg

Institute of Experimental Physics, University of Gdańsk, Wita Stwosza 57, 80-952 Gdańsk, Poland

09.30-09.45 **O.S.II.A.5.**

Enhancing the environmental aspect of mineral recovery: separation of metal carbonate on micro nanofibrillated cellulose

Patrick Gane[1,2], Katarina Dimić Mišić[1], Monireh Imani[1], Ernest Barceló[1]

[1]Aalto University, Department of Bioproducts and Biosystems, School of Chemical Engineering, 00076 Aalto, Helsinki, Finland, [2]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

09.45-10.15 **Break**

10.15-10.30 **O.S.II.A.6.**

Multiscale enhancement to aramid fabric-reinforced composites: electrospun P(An-co-GMA) nanofibrous interlayers

Farzin A. Arpatappeh[1], Cem Ünsal[1], Kaan Bilge[2], Farzin Javanshour[1], Sıla Güngör[3], Melih Papila[4]

[1]Sabanci University, Istanbul, Turkey, TR-34956, Tuzla-Istanbul, Turkey, [2]Piri Reis University, Faculty of Engineering, Department of Naval Architecture and Marine, TR-34940, Tuzla-Istanbul, Turkey, [3]ROKETSAN Industries, Istanbul, Turkey, TR-06780, Elmadag-Ankara, Turkey, [4]BaX Composites, Istanbul, Turkey, TR-34025 Istanbul, Turkey

10.30-10.45 **O.S.II.A.7.**

Structural instabilities of complex oxides and intermetallics probed by in situ x-ray synchrotron powder diffraction

Leonid Vasylechko

Lviv Polytechnic National University, 12 Bandera St., 79013 Lviv, Ukraine

10.45-11.00 **O.S.II.A.8.**

MAX phases-based electro conductive and were resistant coating for application in oxidizing environment at high-temperatures

T. A. Prikhna[1,4], T. B. Serbenyuk[1], O. P. Ostash[2], A. S. Kuprin[3], V.Ya. Podhurska[2], B. Büchner[4], V. B. Sverdun[1], S. S. Ponomaryov[5], M. V. Karpets[1,6], V. E.Moshchil[1], G. N. Tolmachova[3], M. A. Bortnitskaya[3], A. V. Matsenko[1]

[1]Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Kiev, Ukraine, [2]Karpenko Physico-Mechanical Institute of the National Academy of Sciences of Ukraine, Lviv, Ukraine, [3]National Science Center Kharkov Institute of Physics and Technology, Kharkov, Ukraine, [4]Leibniz-Institut für Festkörper und Werkstoffforschung Dresden 01069, Germany, [5]Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine (NASU), Kyiv, Ukraine, [6]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, Ukraine

YUCOMAT SYMPOSIUM B:

ADVANCED MATERIALS FOR HIGH-TECHNOLOGYAPPLICATION

11.00-11.15 **O.S.II.B.1.**

The influence of substrate and thermal annealing on calalytic activity and stability of Pt thin film catalysts

D. V. Tripković, S. I. Stevanović, K. Đ. Popović

Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11 000 Belgrade, Serbia

12.00 **Awards and Closing of the Conference**

12.30 **Cocktail and Greetings for Goodbay**

Third YUCOMAT Oral Session, Small Conference Hall

Session I: **08.30-11.45**
Chairpersons: Piotr Cyganik, Maxim Pogorielev

YUCOMAT SYMPOSIUM C:
NANOSTRUCTURED MATERIALS

08.30-08.45 **O.S.III.C.1.**

$(Gd,Y)VO_4:Eu^{3+}$ nanoparticles as promising theranostic agents

Svetlana Yefimova[1], Pavel Maksimchuk[1], Vladimir Klochkov[1], Kateryna Hubenko[1], Alexander Sorokin[1], Anton Tkachenko[2], Anatolii Onishchenko[2]

[1]Institute for Scintillation Materials, NAS of Ukraine, Ukraine, [2]Research Institute of Experimental and Clinical Medicine, Kharkiv National Medical University, Ukraine

08.45-09.00 **O.S.III.C.2.**

Mechanical behaviour and hydrogen permeability of carbon steel with surface nanocrystalline structure

Olha Zvirko, Olha Maksymiv, Volodymyr Kyryliv

Karpenko Physico-Mechanical Institute of the NAS of Ukraine; Lviv, Ukraine

09.00-09.15 **O.S.III.C.3.**
Improvement of electrochemical properties of ZnO nanoparticles via composites with graphene oxide
S. Marković,[1] A. Stanković,[1] I. Stojković Simatović[2]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

09.15-09.30 **O.S.III.C.4.**
On the contribution of surface chemistry, structure and interactions in GO/WPA nanocomposites for the electrochemical charge storage applications
Zoran Jovanović[1], Željko Mravik[1], Milica Pejčić[1], Sonja Jovanović[1], Milica Vujković[2], Smilja Marković[3], Danica Bajuk-Bogdanović[2]
[1]Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [3]Institute of Technical Sciences, Serbian academy of sciences and arts, Belgrade, Serbia

09.30-09.45 **O.S.III.C.5.**
Features of Influence of the magnetic field on the structure and properties of epoxy composites with lead oxide
Yuliia Bardadym
Institute of Macromolecular Chemistry of the NAS of Ukraine, Ukraine

09.45-10.15 **Break**

10.15-10.30 **O.S.III.C.6.**
The odd-even effect in peptide SAMs-competition of secondary structure and molecule-substrate interaction
Agnieszka Grabarek,[1] Łukasz Walczak,[2] and Piotr Cyganik[1]
[1]Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Krakow, Poland, [2]Science & Research Division, PREVAC sp. z o.o., Raciborska 61, 44-362 Rogow, Poland

10.30-10.45 **O.S.III.C.7.**
Dynamic tuning of quantum light emission from GaN/InGaN nanowire quantum dots by surface acoustic waves
Snežana Lazić[1], Enrique Calleja[2]
[1]Departamento de Física de Materiales, Instituto 'Nicolás Cabrera' and Instituto de Física de Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain, [2]ISOM-DIE, Universidad Politécnica de Madrid, 28040 Madrid, Spain

YUCOMAT SYMPOSIUM D:
ECO-MATERIALS AND ECO-TECHNOLOGIES

10.45-11.00 **O.S.III.D.1.**
Properties of phthalate-free alumina tape prepared by tape casting method
Kostja Makarovič[1,2,3], Matej Klemenčič[1], Robert Dular[1], Barbara Malič[2]
[1]Keko-Equipment d.o.o., Grajski trg15, 8360 Žužemberk, Slovenia, [2]Jožef Stafan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia, [3]CoE NAMASTE, Jamova cesta 39, 1000 Ljubljana, Slovenia

11.00-11.15 **O.S.III.D.2.**

Electronic structure, magnetic properties and magnetocaloric effect of $GdCo_{2-x}Ni_x$

Gabriela Souca[1], Roxana Dudric[1], Karsten Küpper[2], Coriolan Tiusan[1,3], Romulus Tetean[1]

[1]Faculty of Physics, Babes-Bolyai University, Kogalniceanu 1, 400084 Cluj-Napoca, Romania, *[2]University of Osnabrück, Fachbereich Physik, 49069 Osnabrück, Germany*, *[3] National Center of Scientific Research, France*

YUCOMAT SYMPOSIUM E:
BIOMATERIALS

11.15-11.30 **O.S.III.E.1.**

A platform for reliable preclinical testing of anticancer drugs

Jasmina Stojkovska[1,2], Ivana Banićević[1], Jelena Petrović[1,2], Milena Milivojević[3], Milena Stevanović[3,4,5], Miodrag Dragoj[6], Milica Pešić[6], Radmila Janković[7], Bojana Obradović[1]

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[3]University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia, [4]University of Belgrade, Faculty of Biology, Belgrade, Serbia, [5]Serbian Academy of Sciences and Arts, Belgrade, Serbia, [6]University of Belgrade, Institute for Biological Research "Sinisa Stanković", National Institute of the Republic of Serbia, Belgrade, Serbia, [7]University of Belgrade, School of Medicine, Belgrade, Serbia

11.30-11.45 **O.S.III.E.2.**

Pulsed NIR laser for photo-thermal ablation of MXene-loaded cells

Maksym Pogorielov[1,2], Sergiy Kyrylenko[1], Oleksiy Gogotsi[3], Ivan Baginskiy[3], Vitalii Balitskyi[3], Veronika Zahorodna[3], Yevheniia Husak[1,4], Ilya Yanko[1], Mykolay Pernakov[1], Anton Roshchupkin[1], Mykola Lyndin[1], Bernhard B. Singer[5], Volodymyr Buranych[1], Oksana Sulaieva[7], Oleksandr Solodovnyk[1,8], Alexander Pogrebnjak[1,6], Yury Gogotsi[1,9]

[1] Sumy State University, 31 Sanatorna St, Sumy 40007, Ukraine, [2] University of Latvia, 3 Jelgavas St, Riga LV-1004, Latvia, [3]Materials Research Centre, 3 Krzhizhanovskogo St, Kyiv 03680, Ukraine, [4] Silesian University of Technology, 2A Akademicka St, Gliwice 44-100, Poland, [5]University Duisburg-Essen, 171 Virchowstraße, Essen 45147, Germany, [6] Al-Farabi Kazakh National University, Almaty, Kazakhstan, [7]Medical Laboratory CSD, 45 Vasylkivska St, Kyiv 02000, Ukraine, [8] VERBA MEDICAL LTD, 31A Lushpy St, Sumy 40035, Ukraine, [9] Drexel University, 3141 Chestnut St, Philadelphia, PA 19104, United States

12.00 **Awards and Closing of the Conference**

12.30 **Cocktail and Greetings for Goodbay**

Abstracts

Plenary Lectures

MRS-Serbia 2022 Award

Looking back, moving forward: On safari in materials with gun and camera

Richard W. Siegel
Materials Science and Engineering , Rensselaer Polytechnic Institute, Troy, New York, USA

Electron microscopes, with their electron gun at one end and their recording camera at the other, were used to investigate a variety of materials in my research over the past six decades, complemented by a parallel use of a number of macroscopic measurements. This intimate combined use of macro- and micro-scopic methods enabled research spanning from vacancy precipitation in metals to the synthesis, structures, and properties of nanomaterials from ceramics, metals, and polymer nanocomposites, to biomaterials. In 1989, with the newly developing scientific field of nanomaterials still in its infancy, it seemed like a good, if rather bold, time to create the first dedicated commercial venture to manufacture and distribute nanophase materials to the public. Not that the public was yet interested or really aware of these materials, nor were we really yet able to scale up our laboratory process for creating these materials in commercially viable quantities, but we founded a company anyway, which went public in 1997 and is still growing today. Over the intervening 33 years, there have been challenges large and small with some successes and rewarding experiences, leading to commercial activities in several areas: active materials for personal care, including sunscreen ingredients and fully formulated cosmetics; and other advanced nanomaterials for medical diagnostics, architectural and industrial coatings, abrasion-resistant plastics, and surface finishing. A brief reminiscence of these research and commercialization experiences will be presented with examples from the past along with some of the lessons learned, especially those that might prove potentially useful for young researchers.

Y.PL.S.I.1.

Two-dimensional emptiness and its unique properties

Andre K. Geim
University of Manchester, United Kingdom

I shall overview our recent work on atomic-scale cavities fabricated by van der Waals assembly of two-dimensional crystals. These ultimately narrow cavities can be viewed as if an individual atomic plane is extracted from a bulk crystal leaving behind a 2D empty space, essentially an angstrom-scale gap connecting two edge dislocations. Gas, liquid, ion and proton transport has been studied using such 2D cavities down to one atom in height, revealing interesting and sometimes counterintuitive phenomena.

Y.PL.S.I.2.

Materials science with 2D atomic layers

Pulickel M. Ajayan
Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA 77005

There has been tremendous interest in recent years to discover, explore and demonstrate unique properties and applications of 2D materials. This got started with the spectacular discovery of graphene. This talk will focus on the materials science of 2D atomic layers and their hybrid architectures. Several aspects that include synthesis, characterization and manipulation will be discussed with the objective of achieving functional structures based on 2D atomic layers. The concept of artificially stacked van der Waals solids, atomically thin planar heterojunctions, and 2D layers based 3D constructs will be discussed using a number of examples consisting of graphene and other 2D layer compositions. Specifically, the talk will discuss multicomponent 2D alloys and artificially stacked hybrid van der Waals architectures. The talk will explore the emerging landscape of 2D materials systems that include graphene, boron-nitrogen-carbon systems, and a large number of transition metal dichalcogenide compositions.

Y.PL.S.I.3.

Cluster-assembled materials

Horst Hahn, Gleb Iankevich, Ramin Shadkam
Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Germany

Isolated clusters, entities containing a few to a few hundred of atoms, have been studied for decades for their special structures and physical, chemical and quantum properties. Clusters can also be used as building blocks for functional materials, requiring the controlled assembly of individual clusters. At INT, a custom-made UHV-system incorporating a cluster source, a 90° bending magnet for mass selection and controlled deposition positions is available for the preparation of cluster-assembled materials. These materials can consist of crystalline and amorphous clusters of one size and elemental composition, which are deposited on a substrate with controlled impact energy. Alternatively, size-selected clusters can be deposited under controlled conditions and be embedded into a matrix material, with free choice of size and concentration of clusters in the matrix. Several examples of clusterassembled metallic glasses and composite materials consisting of miscible and immiscible elements will be shown. The emphasis is on the description of the synthesis route, the atomic structure and the properties of the clusterassembled materials.

Y.PL.S.I.4.

Probing structure and dynamic behaviors of topological polar solitons by electron microscopy

Xiaoqing Pan
Department of Materials Science and Engineering, Department of Physics and Astronomy, Irvine Materials Research Institute (IMRI), University of California, Irvine, CA 92697, USA

Topological polar solitions such as domain walls, polar voritices, skyrmions, etc, in ferroelectrics have received much attention owing to their unique functionalities and potential applications in electronic devices. Recent advances in transmission electron microscopy (TEM) and electron energy-loss spectroscopy (EELS) provides powerful tools to study the structure, properties, and dynamic behaviors of these nanostructures with atomic resolution. In this talk, I will demonstrate the nucleation, growth and evolution of polar domains, dynamics of domain wall motion by in situ TEM.[1] The electric polarization of nanodomains, vortices and other polar solitons can be mapped by quantitative TEM with the atomic resolution.[2] Recently, we have developed a novel four-dimensional STEM (4D STEM) method that can directly map the local electric field and charge density of crystalline materials in real space with sub-angstrom resolution.[3] Our results provide fundamental understanding of the origins of ferroelectricity and the mechnisms of charge transfer across ferroelectric interfaces. So far, topological polar structures reported in literature, have been observed only in superlattices grown on oxide substrates. We have recently found that two types of skyrmion-like polar nanodomains can be created in lead titanate/strontium titanate bilayers transferred onto silicon and can be switched from one type to another by an applied electric field, which substantially modifies their resistive behaviours.[4] The polar-configuration-modulated resistance is ascribed to the distinct band bending and charge carrier distribution in the core of the two types of polar texture. The integration of high-density (more than 200 gigabits per square inch) switchable skyrmion-like polar nanodomains on silicon may enable non-volatile memory applications using topological polar structures in oxides.

1. C. T. Nelson et al., Science **224**, 968 (2011)
2. C. T. Nelson et al., Nano Letters **11**, 828 (2011)
3. W. P. Gao et al., Nature **575**, 490 (2019)
4. L. Han et al., Nature **603,** 63 (2022).

Y.PL.S.II.1.

Two-dimensional carbides and nitrides pave the road to future technologies

Yury Gogotsi
J. Drexel Nanomaterials Institute, and Department of Materials Science and Engineering,
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Discovery of new materials provides moments of inspiration and shifts in understanding, shaping the dynamic field of materials science. Following the graphene breakthrough, many other 2D materials emerged. Although many of them remain subjects of purely academic interest, others have jumped into the limelight due to their attractive properties, which have led to practical applications. Among the latter are 2D carbides and nitrides of early transition metals known as MXenes [1]. The family of MXenes has been expanding rapidly since the discovery of Ti_3C_2 in 2011. More than 30 different stoichiometric MXenes have been reported, and the structure and properties of numerous other MXenes have been predicted. Moreover, the availability of solid solutions on M and X sites, multi-element high-entropy MXenes, control of surface terminations, and the discovery of out-of-plane ordered double-M o-MXenes (e.g., Mo_2TiC_2), as well as in-plane ordered i-MAX phases and their i-MXenes offer a potential for producing dozens of new distinct structures. Chalcogen terminated carbides, which are crossover between carbides and chalcogenides, 2D borides, and Si-containing nitrides of transition metals further expanded the family of 2D non-oxide materials in the recent years. This presentation will describe the state of the art in the manufacturing of those new 2D compounds, their delamination into single-layer 2D flakes and assembly into films, fibers and 3D structures [2]. Synthesis-structure-properties relations of MXenes will be addressed on the example of Ti_3C_2. Many MXenes offer high electronic conductivity combined with hydrophilic surfaces. This allows environmentally friendly and scalable manufacturing and processing of MXenes from dispersions in water, with no surfactant of binder added. The versatile chemistry of the MXene family renders their properties tunable for a large variety of energy-related, electronic, optical, biomedical and other applications. In particular, the applications of MXenes in electrochemical energy storage and harvesting, electrocatalytic water splitting and water purification/desalination are promising. However, MXene antennas, sensors, actuators, films for electromagnetic interference shielding are equally attractive. Structural, tribological and high-temperature applications of MXenes are being explored as well.

1. VahidMohammadi, J. Rosen, Y. Gogotsi, The World of Two-Dimensional Carbides and Nitrides (MXenes), Science, **372**, eabf1581 (2021)
2. X. Li, Z. Huang, C. E. Shuck, G. Liang, Y. Gogotsi, C. Zhi, MXene chemistry, electrochemistry, and energy storage applications, Nature Reviews Chemistry, **6** (6), 389–404 (2022)

Y.PL.S.II.2.

Advanced materials for health monitoring and haptic interactions

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Advances in materials science, mechanical engineering and manufacturing methods establish the foundations for high performance classes of electronics technologies that have soft, flexible physical properties, sometimes in bioresorbable forms. The resulting devices can mount on the skin, at nearly any location across the body, and they can also implant into the body, to provide continuous, clinical-quality information on physiological status, with options in complex, large-area multi-haptic forms of engagement and feedback. This talk summarizes the key ideas and presents examples in wireless devices for (1) maternal, fetal, neonatal and pediatric care in clinical facilities and home settings, and (2) full-body haptic experiences in virtual/augmented reality environments.

Y.PL.S.II.3.

Correlative imaging of mineral deposits in brain tissue of Alzheimer's Disease patients: application to the valence state of iron deposits by STEM-EELS

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It is known that abnormal mineral deposits containing zinc, aluminum or iron are found in the brain tissue of former patients with severe Alzheimer's Disease (AD). In this work, we have applied correlative imaging methods which are common either in biological or in physical sciences, but rarely together, to characterize such deposits in the same samples (e.g. [1,2]). For iron deposits, it has been suggested that ferrous rather than ferric irons are more responsible for adverse biochemical activity in AD development (e.g. [3,4]). We have used correlative magnetic resonance imaging, histological analysis, optical and scanning electron microscopy methods to locate iron deposits in AD brain tissue, and subsequently site-specific focused ion beam specimen preparation for scanning transmission electron microscopy-electron energy loss spectroscopy (STEM-EELS) to determine the iron valence state [5]. A significent proportion of the ferrous state is formed in three severe AD patients compared to equivalent tissue from healthy patients, showing the usefulness of the combined imaging techniques [6].

1. M. Zeineh et al., Alzheimer's & Dementia: The Journal of the Alzheimer's Association, **13** (7), pp. 1129-1130 (2017).
2. S. J. Madsen et al., J. Alzheimer's Disease Reports, **4**, pp. 525-536 (2020)
3. M.M. Zeineh et al., Neurobiol. Aging **36** (9) pp. 2483-2500 (2015).
4. J.F. Collingwood et al., J. Alzheimer's Disease. **14** (2) pp. 235-245 (2008).
5. Y. Zeng et al., Ultramicroscopy, **231**, pp. 113254-113261 (2021)
6. This work was supported by the National Institute of Aging of the U.S. National Institutes of Health under Award Number R01AG061120.

Y.PL.S.II.4.

Advances in engineering novel materials for nanomedicine

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Pharmaceutical nanocarriers, including liposomes and polymeric micelles, are frequently used for the delivery of a broad variety of both soluble and poorly soluble pharmaceuticals to enhance the in vivo efficiency of many drugs. Now, within the frame of this concept, it is tempting to develop multifunctional stimuli-responsive nanocarriers, i.e. nanocarriers that, depending on the particular requirements, can circulate long; target the site of the disease via both non-specific and/or specific mechanisms, such as enhanced permeability and retention effect (EPR) and ligand(antibody)-mediated recognition; respond local stimuli characteristic of the pathological site by, for example, releasing an entrapped drug or deleting a protective coating facilitating thus the contact between drug-loaded nanocarriers and target cells (especially important for cancer therapy); and even provide an enhanced intracellular delivery of an entrapped drug with its subsequent delivery to specific intracellular organelles, such as nuclei, lysosomes or mitochondria. Such carriers can be additionally supplemented with reporter moieties to follow their real-time biodistribution and target accumulation. Among new developments to be considered in the area of multifunctional pharmaceutical nanocarriers are: drug- or/and RNA-loaded delivery systems additionally decorated with cell-penetrating peptides for the enhanced intracellular delivery; “smart” multifunctional drug delivery systems, which can reveal/expose temporarily hidden functions under the action of certain local stimuli characteristic for the pathological zone (such as lowered pH, redox-conditions, hypoxia, or locally increased expression of certain enzymes); new means for controlled delivery and release of siRNA; approaches for intracellular drug delivery and organelle targeting; and application of nanocarriers co-loaded with siRNA and drugs to treat multidrug resistant tumors.

Y.PL.S.II.5.

SARS-CoV-2: Molecular interaction specifics viewed through the prism of nanotechnologies

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Severe respiratory syndrome coronavirus-2 (SARS-CoV-2) has gripped the world in an ongoing pandemic and timely investigations of various aspects of its nature are of paramount importance. In this lecture I will present arguments supporting the idea that the current absence of antiviral therapeutics that specifically target human coronaviruses, including SARS-CoV-2, is largely due to the underuse of nanotechnologies in viral research. In addition, the effects of single-point mutations on the specifics of the interaction between the receptor-binding domains on the spike proteins of SARS-CoV-2 and SARS-CoV and its targets in the human cells will be elaborated. Such analyses of the structural differences and the impact of mutations on different viral strains and members of the coronavirus genera are an essential aid in the development of effective therapeutic strategies for an infection such as SARS-CoV-2. At the same time, fundamental research focusing on the interface between nanostructures and coronaviruses is of essential importance for building a knowledge base from which more express medical treatments can be produced for a rapidly spreading community-acquired disease such as COVID-19 than it is the case today. Such fundamental knowledge also presents the only route to the rational design of precisely targeted therapeutics for coronavirus infections. The development of COVID-19 vaccines utilizing nanotechnologies ensures that this is a prospective path to follow, assuming that the various technological and socioeconomic obstacles that have appeared in the course of traversing this path are surmountable.

Y.PL.S.II.6.

Air force office of scientific research grant funding opportunities

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European Office of Aerospace Research and Development

This presentaton will highlight various opportunities for reseach grant funding contributed by the U.S. Air Force Office of Scientific Reserach (AFOSR). The european Office of Aerospace Research and Development (EOARD) is the AFOSR office located in London in the United Kingdom and is composed of scientists and engineers who review research topic ideas and make decisions on the best distribution of grant funding for qualified researchers and professors at Euroean universities. This author and presenter is responsible for programs within the material science and structures topic areas.

This presentation will provide an overview of AFOSR and EOARD, as well as give detailed instructions on how professors from any university throughout Europe may inquire about and apply for grant funding opportunities. EOARD provides grants for in-house university research programs, as well as conference support, and visiting scientist travel costs to collaborate in the U.S.A. Various researchers within Universities in nearly every country in Europe are currently supported by the U.S. Air Force. EOARD seeks to financially support innovative basic science that will benefit the aerospace community at large.

Y.PL.S.III.1.

Hard films for industrial applications: Design-synthesis-evaluation

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Hard-phase films have been extensively applied in various parts with superior mechanical properties like high hardness, wear resistance, low friction, etc. for the applications in machining, die-casting processes. Recently, the electrochemical applications of DLC, diamond films are spotlighted for waste-water treatments.

1 Nanocomposite films

Various new materials for the multi-function are designed. For example, various ternary, quaternary, and quinary nano-structured films in the (Ti, Cr, Mo, Al, Si)-(B, C, N) system are compared in sense of not only hardness but also other properties of corrosion, oxidation, friction etc. for the structural applications.

2 DLC and BDD films for the waste-water treatment

Diamond- like carbon (DLC) and boron-doped diamond (BDD) films have superior chemical stability and electrochemical properties. For the applications of waste-water treatment, the hard layers should have ideal interlayer structure and those multi-layered structure must show the excellent properties such as mechanical stability and electrochemical properties.

Y.PL.S.III.2.

Structure and properties of the compounds TZnSb, T = Ti, V, Cr

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Structure and properties of compounds TZnSb (T = Ti,V,Cr) and solid solutions $V_{0.9}M_{0.1}ZnSb$ (M = Ti,Cr) have been evaluated via combined experimental and first-principles studies. Physical properties i.e. electrical resistivity (4.2 - 800 K), Seebeck coefficient (300 - 800 K), specific heat (2 - 110 K), Vickers hardness and elastic moduli (RT) have been defined for the afore mentioned polycrystalline single-phase materials. From X-ray single crystal and Rietveld analyses all these phases, of which TiZnSb and CrZnSb are novel representatives, were found to crystallize with the ordered MnAlGe-type (space group P4/nmm). The thermal stability has been investigated by differential thermal analysis, indicating an upper limit at about ~ 820 K for T = Ti, Cr and ~950 K for T = V.

A detailed analysis of the structure types TZnSb adopted within the series of 3d transition elements clearly reveals that electropositive elements T=Ti,V,Cr,Mn,Fe crystallize with the tetragonal MnAlGe-type but with rising electronegativity T = Fe,Co,Ni incline to the cubic half-Heusler structure or to a (2a×2a×2a) superstructure of it. The case of Fe with three modifications constitutes the border range.

A variety of physical properties for {Ti,V,Cr}ZnSb are derived from first principles such as structural and magnetic structural stabilities, charge transfer and atomic size, elastic properties, electronic structure (density of states, band structure), electronic transport properties (Seebeck coefficient and resistivity) within Boltzmann's transport theory. All the results are obtained for fully relaxed structural parameters. Concerning magnetic ordering the in-plane antiferromagnetic ordering of T-magnetic moments in the tetragonal MnAlGe-type is dominant. The influence of T-vacancies for VZnSb and CrZnSb are investigated and the results emphasize the role of such vacancies.

Y.PL.S.III.3.

Electrical resistivity and thermal expansion (4.2 – 820 K) of nanostructured skutterudites after severe plastic deformation

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Thermoelectric materials, like skutterudites, with a high figure of merit, ZT, are the essential basis to build thermoelectric generators, which can directly convert heat into electricity. Severe plastic deformation (SPD) via high-pressure torsion (HPT) was successfully applied to enhance ZT of ball-milled and hot-pressed skutterudites (p-type: from 1.1 to 1.4, n-type from 1.6 to 2). In addition, it is possible to achieve high-ZT p- and n-type bulk skutterudites (ZT ~ 1.3 at 773 K for p-type $DD_{0.7}Fe_3CoSb_{12}$ and ZT ~ 1.45 at 823 K for n-type $(Mm,Sm)_{0.14}Co_4Sb_{12}$) by processing industrially produced raw powders, applying a custom-built high-pressure torsion (HPT) equipment at elevated temperature. SPD has a big influence on the structural and as a consequence on the transport and mechanical properties of thermoelectric materials, as SPD introduces many defects, mainly dislocations into the sample and in parallel reduces the crystallite size significantly.

It could be demonstrated that the structural changes of HPT-processed p- and n-type skutterudites, which take place during measurement-induced heating, influence the electrical resistivity and thermal expansion more or less simultaneously. For HP+HPT samples, a severe change takes place above 400 K, whereas for the CP+HPT samples thermal expansion exhibits an unexpected decrease between 300 and 400 K. A further anomaly - being more prominent for the electrical resistivity - takes place at around 520 K. As soon as the sample is thermally stable, all HPT-consolidated samples have in common that the temperature-dependent electrical resistivity is linear but higher than that of the HP samples.

Y.PL.S.IV.1. VIRTUAL

The fundamental science and technology applications of triboelectric nanogenerators

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Triboelectric nanogenerators (TENGs) was invented in 2012, which is based on coupling of triboelectrification and electrostatic induction effects, which is the most effective approach for converting mechanical energy into electric power. TENG is playing a vitally important role in the distributed energy and self-powered systems, with applications in internet of things, environmental/infrastructural monitoring, medical science, environmental science and security. In this talk, we first present the physics mechanism of triboelectrification for general materials. Our model is extended to liquid-solid contact electrification, reviving the classical understanding about the formation of electric double layers. Secondly, the fundamental theory of the TENGs is explored based on expanded Maxwell equations for a mechano-driven system. We will present the applications of the TENGs for harvesting all kind mechanical energy that is available but wasted in our daily life, such as human motion, walking, vibration, mechanical triggering, rotating tire, wind, flowing water and more. Then, we will illustrate the networks based on triboelectric TENGs for harvesting ocean water wave energy, for exploring its possibility as a sustainable large-scale blue energy. Lastly, we will show that TENGs as self-powered sensors for actively detecting the static and dynamic processes arising from mechanical agitation using the voltage and current output signals.

1. Z.L. Wang and A.C. Wang “On the origin of contact electrification“ (Review), Materials Today, **30** (2019) 34-51; https://doi.org/10.1016/j.mattod.2019.05.016
2. Shiquan Lin#, Xiangyu Chen#, and Zhong Lin Wang* “Contact-electrification at liquid-solid interface” (Review), Chemical Review, 122 (2022) 5209-5232; https://doi.org/10.1021/acs.chemrev.1c00176
3. Z.L. Wang “From conctact electrication to triboelectric nanogenerators“ (Review), Report on Progress in Physics, **84** (2021) 096502; https://doi.org/10.1088/1361-6633/ac0a50
4. Jiajia Shao, Morten Willatzen*, and Zhong Lin Wang* “Theoretical modelling of triboelectric nanogenerators (TENGs)” （Review）, J. Applied Physics, **128** (2020) 111101; https://doi.org/10.1063/5.0020961
5. Zhong Lin Wang “ On the expanded Maxwell’s equations for moving charged media system – general theory, mathematical solutions and applications in TENG”, Materials Today, 52 (2022) 348-363; https://doi.org/10.1016/j.mattod.2021.10.027

Y.PL.S.IV.2. VIRTUAL

Carbon dot luminophores

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Carbon dots (CDs) – small crystalline or amorphous carbon-based quasi-spherical nanoparticles – have recently attracted much attention as promising fluorescent materials [1]. One of their widely accepted advantages is the simplicity of the formation of highly luminescent CDs from a wide variety of organic precursors. At the same time, several recent studies on these chemically synthesized CDs raised questions about the chemical nature of the resulting products; their strong luminescence can originate from the presence of molecular organic fluorophores [2]. On the other hand, use of proper synthetic procedures yield purely carbon dot samples of different sizes; color-tunable fluorescence of CDs with blue, green, yellow, orange, red [3] and even near-infrared emission [4] can be achieved, with the color depending on size of the π-conjugated domains in the CD graphitic core [5]. Recently, we have extended the family of these light-emitting colloidal carbon nanoparticles towards other shapes, such as nanorods with linearly polarized emission [6], nanobelts and nanorolls [7]. Application of CDs in luminescent solar concentrators has been demonstrated [8].

1. G. Ragazzon, A. Cadranel, E. V. Ushakova, Y. Wang, D. M. Guldi, A. L. Rogach, N. A. Kotov, M. Prato. Optical Processes in Carbon Nanocolloids. Chem. 2021, 7, 606.
2. Y. Xiong, J. Schneider, E. V. Ushakova, A. L. Rogach. Influence of Molecular Fluorophores on the Research Field of Chemically Synthesized Carbon Dots. NanoToday 2018, 23, 124.
3. J. Zhu, X. Bai, X. Chen, H. Shao, Y. Zhai, G. Pan, H. Zhang, E. V. Ushakova, Y. Zhang, H. Song, A. L. Rogach. Spectrally Tunable Solid State Fluorescence and Room-Temperature Phosphorescence of Carbon Dots Synthesized via Seeded Growth Method. Adv. Opt. Mater. 2019, 1801599.
4. D. Li, P. Jing, L. Sun, Y. An, X. Shan, X. Lu, D. Zhou, D. Han, D. Shen, Y. Zhai, S. Qu, R. Zboril, A. L. Rogach. Near-Infrared Excitation/Emission and Multiphoton-Induced Fluorescence of Carbon Dots. Adv. Mater. 2018, 1705913.
5. N. V. Tepliakov, E. V. Kundelev, P. D. Khavlyuk, M. Y. Leonov, W. Zhu, A. V. Baranov, A. V. Fedorov, A. L. Rogach, I. D. Rukhlenko. sp2–sp3-Hybridized Atomic Domains Determine Optical Features of Carbon Dots. ACS Nano 2019, 13, 10737.
6. Y. Xiong, X. Zhang, A. F. Richter, Y. Li, A. Döring, P. Kasak, A. Popelka, J. Schneider, S. V. Kershaw, S. J. Yoo, J.-G. Kim, W. Zhang, W. Zheng, E. V. Ushakova, J. Feldmann, A. L. Rogach. Chemically Synthesized Carbon Nanorods with Dual Polarized Emission. ACS Nano 2019, 13, 12024.
7. T. Liang, E. Liu, M. Li, E. V. Ushakova, S. V. Kershaw, A. L. Rogach, Z. Tang, S. Qu. Morphology Control of Luminescent Carbon Nanomaterials: from Dots to Rolls and Belts. ACS Nano 2021, 15, 1579.
8. L. Zdrazil, S. Kalytchuk, K. Hola, M. Petr, O. Zmeskal, S. Kment, A. L. Rogach, R. Zboril. A Carbon Dot-Based Tandem Luminescent Solar Concentrator. Nanoscale 2020, 12, 6664-6672.

Y.PL.S.IV.3. VIRTUAL

Electron liquid crystals: A materials science minefield

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Our understanding of metals was pioneered by Paul Drude, who imagined it as a gas of free electrons contained in a can. This model was refined by Lorentz and Sommerfeld and corroborated by Landau's Fermi Liquid theory, which successfully accounted for all properties of metals. This textbook explanation has been challenged by discovering "strange metal" behavior in high-T_c cuprates — the resistivity scaling linearly with temperature and magnetic field. This is attributed to the electron correlations, strong enough to invalidate the FL picture. An even more spectacular departure is the spontaneous breaking of the rotation symmetry in the electron fluid, first observed in cuprates but subsequently in other correlated-electron materials such as Fe-pnictides and chalcogenides, Sr_2RuO_4, and twisted double-layer graphene (TDLG).

In principle, the most direct way to detect electronic nematicity is the measurement of the components of the resistivity tensor. However, one must beware of artifacts; symmetry breaking may be due to various extrinsic factors. This calls for careful experimentation, extensive statistics, and some meticulous Materials science. The latter includes characterization by STEM, RHEED, LEEM/PEEM/LEED, AFM, synchrotron-based XRD, XRF, and XAS, THz dichroism, Second-harmonic generation, Cross-polarized Raman scattering, as well as the angle-resolved measurements of transverse resistivity and magnetoresistance.

References: Nature **572**, 493 (2019); **547**, 432 (2017); **536**, 309 (2016); **472**, 458 (2011); **455**, 782 (2008); 4**22**, 873 (2003); **398**, 221 (1999). Science **361**, 479 (2018); **326**, 699 (2009); **316**, 425 (2007); **297**, 581 (2002); **282**, 2067 (1998). Nature Mater. **21**, 11 (2022); **12**, 877 (2013); **12**, 387 (2013); **12**, 1019 (2013); **12**, 47 (2013); **11**, 850 (2012). Nature Phys. **16**, 712 (2020); **10**, 256 (2014); **7**, 298 (2011). Nature Chem. **14**, 377 (2021). Nature Nanotech. **14**, 44 (2019); **9**, 443 (2014); **5**, 516 (2010). Nature Comm. **9**, 5210 (2018). **2**, 272 (2011).

W.PL.S.I.1.

Sintering assisted additive manufacturing

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Additive manufacturing is increasingly used to make porous preforms followed by sintering to fabricate the final component. The effects of fabrication directionality and gravity on micro- and macro-structure of sintered components are still poorly understood. Present technologies of additive manufacturing (such as binder-jetting, stereolithography, robocasting, selective laser sintering, etc.) of complex-shape powder-components necessitate fine-tuning of sintering as applied to porous 3D- printing products. The densification of complex shapes requires control of the gravity-related and anisotropy phenomena to ensure a nearly full and distortion-free densification. The conducted studies address these issues through the involvement of comprehensive finite element simulations, the determination of the additively manufactured powder specimens' sintering behavior, and the experimental validation of the developed models describing sintering of 3D-printed objects. The presentation describes the numerical modeling of macro and micro- defect formation during sintering of 3D-printed powder components. The validation of the developed models is conducted through the comparison with the experimental results obtained for the sintering of the printed powder ceramic and metallic components. An analytical engineering criterion, which can be used for sintered 3D- printed parts' design recommendations, is derived.

W.PL.S.I.2.

Challenges and opportunities for machine learning approaches for sintering and microstructure development

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There have been significant developments in the use of machine learning for guiding the development of sintering protocols for ceramics. The current status of the field will be reviewed with a focus on the challenges and opportunities that this approach presents. One of the primary limitations is the lack of robust and large number of training data sets. One way to address this limitation is thru the use of high throughput experiments. We will present results on one high throughput study. Ultra-fast laser sintering of alumina that achieves the desired density (*e.g.* 80 to 98 % relative density) and microstructure (*e.g.* grain size) for alumina within ~10 seconds was conducted. A sample array of ~80 sample units (~500×500×100 μm each) can be sintered simultaneously under one laser scan, which results in various microstructures for each sample unit due to the laser power distribution. The hardness of each sample unit and corresponding microstructure were characterized to efficiently establish the datasets for machine learning (ML) training. The hardness vs. relative density data obtained from this high throughput method, well match the literature data. We developed convolutional neural network (CNN)-based ML algorithms that can precisely predict the laser-sintered alumina microstructure from the hardness values and precisely predict the hardness of the laser-sintered alumina from the SEM micrographs with less than 5% error. The grain size- density trajectory for laser sintered alumina was compared to furnace sintered samples and the similarities and differences discussed.

W.PL.S.I.3.

Electric field assisted sintering of oxide ceramics: Fields matter!

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Sintering as a consolidation, densification and coarsening process depends on numerous different intrinsic and extrinsic factors: materials composition, particle size distribution and morphology, temperature programme (heating rate, maximum temperature, dwell time), atmosphere, pressure, microstructure of the green body, etc.

The use of external electric fields offers additional degree of freedom to accelerate densification and taylor microstructure. In order to use their full potential, systematic investigations under well-controlled experimental conditions are required.

Taking the example of doped ceria, sintering parameters required for continuum mechanical modeling are significantly affected by very moderate fields without the generation of macroscopic Joule heating in the sample. For example, the decrease in viscous Poisson's ratio observed with fields is correlated to a clear decrease in shear viscosity, which can be attributed to an easier grain boundary sliding.

In addition, by increasing the amplitude of the electric field, transition to flash sintering is correlated with the generation of n-type electronic conductivity in air under direct-current bias. Its origin is attributed to partial reduction of the material which propagates from the cathodic-to-anodic region. When using AC fields, frequency needs to be taken into account, leading to different kinetics compared to DC fields. Current-rate flash sintering with controlled power leads to a uniform density and grain size. Such strategies are required in order to get homogeneous microstructure and high-quality parts of large dimensions on the way to industrial production.

W.PL.S.I.4.

Enhancing powder metallurgy processing using advanced microstructural characterization and physical metallurgy

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This talk addresses problems limiting the application of two powder metallurgy processes. In the first, prior particle boundaries (ppb) observed in Ni-base superalloy powders that have been consolidated by hot isostatic pressing (HIP) have been characterized using a new imaging technique of scanning electron microscopy (SEM). Using this technique to characterize the surfaces of powders produced using three different processes, namely gas atomization, rotary atomization, and plasma rotating electrode processing, and subsequent consolidated samples from each of these powder sources, yields a solution to this problem. The second problem that has been addressed involves the formation of coarse columnar grain morphologies that result when Ti alloys are processed using additive manufacturing. The solution has involved a small, but predicted, modification of alloy composition that has resulted in a columnar-to-equiaxed transition. In addition to effecting an attractive grain morphology, there are other consequences of such alloying, and the manner in which these may be exploited are discussed.

W.PL.S.I.5.

The role of sintering in process design for aerosol synthesis of nanostructured materials

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Sintering largely determines the morphology and size-structure of nanostructured materials made by gas-phase (aerosol) processes. This is crucial in manufacture of pigmentary titania, fumed silica, nanosilver and optical fibers as well as in the assembly of a number of novel sophisticated materials compositions for heterogeneous catalysis, gas sensors and biomaterials 1 . As a result, there is keen interest to establish a functional understanding of sintering and its impact on the characteristics of these materials and subsequently their performance. By now it is reasonably well understood that a multi-scale approach captures the essence of process design and scale-up for manufacturing of aerosol-made nanostructured materials. Here some examples of quantitative description of sintering of metal oxides (Si/TiO 2) and noble metals and their alloys (Ag/Au) will be elucidated by mesoscale and molecular dynamics simulations highlighting the attainment of power laws regardless of sintering mechanism and explain the “curing” of the toxicity of nanosilver by its alloys with gold.

1. G.A. Kelesidis, S.E. Pratsinis, A perspective on gas-phase synthesis of nanomaterials: process design, impact and outlook, *Chem. Eng. J.,* **421**, 129884 (2021). 10.1016/j.cej.2021.129884

W.PL.S.I.6.

Grain growth: the mixed control mechanism of atom transport

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Ever since its inception, the kinetics of boundary migration and grain growth has been described to be linearly proportional to the associated driving force, irrespective of the presence of impurities, second phase particles or a liquid film at the boundary, as well as any anisotropy in energy or mobility of the grain boundary. Whenever diffusional material transport occurs from one place to another, there are always sources and sinks of atoms. Therefore, the resultant transport kinetics can be governed by either the kinetics of atom movement (diffusion) from the source to the sink or the reaction of atoms at the interface of the source or sink. A typical example is the growth of a single crystal from a melt. It is well documented that the crystal growth mechanism and kinetics is highly dependent on the surface structure of the crystal. For a faceted crystal with an atomically ordered surface, the growth mechanism is either interface reaction- or diffusion-controlled below or above a critical driving force. This mechanism is called the mixed control mechanism. A similar idea may also be valid for the migration of grain boundaries as boundary migration occurs via thermal jumping, which can be considered as diffusion, of atoms across the boundary and their placement (interface reaction) on the surface of the growing grain. Some previous HRTEM observations show that the migration of a flat (faceted) boundary occurs via a lateral spreading of atoms from kink sites formed on the surface of the advancing grain, similar to the growth of a faceted crystal from a melt. Our experimental observations indicate that the mixed control mechanism is operative in the migration of faceted (flat) grain boundaries and resultant grain growth.

This presentation first discusses the limits of the conventional concept of boundary migration. It then describes the basis of the mixed control mechanism of atom transport across the boundary. The mixed mechanism principle of microstructural evolution, which we deduced a decade ago, is explained. We provide examples, which were obtained not only from ceramics but also metals, for the generality of the microstructural evolution principle.[1,2] Some future research directions for boundary migration and grain growth will also be commented on and suggested.

1. S.-J. Kang, et al., J. Am. Ceram. Soc., 92, 1464-71 (2009).
2. S.-J. L. Kang et al., J. Am. Ceram. Soc., 98, 347-60 (2015)

W.PL.S.II.1.

From nanoparticles to nanocrystalline solids with designed functionalities

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Sintering of nanoparticles is the most versatile way to produce nanocrystalline solids of various materials. Scaling grains down to nanometer size enhances many properties of polycrystalline solids due to an increase of the grain boundary interfacial volume fraction. It is well established that the main prerequisite for taking full advantage of such size dependent properties in these materials is removing porosity during sintering while preserving nanoscale morphology and grain size.

Furthermore, these nanoparticle building blocks can be engineered by designing and synthesizing core/shell structures. By sintering core/shell nanoparticles to a fully dense solid and preserving their initial core/shell design, novel bulk solid materials can be fabricated with properties controlled by rationally designed core/shell geometries and properties, and the resultant vast network of interfaces.

A few examples will be presented how we exploit this possibility in order to enhance physical and mechanical material properties made by sintering of engineered core/shell nanoparticles.

W.PL.S.II.2.

Studies on the Flash sintering of KNN: Flash variables, mechanisms and material's properties

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Alternative sintering techniques, as Flash sintering, are needed and currently being object of study and development either for a more sustainable production of materials or for improving its performance. In this work we studied the Flash sintering of Potassium Sodium Niobate, K0.5Na0.5NbO3 (KNN), one of the most promising lead-free piezoelectric. In the case of KNN, Flash, an Electrical Field Assisted Sintering (EFAS) technique allows the reduction of both sintering temperature and time; additionally is has the potential to overpass the limitations found in conventional sintering, i.e., secondary phase formation and limited final density (< 95 % of relative density) due to alkalis volatilization at high sintering temperature (> 1100 ºC) and time (> 2 h).

In this work, variables of Flash sintering KNN such as the powder particle size and purity, applied electric field, sintering atmosphere and thermal schedulle were studied using dilatometric experiments with an applied electric field. The research envolved simulations studies with Finite Element Modeling, FEM, as a tool to model the microstructure of particle contacts and calculate the current density and Joule heating. The simulation data were compared to experimental results of the characterization of Flash sintered samples with XRD, Raman Spectroscopy, SEM and TEM analysis.

The Flash temperature (Tf) of KNN was found to vary between ~300 and ~900 ºC, depending on some powder and processing variables, such as the density of contacts and surface conductivity of green compacts, sintering atmosphere and applied electric field. Liquid-phase assisted sintering is shown to be the prevalent FLASH sintering mechanism of KNN and high dense (95 % of relative density) single phase ceramics could be achieved by this technique. Interestingly, and for the first time, we show that FLASH sintered KNN behave very closely to conventionally sintered materials, in terms of permittivity as a function of temperature, with a Curie temperature of FLASH sintered KNN very close to 420 ºC. Moreover, despite some leakage currents, FLASH sintered KNN can be polarized and its ferroelectric characteristic determined.

W.PL.S.II.3.

Capsule free hot isostatic pressing as a way towards transparent structural and functional ceramics

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Capsule free Hot isostatic pressing is a two-step pressure-assisted sintering method comprising a pressure-less sintering to the stage of reaching closed porosity and Hot isostatic pressing (HIP) on the final stage. The present work comprehends a systematic study both stages individually with the aim to produce highly transparent oxide ceramics with high-end properties. It was shown that very important parameter of capsule free HIP is so-called critical density where the pressure-less pre-sintering (stage 1) has to be terminated. After optimization of the whole sintering process, the real in-line transparency for Al_2O_3, $MgAl_2O_4$, and c-ZrO_2 ceramics was acquired as 70.4, 65.8 and 68.8 %, respectively, at a wavelength of 632.8 nm. Special attention was put through to preparation of transparent luminescent alumina ceramics doped by various rare earth elements (Eu, Er, Nd, Tb, Dy) as well as transition metals (Cr, Mn). The combination of superior optical (RIT exceed 55 %), luminescent and mechanical (Vickers hardness exceeded 25 GPa) properties allow these materials to become a promising candidate for number of hi-tech applications.

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W.PL.S.II.4.

Additive manufacturing and spark plasma sintering: Fabrication of powder components with cooling channels

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A novel method combining Additive Manufacturing (AM) technique of solvent jetting and Spark Plasma Sintering (SPS) of producing complex ceramic and metallic parts with designed internal channels is developed. This novel net shaping approach synergistically combines the capabilities of AM and SPS in producing complex components with internal channels. Along with geometric customization of the 3D printed mold, a major advantage of this method is the removal of the need for a long debinding process, usually necessary with other 3D printing methods, by using the SPS. High density ceramic and metallic complex parts with internal channels were successfully produced with close to theoretical densities. The conducted studies include the development of a model that can predict the evolution and/or distortions of the complex-shaped powder assembly during the sintering process. The model is based on the continuum theory of sintering formulations embedded in a finite element code.

W.PL.S.II.5. VIRTUAL PRESENTATION

Thermal stress and deformation in SiC power chip systems having Ag sintered bonding layers for advanced power conversion

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Power devices and modules need highly efficient heat dissipation system having a chip bonding layer with high thermal conductance and high melting temperature. Ag sintered bonding layer has been attracting much attention in power electronics and bonding technology. Ag sintered layer (SL) has the high melting temperature, enabling SiC power chip operations at high temperatures and high-power conversion. Ag SL also has the high thermal conductivity of about 250 W/mK and the thickness much thinner than conventional lead-free solders. Present important subject is to certify the reliabilities of Ag SL and chip system with this sintered bonding.

This paper presents the thermal stress and deformation results at fixed ambient temperature (25 ^{o}C) by 3D multi-physics solver for SiC power chip systems having Ag sintered bonding layers. We performed analysis and simulations assuming the elastic stress-strain relationship. The stress free temperature was set at Ag sintering temperature (250 ^{o}C).

The first target chip system has a Cu clip attached by Ag SL on a chip, a SiC chip with the thickness of 150 μm (6x5 square millimeter), and Ag sintering chip-attachment on AMB (Active Metal Brazing) substrate with Si_3N_4 film. Simulation results show that perpendicular tensile stress appears at the Cu clip contact edges of chip and Ag SLs. The maximum perpendicular tensile stress is at the lower edge of SiC chip near Cu clip bridge. This tensile stress is thought to be caused by thermal contraction and downward bending moment of Cu clip, and by thermal contraction and upward bending of AMB Cu films. In the second target system a 5 mm square SiC chip with the thickness of 180 μm is attached on Cu plate with the thickness over 1 mm by 30 μm Ag SL. At the corner of this system we have obtained the perpendicular compressive stress in both SiC chip and Ag SL. This perpendicular compressive stress is caused by combined action of SiC chip and Cu plate warpages.

In conclusion our analysis approach and results are very useful for designing reliable SiC power chips having Ag sintered boding layers.

W.PL.S.II.6. VIRTUAL PRESENTATION

Excellent heat dissipation performance of power device structures having Ag sintered bonding layers

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Heat dissipation of power devices needs to be more efficient for high power operations. Ag sintered bonding layer has been attracting much attention because this bonding layer has a high thermal conductivity of about 250 W/mK and a thickness of about 30 µm. In this paper we present an analysis and simulation results by 3D Multiphysics solver on the temperature profile and heat dissipation performance of power device structures using Ag sintered bonding layers. Target structure consists of a 10 mm square Si chip with the thickness of 100 µm, a 20 mm square DCB substrate having 320 µm Cu, 320 µm Si_3N_4 and 290 µm Cu, a 45 mm square Cu heat spreader with the thickness of 3 mm, and a 55 mm square Al heat sink with the thickness of 5 mm. We minimized the heat spreader size, keeping Tjmax increase within 0.5 degrees from the minimum value. This structure has bonding layers (a), (b), (c) under a chip, a DCB substrate, and a heat spreader, respectively. We performed the simulations under the condition where the chip power is 400 W, and the bottom surface of heat sink is fixed at Ta (ambient temperature) of 70 degrees Celsius. Other boundary surfaces are set at heat insulation.
Reference structure for evaluating Ag sintered bonding has 150 µm conventional lead-free solders as bonding layers (a) and (b), and 100 µm thick grease as a bonding (c). Simulated Tjmax of Si chip in the reference structure was 166.8 degrees Celsius. The structure-1 having Ag sintered layers (SL) as bonding layers (a) and (b), and grease as a bonding (c) showed Tjmax of 147.9 degrees Celsius, and 19 degrees lower than the reference structure Tjmax (Tjmax_0). The structure-2 having Ag SLs as all bonding layers (a), (b) and (c) showed Tjmax of 133.4 degrees, and 33 degrees lower than Tjmax_0. The structure-3 without heat spreader having Ag SLs as bonding layers (a) and (b), and Ag sintered bonding between a DCB substrate and a heat sink showed Tjmax of 138.7 degrees, and 5 degrees higher than Tjmax of the structure-2. It was also found that Tjmax of the structure-1 with Ag sintered bonding and grease is still about 7 degrees lower than Tjmax (154.7 degrees) of the structure-4 using conventional solders for all bonding layers. In conclusion our analysis and simulations have revealed remarkable heat dissipation improvement by Ag sintered bonding for Si power chip systems.

Oral Presentations

O.S.I.A.1.

Characterization of thin films obtained using pulsed laser deposition technique

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One of the most important changes in the domain of current surface engineering consists in the discovery and application of modern materials and techniques of the production, as well as their application in nanotechnology, biophysics, power engineering, optoelectronics and other, dynamically developing field of science and common applications of the technology. Therefore, to produce thin films, which are widely used in the above-mentioned industries the new technology namely pulsed laser deposition (PLD) was applied. The present study is focused mainly on the characterisation of the morphology, microstructure, phase and chemical composition, nanohardness of Al-Mg thin films deposited by the pulsed laser deposition (PLD). These aluminium based films can be easily deposited from pure metallic target by modification of process parameters. The research was carried out by scanning electron microscope (SEM) and the transmission electron microscope (TEM). For the purpose of the determining the phase composition of the obtained films the X-ray diffraction and electron diffraction techniques were used. The results of the own research showed that the low homological temperature of the substrate (T_h <0.44) contributes to the formation of thin layers with the nanocrystalline-amorphous structure. The changes of the target-substrate distance led to a structure composed of nanometric crystallites and structural defects. The generation of different harmonic from a nanosecond Nd:YAG laser led to the changes of the microstructure of the thin films. Highly efficient first harmonic of the laser resulted in the nanostructured films with the large clusters of droplets. A significant change in the morphology was essential for the functional properties of the layers the surface of the layers, depending on the energy of the laser radiation photons. The hardness of the thin layers was approx. 265 HV and was slightly higher than the hardness of the target (251 HV).

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O.S.I.A.2.

Selective Laser Melting technology of hot work tool steel influenced by remelting method without preheating of the base plate

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Hot-working steels, used commonly for tools such as dies or hammers in metal forming processes, are known widely for their excellent mechanical properties. Toughness, tensile strength and wear resistance are the main requirements for these steels and are determined by harsh working conditions related to a higher temperature, abrasion and fatigue. Because of these conditions, hot work tool steels are under consistent development focused on heat treatment and manufacturing processes. When it comes to the fabrication of tools, that often have complex geometry, a lately trending technology Selective Laser Melting (SLM) grabs much attraction. Selective Laser Melting technology belongs to a group of processes developed and implemented for additive manufacturing. Utilizing metallic powder with micro-scaled particle sizes and a laser source with a tenth of a millimetre beam diameter can offer industrial level printing precision alongside fine material properties. This, combined with the ability to produce complex geometries or internal structures in metallic parts, is the reason behind the broad usage of this technology. However, due to SLM methodology, the melted powder material is being solidified with high cooling rates, which causes high material internal stresses and, as a result, leads to cracks formation. To limit the thermal gradient during printing, a method of additional heating of the base plate before and during printing has been developed. However, this method aims at the heating base plate to Martensite Start temperature, which is often beyond the limitations of SLM printing machines due to thermal expansion and resulting jamming of mechanical parts. A remelting scanning strategy is proposed to allow the printing of crack sensible materials such as hot working tool steels with SLM technology. It is based on additional melting of the previously melted powder layer, often used to enhance printouts' porosity. However, this approach delivers additional heat to the printout and changes its thermal conditions, influencing the material's internal stresses, phase transformations and resulting microstructure. Preliminary results of scanning electron microscopy observations and light microscopy observations show that remelting can enhance porosity, limit the cracks density and influence the microstructure of hot work tool steel, which makes it a potential solution for additive manufacturing of crack sensible materials in SLM technology.

O.S.I.A.3.

Effect of sodium on phase transformation of gamma-alumina

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Alumina is the most advanced ceramic material that is highly available powder, and γ-alumina is the most common alumina phase. To obtain high-density ceramic, gamma-alumina undergoes several polymorphic transformations. This phase consists of the transition phase of alumina, θ-alumina, which occurs in a specific order before converting to α-alumina. Although significant progress has been made so far in considering the effect of Na on the properties of alumina, its influence on gamma-alumina is still incomplete.

This work aims to investigate the effects of the Sodium on the phase transformation of gamma-alumina. The transition behavior and the microstructure of the samples have been investigated. The results show that the ratio of sodium affects the transition behavior of alumina.

O.S.I.A.4.

Densification and microstructural evolution of Na-doped alpha alumina

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Effect of sodium in various amounts on densification, microstructure, and consequently its mechanical properties of commercial α-alumina was investigated as a function of sintering temperature. Most of the commercial α-alumina is produced by the Bayer process. In the Bayer process, NaOH is used as a digestion agent to dissolve aluminum hydroxide inside the bauxite. Alumina powders thus produced contain significant amount of Na (>0.1wt.%). The increased amount of sodium in alumina ceramics retards sintering and can cause abnormal grain growth (AGG). Sodium also has very low solubility in alumina. Elongated grains were usually observed at low sodium concentrations in alumina ceramics sintered at high temperatures. To determine sodium's effect on the microstructure and consequently, on the mechanical properties, alpha-alumina with varying amounts of sodium were prepared and sintered at 1450℃-1600℃ for 2h. Inhibition of sintering resulted in low sintered density. Elongated abnormally grown grains deteriorated the mechanical property, i.e., flexural strength and hardness. Characterization of samples was done using electron microscopy (SEM/TEM), XRF, flexural strength, and thermal analysis (DTA/TGA). The best densities (≥99%) and mechanical properties were obtained in samples sintered at 1600 C for 2 hours.

O.S.I.B.1.

Graphene supported PdAu nanoparticles as catalyst for hydrogen evolution reaction

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Platinum group metals are the most common catalysts for the studies of hydrogen evolution reaction (HER) from both a fundamental and practical point of view. Such catalysts are expensive and scarce so for practical use their design aims to limit the amount of metals used. The synthesis of cost effective catalysts goes in the direction of bimetallic nanoparticles supported by a conductive and cheap material such as carbon based graphene and glassy carbon. In this work, activity of Au and PdAu nanoparticles supported on reduced graphene oxide (rGO) was examined for HER in acid solution. Reduced graphene oxide was spread using a drop of suspension over the glassy carbon (GC) support. PdAu nanoparticles were obtained by a spontaneous deposition of Au on the rGO/GC, followed by a subsequent spontaneous deposition of Pd. Surface morphology and chemical analysis of rGO/GC, and rGO-supported Au and PdAu nanoparticles were performed using atomic force microscopy (AFM), and X-ray photoelectron spectroscopy (XPS). Phase AFM images have shown that the edges of the rGO sheets were active sites for the deposition of both Au and Pd. XPS analysis revealed that the atomic percentages of both Au and PdAu nanoparticles were slightly higher than 1%. Electrochemical characterization was performed by cyclic voltammetry (CV), while linear sweep voltammetry (LSV) was used to gain insight into the electrocatalytic activity of these electrodes for HER. Test stability and activity measurements of the electrodes were performed by CV, LSV, and chronoamperometry (CA). The activity of the PdAu/rGO electrode for the HER was remarkably high, with the overpotential close to zero with a Tafel slope of −65 mV/dec. HER activity was stable over a 3 h testing time, with a low Tafel slope of approx. −46 mV/dec achieved after prolonged hydrogen evolution at a constant potential indicating faster kinetics.

O.S.I.B.2.

Metal-ceramic composites based on reinforced ceramics

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The microstructure of composites viewed at different levels allows property control and optimization for a specific application. In many cases, there are at least two functional parameters with opposite tendencies that should be simultaneously improved for a superior general performance. The straightforward example is the need for composites with a high ductility or fracture toughness and strength or strength-to-weight ratio. To achieve this goal, the literature presents different solutions in which the microstructural concept is defined as a range of uniquely multi-scale hierarchical structures obtained as a result of planning, design, and use of adequate processing technologies. Under these circumstances, selection of the building elements of a composite, their compatibility, relationships, arrangement and how these elements and their structures are formed considering the raw materials, are essential.

The work contains results of the R&D of a new class of metal-ceramic composite materials based on reinforced composites and high entropy alloy (HEA) as a binder. AlCrFeCoNiV(Ti) HEA was used for the densification of WC-W_2C(B_4C–TiB_2) eutectic particles by spark plasma sintering. Thermodynamic, kinetic, thermomechanical compatibility of AlFeCoNiCr(V)Ti –(WC-W_2C)/(B_4C–TiB_2) composites were investigated. In the case of using WC-W_2C eutectic particles, the W_2C phase dissolves in the HEA matrix and forms a core-rim structure leads to the formation of a reinforced boundary and grain refinement. Also, the interaction of the boron carbide phase of the eutectic particles B_4C-TiB_2 with HEA leads to the formation of a unique reinforced grand boundary. As a result, the average value of the hardness of (WC-W_2C) – HEA and (B_4C–TiB_2) – HEA composites reaches 93 HRA (HV = 16 GPa) and 21 GPa, respectively, while the Palmqvist fracture toughness reaches 17 $MPa\cdot m^{1/2}$ and 14 $MPa\cdot m^{1/2}$.

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O.S.I.B.3.

Suspension plasma spraying of $BaTiO_3$ and $BaTiO_3/ZrO_2$

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In this work, thermal spraying of barium titanate-based ceramic composites was investigated. This lead-free electroceramic material can be combined with other ceramics, such as yttria stabilised zirconia, to increase its mechanical response while maintaining the material's dielectric and piezoelectric properties. Suspension plasma spraying was used to manufacture homogeneously dispersed composites with fine ceramic particles. The concentration of ZrO_2 in $BaTiO_3$ ranged from 0 to 50 wt. %. The microstructure of the coatings was columnar, with distinct and dense columns. An increasing amount of ZrO_2 in the suspension changed particle size and chemical composition, which led to changes in the microstructure of the coatings. X-ray diffraction analysis suggested that incorporating a small amount of ZrO_2 could substantially influence the crystalline structure of the matrix. The influence of ZrO_2 on the phase composition and chemical composition was further studied by X-ray dispersive spectroscopy and Raman spectroscopy. The influence of the microstructure and the chemical composition on the mechanical properties was evaluated by the Vicker's hardness test.

O.S.I.B.4.

Investigation of the dynamics of deformation mechanisms in Mg-Gd alloys

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The dynamics of the deformation mechanisms activated in cast binary magnesium-gadolinium (Mg-Gd) alloys with respect to the concentration of Gd was studied with in-situ experimental methods. Alloys were characterized by random texture and homogenous microstructure. Acoustic emission (AE) technique was recorded simultaneously during compression tests to determine the dominant deformation mechanism activated in different stages of the deformation. Deformation test were repeated in the chamber of scanning electron microscope (in-situ SEM). The development of the microstructure was concurrently followed by secondary electrons and electron back-scatter diffraction (EBSD). The main goal of these measurements was to identify the activated slip systems in particular stages of the deformation and the progress of twin volume fraction. Results of the combination of AE and in-situ SEM indicate higher activity of non-basal slip systems with increasing Gd content. Lateral growth of twins decreases also with higher Gd concentration as a result of decreased mobility of twin boundaries caused by solute Gd atoms. High speed camera was used to investigate the dynamics of twinning, mainly to estimate the velocity of twin propagation. The results clearly indicate that the rate of twin propagation is in order of 10 m/s.

O.S.I.B.5.

Investigations of pressed and sintered components using 17-4PH powder collected in the chamber of an SLM printer

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In this study, a precipitation-hardened, water-atomized martensitic stainless steel powder (17-4PH, 100-mesh) was investigated in its original and used states. The 17-4PH powder used was taken from the chamber of a selective laser melting machine (SLM). Cylindrical components were produced from both powders by cold pressing and sintering. The density, microstructure, strength, and workability of the various manufactured components were determined using different measurement techniques. The results showed that the properties of the components produced with the used powder are almost the same as those of the original powder. Thus, it is practicable to produce components from used 17-4PH powder via cold pressing and sintering.

O.S.I.C.1.

Electrochemically-grown Cu_2O nanocubes favorably electroreduce CO_2 to methane: What triggers the activity?

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Recently, CO_2 electroreduction reaction (CO_2RR) has been established as a promising approach for transforming greenhouse gas into fuels and commodity chemicals. Copper is an appealing catalyst and it is the only monometallic catalyst that can produce hydrocarbons and alcohols in decent amounts.[1] Among the complex interplay of various Cu-based catalyst parameters (morphology, composition, shape, size, interparticle distance, loading, etc.) to improve the CO_2RR reactivity, the shape effect has attracted significant interest due to the tunable approach toward selectivity of certain facets. Cube-shaped copper (Cu NCs) nanoparticles with Cu (100)-rich surfaces have been recognized in the CO_2RR community as the propitious catalyst for the production of ethylene (C_2H_4) for future industrial applications.[2] However, since the copper-based catalysts are highly vulnerable to dynamic reconstruction during CO_2RR-relevant conditions, the working morphology/composition needs to be assessed to unambiguously interpret the selectivity of any given catalyst system.[3] In this study, electrochemically-grown chloride-free Cu_2O nanocubes with optimized size and coverage are employed for CO_2RR. Concerning selectivity, electrochemically-grown Cu NCs showed surprisingly different behavior than commonly reported Cu (100) abundant surfaces.[4] The unexpected behavior of as-prepared nanocubes is reflected in inactivity towards hydrocarbons when they are employed in electrolysis even at high overpotentials. However, interestingly, when the catalyst undergoes "pre-treatment" in the form of a double-layer capacitive cycling method for the determination of electrochemical surface area (ECSA), often considered a non-invasive method, it becomes active for methane formation. In this study, the influence of potential window width in which the ECSA is employed and its correlations with the selectivity is presented. We will underline the importance of the employment of the ECSA determination method as a triggering factor for the activity/selectivity of particular Cu NCs catalysts for CO_2RR and further emphasize the reconstructive nature of Cu-based catalysts during a reaction.

O.S.I.C.2.

N-Heterocyclic carbenes - the design concept for densely packed and thermally ultra-stable aromatic self-assembled monolayers

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One of the prominent platform for use in molecular/organic electronics are self-assembled monolayers (SAMs). The majority of SAMs-related research is based on sulfur-metal bonding. However, thiol-based coatings suffer from low thermal and chemical stability. Recently, Crudden et al. proposed a new promising strategy for bonding molecules to noble metal substrates using N-heterocyclic carbenes (NHCs) [1,2]. Experiments and calculations shows that only carbenes with bulky (e.g. isopropyl) side groups can form vertically oriented monolayers that are crucial for the surface functionalization. However, this design leads to three times lower surface density of NHC SAMs compared to thiols [3], which strongly decreases the impact of the surface modification. Following our recent successful example of densely packed NHC SAMs formation [4], in the current work [5] we conducted a systematic experimental analysis (XPS, HRXPS, NEXAFS, SIMS, TP-SIMS, WCA) for a series of such monolayers. We demonstrated, that, contrary to other reports, the perpendicular orientation of NHC molecules can be achieved using short (methyl) side groups, thus doubling the surface density compared to the NHC SAMs reported before. Moreover, we were able to increase the thermal stability by ca. 160 K (~0.5 eV increase in desorption energy) compared to NHC monolayers considered currently [3] as a model system. Altogether, the obtained results provide a well-defined concept of molecular design, paving the way to the fabrication of densely packed and thermally ultra-stable functional aromatic SAMs on the NHC basis.

1. Crudden, C. M. et al. **Nat. Chem. 2014**, 6, 409–414.
2. Smith et al. , C. A. et al. **Chem. Rev. 2019**, 119, 4986–5056.
3. Inayeh, A. et al. **Nat. Commun. 2021**, 12, 4034.
4. Krzykawska et al. **ACS Nano 2020**, 14, 6043–6057.
5. Wróbel et al. **Nat. Chem**. **2022** in review

O.S.I.C.3.

Probing improper ferroelectricity in oxygen-deficient $YMnO_3$ ultrathin films

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Hexagonal manganites (*h*-$REMnO_3$, RE = rare earth) belong to the exciting class of multiferroic materials exhibiting coexistence of ferroelectricity and antiferromagnetism in a single phase. This coexistence of separate ferroic orders allows for a large amount of tunable parameters, making them compelling candidates for various novel functional applications, such as non-volatile memory devices. $YMnO_3$ (YMO) is the most studied of the *h*-$RMnO_3$ series. At room temperature, it crystalizes in the polar $P6_3cm$ space group and exhibits improper ferroelectricity, driven by a lattice-trimerizing structural distortion of the MnO_5 bipyramids around the Y^{3+} ion.

In this contribution, we present a systematic study on the lattice trimerization in off-stoichiometric YMO ultrathin epitaxial films grown on single crystalline Pt-buffered $SrTiO_3$(111) substrates. A combination of high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) and electron energy-loss spectroscopy (EELS) is used to quantify the effect of nanoscale confinement on the lattice trimerization, revealing the presence of a critical thickness for improper ferroelectricity and below a 3 unit cell thickness, the polarization is suppressed in the YMO films.

Particularly, an attenuation of the Y-ion corrugation is observed at the top and bottom interfaces, which corresponds to an increase in oxygen vacancy concentration, as evidenced by a reduction of the Mn valence state. The strongest Mn ion reduction is detected for the two unit cell (u.c.) thick films with $Mn^{+2.3}$, while $Mn^{+2.98}$ is found in the bulk of a 14 u.c. thick film. Simultaneously, the amplitude of the Y-layer corrugation drops from ~50 pm in 14 u.c. films down to ~13 pm in 2 u.c. films. The derived ferroelectric polarization shows a similar reduction of about 80% in the thinner film (to ~1 $\mu C/cm^2$) compared to YMO single crystals. Our results advance the understanding of improper ferroelectricity within the confinement of ultrathin films, which is essential for their successful implementation in the next-generation computing and storage devices.

O.S.I.D.1.

Effect of metakaolin and lime on strength development of blended cement paste

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The influence of co-calcined kaolinite and limestone on the hydration of blended cement was investigated. Calcination of kaolinite (with ~50 wt% quartz impurity) and a mixture of kaolinite/limestone was done at the temperatures 700 and 800°C, respectively. These supplementary cementitious materials (SCMs) were added to ordinary Portland cement (OPC) on the order of 30 wt% replacement. The compressive strength of blended cement paste samples was measured after 28 and 90 days. Hydration products and microstructural development in blended cement pastes were studied by X-ray diffraction (XRD), thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). The results indicated that addition of free lime (CaO) together with metakaolin (MK) to OPC leads to an enhancement in mechanical performance. This is due to the increased consumption of Portlandite (CH), formation of calcium aluminosilicate hydrate (CASH), and reduction of porosity in the sample containing free lime and metakaolin.

O.S.I.E.1.

Nanoparticles in our brains

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Calcifications of the dura mater (DM) are an accidental finding during computed tomography. They are found even more often during autopsies. However, how common is DM calcification and what is its biological significance? Is it a manifestation of age-related changes or a pathological process? These questions remain open. The focus of this work is to study the structural and elemental composition of inclusions in the tissue of DM in patients whose death was caused by intracerebral hemorrhage in the background of hypertension. The study was approved by the Ethics Committee of the Medical Institute of Sumy State University (proceedings 6/02, 09.02.2022). Thirty specimens of the DM obtained during autopsies at Sumy Regional Hospital were involved in our research protocol. We removed tissue from the falx cerebri area and then fixed it in a 10% formalin solution for 24 hours. After that, we cut strips of 2.0x0.5x0.1 cm from them, routinely stained with hematoxylin-eosin. To confirm the presence of calcium compounds, we stained the samples by histochemical methods: the von Cossa and the alizarin red staining's. We performed scanning electron microscopy (SEM) on an SEO-SEM Inspect S50-B with a resolution of 10 nm. We obtained elemental composition data from the analysis of EDX spectra activated by an electronic probe. We performed spectrum processing using the standard software of the microanalysis system. The staining of DM tissue with alizarin red confirmed the presence of calcium compounds (orange-red color) in 86.6% of the DM samples. According to the results of von Cossa staining, 50% of samples of the DM contained calcium compounds. During the SEM study of the DM samples, we found a significant number of calcifications of various sizes (1 to 50 μm). Some of them were extremely small and correspond to the size of nanoparticles. The role of DM calcifications remains unclear and requires further research.

O.S.I.E.2.

Sintering of biodegradable Mg-Y and Mg-Nd magnesium alloys fabricated for medical applications

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The Mg-Y and Mg-Nd biodegradable mischmetal-free magnesium alloys were prepared by the powder metallurgy method. A modern spark plasma sintering technique was used to effectively produce almost fully dense samples from the gas-atomized powders. Different sintering temperatures from 450 °C to 550 °C were used during the sintering compactization. The effect of the alloying elements and the effect of the sintering temperature on the microstructure and corrosion properties were investigated. The microstructures of powders and compacted samples were characterized by scanning and transition electron microscopy. Corrosion properties of compacted samples were evaluated by immersion and electrochemical tests using NaCl solution. Moreover, the results were compared and discused with those of the ternary magnesium alloy Mg-Y-Nd, prepared identically.

O.S.II.A.1.

Influence of brazing conditions on crystallization mechanism and mechanical properties of the TiAlV/TiCuZrPd/TiAlV brazed joints

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Research in the field of brazing titanium alloys using amorphous foils is very intensively carried out around the world. Currently, finding environmentally friendly solutions is of particular importance, by minimizing the energy used for industrial brazing processes in the aerospace, automotive and energy industries. This paper presents a complex analysis of research results describing the fundamentals of phenomena and processes occurring in the filler metal and at the interphase boundaries of brazed connections. The results obtained for the amorphous Ti-Cu-Zr alloys with the Pd addition proved that the kinetics of nucleation and growth at high rates of heating determined character and course of primary and secondary crystallization. Process of multi-phase crystallization became reduced to CuTi phase crystallization.

The use of amorphous, Ti-based alloy brazing foils allowed to lower the process temperature by about 100ºC and to distance the soldering process temperature from the α-β phase transition temperature occurring in the Ti-based alloys. Lowering the temperature to 770 ºC eliminated the problem of crystallization of the fragile Laves phase, which weakens the mechanical and plastic properties of the joint. The use of amorphous foil as a bonding material without the need for flux, allowed to obtain a homogeneous, non-porous joint of high quality and strength. The amorphous foil can easily be placed between the soldered parts due to its flexibility, reducing the time of configuration/assembly, improving the strength and hardness of the joint. The overall strength of the joints was determined by shear tests at room temperature; the mechanical response coupled with fracture path detected by post mortem analysis was related to the microstructures and process parameters.

The results of the studies allowed to describe between the structure of the joint, and its behavior in various conditions (temperature, load) depending on the chemical composition, the crystallization mechanism and mechanical and thermal properties of the alloy used as filler material.

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O.S.II.A.2.

Structure integrity of high-entropy alloys (HEA) manufactured by Selective Laser Melting (SLM) using in-situ alloying of elementary powders

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In recent years, additive manufacturing technologies have become widespread and commonly used. One of the main methods used in industry and research is Selective Laser Melting (SLM). This technique allows obtaining complex elements with high repeatability. It is also characterized by the possibility of precise control of many process parameters. High-entropy alloys (HEAs) are metal alloys containing at least five components in atomic ratio from 5 to 35 %. Their characteristic feature is the ability to form a single phase of high mixing entropy. The ongoing research addresses one of the HEAs' main problems, the efficiency of their fabrication processes. In-situ alloying during the fabrication process has been attempted using mixtures of elementary powders prepared for SLM. Five batches of powder mixtures with different atomic ratios and mixing entropy were prepared to produce alloys. The blends included metal powders such as Ni, Co, Fe, Mn, Ti, and Al. All alloys were fabricated using a Renishaw AM400 machine using a Reduced Build Volume (RBV) module. Eight samples were obtained from each alloy, each for different process parameters. The variables were laser power and exposure time, and the linear energy density ranged from 148 J/mm^3 to 580 J/mm^3. The process was carried out in a protective argon atmosphere with oxygen levels not exceeding 1200 ppm. Light microscopy and scanning electron microscopy (SEM) studies were performed. Based on the preliminary studies, it was found that for the selected alloy and parameter combinations, a homogeneous material could be obtained. Investigations of porosity showed the dependence between the process parameters and the number of gas pores in the structure of the materials. Remelting deficiencies were also observed for the lower linear energy density values. The discontinuities in the structure counted for each sample on a cross-section area of at least 55 mm^2 ranged from 0.012% up to 3.2%, and for each material, there was a different optimal combination of parameters. Overall, the higher laser power values and longer exposure times promoted less porosity and higher homogeneity in the alloys.

O.S.II.A.3.

Non-destructive testing of composites using terahertz radiation

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In recent years, terahertz radiation has been of great interest. In the field of electromagnetic radiation, the terahertz band is located between infrared radiation and microwaves. Therefore, it is often referred to as far infrared radiation or is included in the microwave band range. The terahertz band includes waves in the range from 0.1 to 10 THz. Electromagnetic waves in this spectral range are strongly attenuated in electrically conductive substances such as metals, as well as in water and electrolytes, while they are very poorly attenuated in dielectrics. Therefore, terahertz radiation can be used in non-destructive testing of composites with polymer and ceramic matrix. In non-destructive testing, terahertz radiation is used in two "classic" research methods: reflection and transmission. In both of these methods, there must be both a source of terahertz radiation and a receiver through which changes in the terahertz signal are recorded. As a result of absorption and reflection by the tested material and discontinuities in its internal structure. In the reflection method, both the radiation source and the receiver are on the same side of the tested object. In the transmission method, the source of terahertz radiation and the receiver (THz detector) are on opposite sides of the tested object. The paper presents the results of tests of glass and aramid fiber reinforced composites with deliberately introduced defects. The tests was carried out using the transmission method.

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O.S.II.A.4.

The role of compensation defects in the stabilization of multivalent inorganic systems doped with europium ions

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The functional materials characterized by the strictly defined properties are highly desired to use in many technological processes. Catalysis, water splitting and solid state lighting among many others use systems consisting of an inorganic matrix and multivalent active centers incorporated into the matrix.

Taking into account the requirements that have to be met in the case of luminescent materials used in modern white light sources, such as high CRI and quantum efficiency, low cost of the phosphors, the aforementioned systems are perspective in lighting technologies. The procedure typically used to obtain the source of white light is ineffective and can be replaced by a synthesis of a system consisting of a matrix activated by lanthanide ions in two different oxidation states. Due to the high efficient emission observed in the both oxidation states as well as facility in controlling of emission energy the europium ions are the most extensively studied. However, in such systems the most crucial factor for obtaining the white emission is precise control of the $[Eu^{2+}]/[Eu^{3+}]$ concentration ratio.

The recent studies show that this control can be achieved by aliovalent co-doping of a matrix - lanthanide system. These co-dopants can be considered as compensators for the charge of $Ln_{Me}^{\bullet}$ defect and, thus, Eu^{3+} stabilizers. Some of the results show that if more stable the compensator is, the more stable Eu^{3+} ion under reductive conditions will be.

The introduction of the co-dopants and thus the creation of chemically induced compensating defects can be executed using several strategies that will be presented in this contribution. Moreover, the qualitative explanation of the influence of the compensation defects created via above mentioned strategies on the stabilization of multivalent europium systems will be shown.

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O.S.II.A.5.

Enhancing the environmental aspect of mineral recovery: separation of metal carbonate on micro nanofibrillated cellulose

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The demand for mineral resources continues to expand unabated, driven by the rapid technology direction change toward the electrification of vehicular transport and the exponential growth of microelectronic and power storage systems. The focus on rare earth element (REE) beneficiation features as one of the major newly emerging environmental impact factors facing the future extraction industry, governmental policy-makers and regulatory protection agencies alike. Traditionally, flotation beneficiation adopts surfactant chemistry enabling surface energy-driven separation of mineral components in aqueous medium. Whilst efficient for high-bearing ores, the chemical load on the environment caused by flotation tailings has been a matter for concern. When considering the winning of elements such as lithium alongside REE the paucity of the desired component in the ore results in extremely large deposits of ancillary mineral waste, not all of which is environmentally acceptable, and made even more problematic if carrying aquatic-damaging surfactant. To help overcome these barriers to mining implementation much work is progressing in the area of using cellulose as a separation agent, primarily by chemical modification to enable compatibility with silica, iron or heavy metals, for example. Based on our prior observations that when placed under ultralow shear ($< 0.01\ s^{-1}$), acting below the yield stress of the aqueous gel formed using micro nanofibrillated cellulose (MNFC), adsorption of calcium carbonate nanoparticles onto cellulose nanofibrils occurs without particle–particle preflocculation. The action of surface bound water on the nanofibril is considered to initiate the adsorption, and the condition of ultralow shear suggests that the residence time of the mineral particle in contact with the nanofibril, acting under controlled strain against diffusion in the gel, is critical. Given the specificity of this interaction, we here illustrate that mineral separation can be implemented, exemplified by the free removal of silica whilst capturing calcium carbonate. Use of the cellulose-carbonate composite thus formed is currently another field we are pursuing in circular economy, which together with the biodegradability of cellulose renders the concept a positive contribution to enabling the future extraction of the much sought-after REE residing, for example, in carbonatite ore under enhanced environmental conditions.

1. Liu, G., Maloney, T., Dimić Mišić. K., Gane, P., (2017) Acid dissociation of surface bound water on cellulose nanofibrils in aqueous micro nanofibrillated cellulose (MNFC) gel revealed by adsorption of calcium carbonate nanoparticles under the application of ultralow shear. Cellulose 24:3155-3178: DOI 10.1007/s10570-017-1371-1

O.S.II.A.6.

Multiscale enhancement to aramid fabric-reinforced composites: electrospun P(An-co-GMA) nanofibrous interlayers

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This study reports the effect of electrospinning nanofiber interlayers of epoxy-compatible poly[acrylonitrile-co-(glycidyl methacrylate)], hereafter P(An-co-GMA), in the tensile properties of plain-weave aramid fabric-reinforced composites. Laminates of composites were interleaved by nanofiber mats of commercially available polyacrylonitrile and the copolymerized acrylonitrile with glycidyl methacrylate; a molecule containing an epoxide. This ring was supposed to break by the heat of provided in the composite processing and make bonds to the same broken groups on the epoxy matrix. Free-radical polymerization was run in solution environment and the success of the polymerization was verified with FT-IR. Nanofibers mats were collected electrospinning of both PAN and P(An-co-GMA) and analyzed morphologically using FE-SEM. Laminates were prepared using vacuum bag-assisted hot-press molding and cut into desired geometry using a waterjet. The samples were tested according to the standard tensile tests. The results revealed that the interlayers of P(An-co-GMA) in epoxy-matrix increased the stiffnesstensile modulus, E, by 34%, the strength, σ_u, by 8%, and reduced the ductility , ϵ_b, by 2.5% when compared to virgin laminates. Polyacrylonitrile also improved the mechanical properties; increased E by 26%, reduced σ_u by 13%, and reduced the ϵ_b by 2.4%. Comparing the effect of these two interlayers, the presence of epoxide rings caused 8% excess increase in E, 5% extra decrease in σ_u, and almost no change in ϵ_b. When nanofibers interlayers of epoxy-compatible polymer laminated with phenolic matrix, the reinforcement mechanism changed from the improvement in elastic modulus to an improvement in σ_u by 18%. In conclusion, epoxy compatible polymers showed promising results in improving the mechanical properties of composites both with their morphological advantages, and covalent bonding they created with the epoxy matrix. The approach can be applied for tailoring the properties of aramid fiber-reinforced composites in automotive and aerospace structures.

O.S.II.A.7.

Structural instabilities of complex oxides and intermetallics probed by in situ X-ray synchrotron powder diffraction

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In situ temperature-dependence powder diffraction examinations and analysis of thermal expansion is very sensitive tool not only for the study of structural phase transformations, but also for the investigation of diverse electronic and magnetic phase transitions occurred in complex oxide and intermetallic systems. Especially this is important for the Pr- and Nd-based compositions, where the spin-state transition is seen much better in the thermal expansion data than in the magnetic susceptibility due to the large contribution of the 4f moments of Pr and Nd ions on the magnetic properties.

This presentation outlines our twenty years experience of the comprehensive investigations of thermal behaviour of several classes of complex oxide and intermetallic materials by in situ high-resolution X-ray synchrotron powder diffraction at the large scale facilities of leading European synchrotron radiation sources such as ESRF (Grenoble), HASYLAB@DESY (Hamburg) and ALBA (Barcelona).

Numerous investigations of several series of mixed rare earth (RE) cobaltites $R_{1-x}R'_xCoO_3$, cobaltites-ferrites, cobaltites-chromites and cobaltites-gallates $RCo_{1-x}M_xO_3$ (M = Fe, Cr, Ga) revealed pronounced anomalies in the lattice expansion, which are reflected in a sigmoidal dependence of the unit cell dimensions and in abnormal anisotropic increase of the thermal expansion coefficients with (several) maxima at the specific temperature. It was shown that these anomalies are caused by a thermally driven transitions from a low-spin (LS) to the excited spin states (IS or HS) of Co^{3+} ions and the coupled magnetic and metal-insulator transitions.

In the RE perovskite ferrite series, clear signs of magnetoelastic coupling was discovered in $SmFeO_3$ and in the mixed $SmFeO_3$–Pr(Nd)FeO_3 systems, in which subtle deviations of the thermal expansion were observed at the magnetic ordering temperature T_N.

Several kinds of concentration and temperature induced structural phase transitions and diverse sorts of lattice expansion anomalies have been detected in the RE–(Ni,Pd)–Ga intermetallic systems. In particular, diverse sequences of structural phase transitions were found in the La(Ce)$Ni_{13-x}Ga_x$ solid solution series. In YbNiGa and YbPdGa compounds, pronounces anomalous lattice expansion and negative thermal expansion (NTE) phenomena was discovered in a broad temperature range of 8 K–1173 K.

O.S.II.A.8.

MAX phases-based electro conductive and were resistant coating for application in oxidizing environment at high-temperatures

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The results of variations of structure, oxidation and wear-resistance, and electrical conductivity of novel MAX-phase Ti,Nb-Al-C-based bulk composites and vacuum-arc deposited coating are presented. The stability in air was studied at 600 °C for 1000 h. High electrical conductivity (σ=1.3·10 6 S/m) of the highly resistant toward oxidation ($\Delta m/S$=0.07 mg/cm^2) Ti-Al-C coating was preserved after long-term heating in air. High oxidation- and wear-resistance of the coatings, high mechanical characteristics after long-term oxydaytion, namely nanohardness H (10 mN)= 9.5±1.5 GPa, and Young's modulus E =190±10 GPa, make them very promising for interconnects of solid oxide fuel cells (SOFCs) and for blades of gas turbine engine compressor, as well as plain bearings operating under fretting corrosion conditions at temperatures up to 600 °C.

O.S.II.B.1.

The influence of substrate and thermal annealing on calalytic activity and stability of Pt thin film catalysts

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The electrocatalytic oxidation of small organic molecules, such as methanol, ethanol and formic acid has been extensively studied due to their properties that make them suitable for use in fuel cells. Particularly, the electrochemical oxidation of formic acid has been comprehensively examined as the anodic reaction in direct formic acid fuel cell (DFAFC).

In this study, we have investigated how the change in surface composition of Pt thin film deposited on Ni and Cr supports, induced by the controlled thermal treatment, reflects on catalyst performance for the electrooxidation of formic acid.

The results presented unequivocally show that the exceptional activity for formic acid electrooxidation, measured on annealed Pt/Ni and Pt/Cr catalysts, is a direct consequence of the nature of the substrate which manifests itself after controlled heat treatment trough bifunctional effect at Pt/Ni and through surface reconstruction at Pt/Cr catalyst.

In the case of Pt/Ni catalysts, exactly what makes it active leads to instability, which means that the increase in activity goes at the expense of stability. In contrast, at Pt/Cr catalysts, by using the controlled thermal treatment we increase both activity and stability, and actually to a significant extent for the catalyst annealed to 500 ^{o}C

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O.S.III.C.1.

$(Gd,Y)VO_4:Eu^{3+}$ nanoparticles as promising theranostic agents

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Theranostics is a novel concept, which involves the integration of diagnosis and therapy in a single platform using nanomaterials. This approach implies the application of novel therapeutics on the base of various nanoparticles (NPs) as delivery systems, which are functionalized by combining imaging and therapeutic agents, that allows both effective drug delivering, treatment and diagnostic of the treatment process to be realized. Redox active nanoparticles, which are able to participate in reactive oxygen species (ROS) control at the cellular level, are of great prospect for theranostics applications, because it is now generally accepted that an imbalance of ROS production and scavenging is closely related to a broad spectrum of diseases including cancer. Thus, besides the delivering function, such NPs could be considered as a therapeutic agent themselves.

In this concern, $(Gd,Y)VO_4:Eu^{3+}$ NPs (d= 2 nm) stand out in the NPs family. Due to doping with Eu^{3+} ions and paramagnetic features of gadolinium ions, they could serve as diagnostic agents. Besides imaging and contrast enhanced abilities, $(Gd,Y)VO_4:Eu^{3+}$ NPs could serve as containers for the delivery of active compounds inside cells and tissues. Moreover, $(Gd,Y)VO_4:Eu^{3+}$ NPs were found to exhibit dual (pro- and antioxidant) action, which could be controlled, that allows them to be used as ROS-regulating agents.

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O.S.III.C.2.

Mechanical behaviour and hydrogen permeability of carbon steel with surface nanocrystalline structure

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Extreme operating conditions, namely mutual action of mechanical loads, corrosion and wear, demand the highest performance of the materials used in many industries. Since recently, it is known that heterostructured materials with nanocrystalline structures on the surface [1–3] can be promising candidates to be operated in such severe conditions. Nanocrystalization is one of the most effective methods of protection of the metal surface and significantly improvement of the overall properties.

The main objective of the study was to assess mechanical behaviour and hydrogen permeability of the carbon steel with surface nanocrystalline structure generated by mechanical-pulse treatment using different technological environments. In this technique high-speed friction is used for severe plastic deformation of the surface layer of the steel specimens. The fragmentation of the surface layer's structure to the nano sizes with its simultaneous saturation by components and alloying elements took place during treatment. Parameters of nanocrystalline surface layer and its physical and mechanical properties depended on treatment regime and type of technological environment, which enabled forming a surface layer with desirable structure and properties. The size value of crystallites was the smallest (in the range of 15–60 nm) on the surface. Microhardness of the treated surface was influenced by the size of crystallites of the nanocrystalline structure: it increased with decreasing size of crystallites. It was revealed that the nanocrystalline surface layer served as a barrier for hydrogen penetration into the bulk metal: it was characterized by lower hydrogen permeability and higher efficiency of hydrogen trapping in comparison with the untreated steel.

References

1. Umemoto M., Todaka K., Tsuchiya K. Formation of nanocrystalline structure in carbon steels by ball drop and particle impact techniques. Mater. Sci. Eng. A. 2004; 375–377: 899–904.
2. Dai K., Shaw L. Comparison between shot peening and surface nanocrystallization and hardening processes. Mater. Sci. Eng. A. 2007; 463: 46–53.
3. Maksymiv O., Kyryliv V., Zvirko O., Nykyforchyn H. Behavior of tempered surface nanocrystalline structures obtained by mechanical-pulse treatment. Springer Proceedings in Physics. 2019; 221: 125–134.

O.S.III.C.3.

Improvement of electrochemical properties of ZnO nanoparticles via composites with graphene oxide

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Due to their tunable multifunctional properties zinc oxide (ZnO) based materials have attracted extensive scientific and technological attention. Since they combines different properties such as electrochemical activities, chemical and photochemical stability, non-toxicity, biocompatibility, etc. ZnO-based materials have been used for variety of applications in electronics, opto-electronics, biosensing, bioimaging, drug and gene delivery, implants, antimicrobial and anticancer agents, as well as sensing in environmental applications.

The main aim of this study was to improve efficiency of ZnO particles toward both electrochemical sensing for environmental application and electrocatalysis. To vary electrochemical properties, series of zinc oxide/graphene oxide (ZnO/GO) composites were synthesized by microwave processing of precipitate in the presence of a different amount (0.1 and 0.5 wt.%) of previously prepared GO as well as reduced GO (rGO). The particles crystal structure and phase composition were investigated by X-ray diffraction and Raman spectroscopy. The particles morphology was observed with FE–SEM while the textural properties (BET surface area and pore volume) were determined by low-temperature adsorption-desorption of nitrogen. The optical properties were studied using UV–Vis DRS and PL spectroscopy. The electrochemical sensing activity of ZnO, ZnO/GO and ZnO/rGO electrodes was tested for detection of bisphenol A in water solution while electrocatalytic activity was tested for water splitting when samples were used as anode materials and evaluated by linear sweep voltammetry in several different electrolytes. Differences in electrochemical activity between the composites were correlated with presence of GO, particles morphology and textural properties.

O.S.III.C.4.

On the contribution of surface chemistry, structure and interactions in GO/WPA nanocomposites for the electrochemical charge storage applications

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Gaining a momentum from newly emerging properties of nanomaterials the further enhancement and integration of various functionalities have been made possible. Also, it became apparent that interaction between nano-objects can provide additional synergy capable of yielding new or significantly improved properties. This particularly applies to the surfaces and interfaces of nanomaterials where the intimate contact between components amplifies possible contributions of interfacial interactions. Since this aspect of interaction-property relation in many nanocomposites is still insufficiently explored, it is of interest to identify to what extent the properties emerge as a result of interaction-based synergy. To address these aspects, we have investigated a nano-composite of graphene oxide (GO) and 12-tungstophosporic acid (WPA) – a combination of materials that are known for the rich "portfolio" of properties. We will present results that contribute to better the understanding of interactions between nano-objects. The results are showing how simple temperature treatment and weight ratio of components is influencing the evolution of surface, structural properties and charge storage properties – all closely connected to interactions between components. Finally, the implications on synthetic approaches and fine-tuning of the functionality of GO/WPA nanocomposites will be discussed from the perspective of the obtained results.

O.S.III.C.5.

Features of Influence of the magnetic field on the structure and properties of epoxy composites with lead oxide

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Epoxy resins, an important class of thermosets, have been deeply rooted in almost everything both in industry and in our daily lives. They have excellent dimensional stability, thermal stability, mechanical strength, creep and chemical resistance. Functional materials with pronounced physical and chemical properties can be obtained by exposing a polymer composite to a constant magnetic field [1].

The present work aims to explore the influence of the constant magnetic field on the structure and properties of epoxy polymers with lead oxide (PbO). Samples of nanocomposites were formed from epoxy resin ED-20 and triethylenetetramine. Powder PbO was used as fillers. The content of metal oxide was 3 vol. %. The influence of constant magnetic field was $2 \cdot 10^5$ A/m. All curing processes were done at 293 – 297 K for 24 hours.

Epoxy polymer has an amorphous structure, while epoxy composites have an amorphous-crystalline structure. Composites containing PbO were characterized by the presence of 17 main reflexes in the region $2\theta = 28 - 58^o$. The average crystallite size for all samples was 6 – 18 nm. The introduction of fillers into the composition of the epoxy composite has contributed to decline the specific heat and increased the glass transition temperature for the all samples. This is explained by an increase the packing density of the macrochains of the epoxy polymer and the free volume. The relative deformation of filled epoxy composite materials have cured in a constant magnetic field has changed within 5 - 15% and the dynamic modulus of elasticity declined to 10%. An increase in the linear expansion coefficient was also observed. The more stable structure of epoxy composites was formed as a result of treatment with a constant magnetic field.

1. Y. Bardadym, E. Sporyagin, The Influence of the Physical Fields on the Structure and Physical Properties Nanocomposites, 2018 IEEE 8th International Conference Nanomaterials: Application & Properties (NAP), ISSN 978-1-5386-5334-0, Zatoka, Ukraine, 1-5 (2018).

O.S.III.C.6.

The odd-even effect in peptide SAMs – competition of secondary structure and molecule-substrate interaction

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Peptide based Self-Assembled Monolayers (SAMs) are known to be crucial for biocompatible surface on inorganic substrates applied for implants, biosensors or tissue engineering. Recently these bioinspired nanostructures are also considered interesting for molecular electronics due to their surprisingly high conductance [1] and thickness independent capacitance [2] which make them promising for organic field effect transistors (OFETs). Our analysis conducted for a series of homooligopeptides based on glycine (Gly) with cysteine (Cys) as a substrate bonding group on Au and Ag substrates ($Gly_nCys/Au(Ag)$, n = 1-9) exhibits secondary b-sheet structure formation by these monolayers with pronounced odd-even structural effect affecting packing density and conformation of molecules in the monolayer which depend on the length of molecules and the type of metal substrate [3]. Our experiments indicate that the origin of these structural effects are related to the either cooperative or competitive relation between the type of secondary structure formed by these molecules and the directional character of their chemical bonding to the metal substrate. Current analysis opens up the opportunity for rational design of these biologically-inspired nanostructures which is crucial both for mentioned biological and electronic applications.

1. Baghbanzadeh, M.; Bowers, C. M.; Rappoport, D.; Żaba, T.; Yuan, L.; Kang, K.; Liao, K. C.; Gonidec, M.; Rothemund, P.; Cyganik, P.; Aspuru-Guzik, A.; Whitesides, G. M. *J. Am. Chem. Soc.* 2017, 139, 7624−7631
2. Chen, X.; Salim, T.; Zhang, Z.; Yu, X.; Volkova, I.; Nijhuis, C. A. *ACS Appl. Mat. Interfaces* 2020, 12, 45111–45121.
3. Grabarek, A.; Walczak, Ł.; Cyganik, P. *J. Phys. Chem. B*, 2021, 125, 10964-10971

O.S.III.C.7.

Dynamic tuning of quantum light emission from GaN/InGaN nanowire quantum dots by surface acoustic waves

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Future on-chip quantum photonics requires controllable quantum emitters that can be operated on-demand and with the possibility of in situ control of the photon emission wavelength and its polarization state. Here, we report the first proof-of-principle demonstration of the dynamic real-time control, using radio frequency surface acoustic waves (SAWs), of the optical emission from quantum dots (QDs) embedded in epitaxially grown core-shell GaN/InGaN nanowire (NW) heterostructures. Luminescent QD-like exciton localization centers, induced by indium content fluctuations within the InGaN nanoshell, are identified using spatially, polarization- and time-resolved stroboscopic micro-photoluminescence (μ-PL) spectroscopy. They exhibit narrow and highly linearly polarized emission lines in the μ-PL spectra and a pronounced antibunching signature of single-photon emission in the photon correlation experiments. Depending on their location within the InGaN nanoshell, nonpolar (m-), semipolar (r-) or polar (c-facet) QDs are discerned, thereby making these NWs the first single nanostructures able to host non-classical light emitters with both high- as well as low-polarity crystallographic orientations. Owing to their shorter radiative lifetimes resulting from weak built-in electric field values along the growth axis, the III-nitride QDs grown on alternative low-polarity crystallographic planes are greatly beneficial for future high-speed quantum information technologies. When such NWs are perturbed by the propagating SAW, the embedded QDs are periodically strained and their excitonic transitions are dynamically modulated by the acousto-mechanical coupling, giving rise to a spectral fine-tuning within a ~2 meV bandwidth at the acoustic frequency of ~330 MHz. This outcome is further combined with spectral detection filtering for temporal control of the emitted photons. In this way, both spectral tunability and on-demand emission of single photons is achieved simultaneously. Moreover, the SAW-triggered acousto-electric effect inflicts changes (up to 30%) in the QD charge population and its optical polarization. This is an important advance since, to date, the photon polarization state of III-nitride QDs has been either probabilistic or pre-determined by electronic properties of the system.

O.S.III.D.1.

Properties of phthalate-free alumina tape prepared by tape casting method

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The majority of multilayer ceramic electronic components are nowadays fabricated from ceramic tapes. The latter are produced from slurries containing ceramic powder, binder, plasticiser, solvent, and other additives. The slurry is cast by tape casting, slot-die, and other less common casting technologies. A plasticiser is one of the slurry components that enables the tape's flexibility. For historical reasons and widespread use of phthalates, they were utilized also in this field. With the restriction of some phthalates from the REACH (Registration, Evaluation, Authorisation, and Restriction of Chemicals) directive, the slurries' formulations should also be changed. Some non-phthalate, environmentally accepted, non-dangerous compounds were evaluated as plasticisers in alumina tapes. The castability of the slurries, the adhesion to the carrier film, and mechanical properties, density, and homogeneity of the tapes were evaluated. The alternative solutions do not directly replace the phthalate plasticiser's formulation with a non-phthalate plasticiser. However, some of them only need a slight change in the formulation to obtain similar or even better workability, stability, and properties of the unfired ceramic tape.

O.S.III.D.2.

Electronic structure, magnetic properties and magnetocaloric effect of $GdCo_{2-x}Ni_x$

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The electronic structure, magnetic properties and magnetocaloric effect of $GdCo_{2-x}Ni_x$ with x = 0.2, 0.25 and 0.3 effect were investigated. X-ray diffraction measurements showed that that all studied samples are single phase with the cubic $MgCu_2$ - Laves type structure. In agreement with experiments, the band structure calculations explain the following issues: the antiferromagnetic ground state of the system, the coupling between Gd and the transition metals (TM) mediated by the 5d electrons of Gd hybridized with the 3d electrons of the TM (Co, Ni), the reduction of the spin magnetic moment of Co when substituting with Ni related to Co-Ni hybridization. XPS measurements showed no significant shift in the binding energy of the investigated Co core levels with the change of Ni concentration. For all investigated samples the exchange splitting estimated to about 3.2 eV between the high spin final state and the low spin final state of the Co 3s core level gives direct evidence of the local magnetic moments on Co sites. The measured increase of the saturation magnetizations when substituting cobalt by nickel confirms the ferrimagnetic-type ordering. The decrease of the Co magnetic moments is related to Co-Ni hybridization and filling of bands with extra-electrons provided by Ni with respect to Co. Moreover, the Arrott plots, the temperature dependence of Landau coefficients and the shapes of magnetic entropy changes confirm the presence of a second order magnetic phase transition. The $RCP(\Delta S)/\Delta B$ values decreases slowly when the Ni concentration increases and could be attributed to the narrowing of the $|\Delta S_m|$ peaks. The temperature-averaged entropy change values are high enough in order to consider these compounds for magnetocaloric cooling applications.

O.S.III.E.1.

A platform for reliable preclinical testing of anticancer drugs

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Development of anticancer drugs is a slow and cumbersome process owing in part to inadequacies of the traditional preclinical testing methods based on in vitro monolayer cell cultures and in vivo animal experimentation. Thus, an urgent need for physiologically relevant in vitro models has been stressed. The aim of this work was to develop a novel 3D platform for anticancer drug screening, based on alginate carriers with cancer cells followed by cultivation in a biomimetic perfusion bioreactor under physiologically relevant conditions. Alginate hydrogels in forms of microfibers and microbeads with immobilized different cancer cell lines (cervical carcinoma SiHa, embryonal carcinoma NT2/D1, rat glioma C6, human U87 and U251 glioblastoma and human lung cancer NCI-H460) were obtained by extrusion techniques, while macroporous composites based on alginate and bioactive inorganic particles (hydroxyapatite and ß-tricalcium phosphate) were prepared by a simple controlled gelation and freeze-drying method followed by manual seeding of murine K7M2-wt osteosarcoma cells onto the rehydrated scaffolds. The obtained carriers with cells were cultivated in perfusion bioreactors under continuous medium flow (superficial velocities: 15 – 100 µm s^{-1}) in short term studies up to 7 days. After cultivation under biomimetic conditions cells retained viability and exhibited higher metabolic activity as compared to cells in static cultures due to the flow providing efficient mass transport. In addition, evaluation of this platform for anticancer drug screening has shown that U87 glioblastoma cells significantly increased drug resistance-related gene expression in 3D cultures as compared to control 2D cultures. Overall, results of this study have shown high potentials of the novel 3D platform for further utilization in medicine and pharmacy.

O.S.III.E.2.

Pulsed NIR laser for photo-thermal ablation of MXene-loaded cells

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Photo-thermal therapy (PTT) is one of the most promising non-invasive methods for contact cell ablation using conversion of near-infrared (NIR) light into localized thermal energy. MXenes, a new class of 2D nanomaterials, are intensively studied as an effective PTT agent. Numerous research demonstrates beneficial effect of $T_3C_2T_x$ MXene for PTT using 808 nm continuous mode lasers with total irradiation energy up to 900 W/cm^2. Such energy densities however can lead to long-term side effects in the surrounding healthy tissues. As an alternative, 1064 nm laser with lower energy and deep tissue penetration could be utilized for PTT in a pulsed laser mode that significantly decreases the total irradiation energy. Here we report on the first application of the pulsed laser in 1064 nm (NIR-II region) for the development of the PPT protocol for cells ablation with $T_3C_2T_x$ MXene.

We demonstrated low toxicity of MXenes in effective concentrations in various cell types (CHO, MSCs and MKN28 cell lines). Moreover, we showed for the first time an effect of the direct autocatalytic reduction of resazurin by MXenes, which needs to be taken into account in cytotoxicity experiments. Importantly, $T_3C_2T_x$ MXene demonstrated significant cell ablation in low concentrations of 0.75 and 3.75 µg/ml during 60 and 80 sec irradiation of 1064 nm pulsed laser with total irradiation energy from 24.8 to 49.6 W/cm^2. The combined treatment with the MXene injection and laser irradiation in rats also demonstrated the lack of local and systemic toxicity in vivo. Overall, this study demonstrated significant advantages of the pulsed 1064 nm NIR laser over the continuous mode lasers for development of safe and effective PTT protocols.

YUCOMAT
Poster Presentations

P.S.I.A.1.

Silica-based organo-inorganic hybrid materials with carboxyl groups for water purification

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The purpose of this work was to develop organo-inorganic materials capable of combining unique properties including improved mechanical, chemical and thermal characteristics. The materials presented in this study enclose carboxyl groups derived from a variety of polymers incorporating into inorganic matrice obtained by sol-gel methods. Tetraethyl orthosilicate (TEOS) serves as a sourse for inorganic matrix, constituted by ≡Si-O-Si≡ and ≡Si-OH groupings. The organic part consists of three different polymers: 1) poly D,L,lactic-co-glycolic acid (PLGA); 2) polystyrene-acrylic polymer (Tubifast 4010®), and 3) carboxyethylsilanetriol disodium salt (CEST). The resulting hybrids in combination with the organic and inorganic parts to gives:

1) $(SiO_2)_x(\equiv SiO\text{-}(C_2H_4)_n((CH(CH_3)(CO))_y(CH(CH_3)COOH)$;
2) $(SiO_2)_x(\equiv SiO(CO)\ (CH)(CH_2)\ (CH)\ (C_6H_5)(CH_2)_n(CH)COOH)$, and
3) $(SiO_2)_x(\equiv Si(CH_2)_2COOH)$.

Table 1. Composition and structure of hybrid materials

Samples	Content, mass.%	EDX, wt.%	pI	C_{acid} / mmol g-1	S_{sp} / m^2 g$_{-1}$
	C	Si			
SiO_2/PLGA	5.1	49.7	3.5	1.29	467
SiO_2/Tubifast 4010®	9.5	41.6	2.7	1.76	484
SiO_2/CEST	6.8	46.5	2.3	6.00	27

Thus, based on Table 1, silica materials containing acidic groups on their surface may be used as high-performance sorbents for cationic pollutants. That is, SiO_2/PLGA was applied for effective selective adsorption of Fe(III) ions [1]; SiO_2/Tubifast 4010® has demonstrated the maximum sorption capacities up to 35.6 mg/g for Methylene blue [2] and 52.4 mg/g for Rhodamine 6G; the SiO_2/CEST was tested for the removal of heavy metal ions (Ni^{2+}, Mn^{2+}, Co^{2+}).

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References:

1. V. Kyshkarova et al. (2022) Hybrid composite sorbents based on SiO_2/PLGA for Fe(III) ions removal. In Applied Nanoscience, vol. 12, no.4, p. 1201-1212.
2. V. Kyshkarova, I. Melnyk (2021) Organo-inorganic hybrid composites, their structure and application for the cationic dye removal from aqueous solution. In 15th International conference on materials chemistry: Book of poster abstract "MC15'', P33, p.60.

P.S.I.A.2.

Mg/Fe layered double hydroxides-based adsorbents for removal of inorganic toxicants commonly found in aquatic environments

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Pyroaurite-type minerals ($Mg_3Fe(OH)_8[(CO_3)_{0.5}\cdot 2H_2O]$) are iron-bearing layered double hydroxides (LDHs). Mg/Fe-LDH are excellent materials in a wide range of important application such as catalysis, energy storage, electrochemistry, environmental remediation, etc. The adsorption capacity of LDHs coupled with thermal stability and developed specific surface area, makes these minerals attractive as a potential adsorbent for environmentally relevant contaminants.

The main purpose of this study is to develop new, low-cost adsorbents for wastewater treatment, combined with the desire to acquire knowledge on LDH ion-exchange properties, led to the synthesis of series of Mg/Fe-LDH-based adsorbents. The Mg/Fe-LDH samples were prepared with the different molar ratio of Mg(II) to Fe(III) (2:1; 3:1; 4:1) and the charge density. They were obtained by two different routes. First, a co-precipitation method in simple conditions at room temperature was used. In the second rout, Mg/Fe-LDH samples were synthesised under hydrothermal conditions with different thermal treatments (at 80-300 °C). In both cases the excessive use of excess chemical reagents was avoided substituting them by low cost analogies. All obtained LDHs samples were characterized using various instrumental methods (XRD, TEM, SEM, FTIR, TGA and N_2 adsorption/desorption isotherms).

Depending on the metal relationship, the samples exhibited a clear shift of the XRD basal reflections, and different carbonate species in interlayer space were identified by spectroscopic methods too. Experimental data showed that despite using different amounts of metal precursors, the formation of layered materials similar to LDHs only with Mg(II) to Fe(III) molar ratio of 2:1 a possible in hydrothermal synthesis conditions. It should be noted that the chemical stability of Mg/Fe-LDH samples obtained in hydrothermal conditions was higher than that ones prepared by co-precipitation method.

Both synthesis approaches of Mg/Fe-LDH were evaluated in adsorption studies to determine the influence of different interlayer anions (CO_3^{2-}, $EDTAH_2^{2-}$, et) on the uptake of dissolved inorganic contaminates. Mg/Fe-LDH intercalated with EDTA acid is capable of taking up heavy metal ions from aqueous solutions. The main of synthesized Mg/Fe-LDH effectively removed metal ions from aqueous medium with digestible adsorption capacity, making them potentially useful for environmental remediation.

P.S.I.A.3.

Supercritical CO_2 assisted deposition of $MAPbBr_3$ perovskite onto TiO_2 nanotubes

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Supercritical carbon dioxide (sCO_2) is an ideal low-temperature cosolvent for perovskite deposition due to its relatively low critical point (31.2 °C, 73.8 bar), no surface tension, liquid-like density, gas-like viscosity, and diffusivity. It enables faster mass transfer which allows penetration of crystals in nanoporous structure. The study investigates the influence of time of deposition of perovskite assisted with supercritical carbon dioxide on the filling of nanotubes. Perovskite solar cell technology has been developed so fast due to several factors including a tunable band gap, high absorption coefficient, and low-cost fabrication. The quality of the perovskite film is important for the high efficiency of perovskite solar cells. Perovskite precursors are usually deposited from the solution onto a substrate using spin-coating followed by post-deposition treatments, but often it results in low-quality films that cannot provide good photovoltaic performances. Deposition of perovskite in the presence of sCO_2 is a promising method for the formation of high-quality perovskite layers. In this work, methylammonium lead bromide perovskite ($MAPbBr_3$) was deposited on TiO_2 nanotubes from the solution in dimethylformamide (DMF) by application of sCO_2 at 35 °C and 200 bar for 1 h, and 3 h. FESEM results show that TiO_2 nanotubes were filled with perovskite material in both cases. The diffuse reflectance spectroscopy measurement of samples proved that the absorption edge of prepared TiO_2 nanotubes/$MAPbBr_3$ was extended to the visible range. Measurement of I-V characteristics showed that the sample made for 3 h had a higher value of current than the sample prepared for 1 h. The application of sCO_2 during the deposition of perovskite has enabled the preparation of a photodiode with a better contact between TiO_2 nanotubes and perovskite which is important for the future development of solar cells.

P.S.I.B.1.

Crystal structure prediction and investigation of mechanical properties of the SiB_6 compound through ab initio calculations

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Silicon borides are lightweight ceramics discovered at the beginning of the XX century, but the crystal structure of this enigmatic compound is yet not fully understood. Within this study of the SiB_6 compound, we have undertaken calculations using the ab initio minimization data mining approach combined with the PCAE method. Several promising structure candidates have been found and each of the newly found structure candidates was locally optimized on the DFT level, employing the LDA-PZ and the GGA-PBE functional. Two novel structures have been discovered, for which there are no previous experimental or theoretical data and are denoted as α-SiB_6-type, and as δ-SiB_6-type. Calculations performed on the experimentally known cubic γ-SiB_6 and recently proposed orthorhombic β-SiB_6 phase are in very good agreement with previous findings. For each of the predicted and experimentally observed modifications mechanical and elastic properties have been investigated. Data obtained from calculated elastic constants regarded α-SiB_6 and β-SiB_6 phases as mechanically stable ones. Moreover, according to the calculated Poison's ratio and Pugh's criterion (B/K) using both GGA and LDA methods, it can be assumed that the β-SiB_6 phase will have a brittle character, while α and γ-phase seem to be ductile. Considering their exceptional properties and very wide application, we believe that it is very important to further explore these newly discovered phases and investigate in detail their properties, in order to find new possibilities for future industrial and technological applications.

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P.S.I.B.2.

The influence of high-temperature annealing on the evolution of precipitates in Inconel 625 superalloy additively manufactured by laser powder bed fusion

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Nowadays, interest in additive manufacturing of nickel-based superalloys is increasing due to the ability to shape the components with complex geometry without additional machining. Due to its high strength, corrosion resistance in harmful environments, as well as good performance in additively manufactured form, Inconel 625 is widely used for the fabrication of parts for high-temperature applications by laser-assisted powder bed fusion, L-PBF.

To meet the requirements of long-term high-temperature operation, understanding changes in the microstructure is of key importance. Therefore, the aim of this study was to investigate the evolution of precipitates in L-PBF Inconel 625 after annealing at a temperature of 700 and 800 °C and various duration up to 1000 h.

Microstructural analysis was performed using scanning electron microscopy (SEM). The quantitative characterization of the precipitates was carried out using image processing and analysis by ImageJ/Fiji software. In samples subjected to annealing at a temperature of 700 °C for 5 hours, no significant changes in microstructure were observed. Along with the prolongation of the annealing time to 100 and 500 hours, intragranular precipitates of Ni_3Nb δ phase with plate-like morphology as well intergranular $M_{23}C_6$ carbide and Laves phase precipitates with globular morphology were developed. Similar microstructure characteristics were observed in the samples subjected to annealing at a temperature of 800 °C for 5, 100, 250, 500 and 1000 hours.

The detemined changes in the size distribution, number density and area fraction of precipitates alowed for the quatitative description of their evolution at high temperature exposure.

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P.S.I.B.3.

The kinetics of γ'' and δ phase precipitation during the high temperature annealing of Inconel 625 additively manufactured by laser powder bed fusion

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The microstructure of the Laser-Powder Bed Fused (L-PBF) Inconel 625 consists of elongated grains with the cellular-dendritic substructure, which is a consequence of high solidification rate of the melt pools. Moreover, the unique substructure is associated with the microsegregation of Nb and Mo to cell boundaries, which has influence on the kinetics of secondary phase precipitation. Thus, the aim of this work was to characterize the high temperature evolution of the microstructure of L-PBF Inconel 625. After manufacturing the samples were subjected to stress relief annealing at a temperature of 980 °C for 1 hour. Subsequently, high temperature annealing in a temperature range from 600 to 800 °C at various duration was conducted. The microstructure of the heat treated samples was investigated by using scanning (SEM), transmission (TEM) and scanning-transmission (STEM) electron microcopy.

Annealing at 600 °C was associated with precipitation of the metastable γ'' (Ni_3Nb) intermetallic phase with body-centred tetragonal structure (I4/mmm). The particles of nanometric size were observed by TEM already after 5 h and were present even after 2000 h of annealing. The γ'' precipitates start nucleate at the cell walls that are supersaturated in Nb and Mo. After longer time the γ'' was also observed inside cells. Curiously, the γ'' phase was also revealed after annealing at 700 °C for 5 h. Further extension of annealing time up to 2000 h at 700 °C resulted in the nucleation and growth of the stable δ (Ni_3Nb) phase with the orthorhombic structure (Pmmn). This phase was also revealed after annealing at 800 °C in the time range from 5 to 2000 h.

It was determined that in L-PBF Inconel 625 the nucleation of the γ'' and δ phase occurs after shorter annealing time compared to the conventionally produced. Moreover, in contrast to wrought Inconel 625 in our samples the coexistence of the γ'' and δ phase was not observed. Therefore, the kinetics of phases precipitation is strongly influenced by initial microstructure created by the manufacturing process.

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P.S.I.B.4.

Cellulose nanocrystals with different surface functionalities as outstanding scaffolds for supercapacitor materials

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Recently, as a class of green nanomaterial, cellulose nanocrystals (CNC) have received extensive attention in energy storage applications. CNCs can be readily extracted from cellulose, the most abundantly available biopolymer on earth. Combining a high aspect ratio and mechanical strength, the ability to readily assembly into 3D ordered structures from aqueous suspension, and a large amount of surface hydroxyl functional groups rendering tunable surface chemistry, make this material extremely suitable for use as a functional scaffold to construct structured electrodes that enable easier ion transport and improved cycling performance.

This work focuses on the development of conductive CNC systems as electrodes for supercapacitor applications. Polypyrrole (PPy), an intrinsically conductive polymer, was combined with CNCs to introduce the desired electrochemical properties. The effect of different CNC surface functionalities on the polymer growth and electrochemical properties was investigated. Three dimensional homogeneous composite electrodes were formed by electrochemical polymerization of the pyrrole monomer on the surface of individual CNCs. The highest areal capacitance achieved was 1.8 F/cm^2 at a current density of 1 mA/cm^2 (corresponding to a specific capacitance of 257 F/g at 0.15 A/g), with 67% capacitance retention at a high current density of 20 mA/cm^2 (3 A/g). Moreover, a symmetric supercapacitor was assembled and exhibited an energy density of 48.5 µW h/cm^2 (6.9 W h/kg) with outstanding cycling performance that can be attributed to the CNC template. The results herein obtained point out CNC-PPy composite material as a promising system for the development of sustainable energy storage devices.

P.S.I.B.5.

A hierarchically porous all-polysaccharide composite anode for an asymmetric supercapacitor

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Electrochemical capacitors are energy storage devices that store charge via capacitive or pseudo-capacitive surface mechanisms. They possess a high power density but a rather low energy density when compared to batteries. To upgrade their energy density, the focus is slowly turning towards the development of hybrid devices that use a combination of two electrodes using the two different capacitive charge storage mechanisms. The complementary electrodes could potentially increase the energy density of a device while retaining the high power density. Thus, we set out to develop an aqueous asymmetric supercapacitor working with a metal oxide, conductive polymer, and polysaccharide scaffolding tertiary composite cathode and a carbonaceous anode. To balance the charges in the electrodes, the anode needs to be thicker to compensate for its intrinsic lower energy density. However, thicker electrodes usually come at the cost of more sluggish ion movement to compensate for the potential at the electrolyte/electrode interface. Hence, the idea is to create a hierarchical structure where small pores feed on bigger cavities to reduce the insertion distance of the ions. Previous work has shown that the best-performing negative electrodes in asymmetric capacitors are based on carbon materials with a high specific surface area. However, little is known about the optimal structure and surface chemistry.

Therefore, herein we have prepared negative electrode materials by controlled pyrolysis of nanostructured networks of polysaccharides. This network is created by tuning the initial composition of multiscale polysaccharide materials: Cellulose nanocrystals (rodlike cellulose) and micro-fibrillated cellulose. Chemical activation was used to carefully control the hierarchical structure, pore dimensions, and surface chemistry. The specific surface area was measured in a very systematic way using the design of experiments to pinpoint the ideal structure. Electrochemical Analysis of the material is processed via Galvanostatic charge-discharge, Cyclic voltammetry, and impedance spectroscopy. Material physical and chemical properties are analyzed via BET, SEM, Raman, and TGA. The result showed a good retention of the specific capacitance with an increase in the thickness of the electrode.

P.S.I.B.6.

Aqueous multivalent-ion chemistry of vanadium oxides: Novelties and challenges

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Although we are aware of the importance of Li-ion batteries and the digital revolution that they brought through laptops and mobiles, limited lithium resources and safety issues have prompted research towards alternative energy storage technologies [1]. Herein, the most important results realized within the Hisuperbat project, focused on developing electrode materials for alternative energy storage devices, will be presented [2,3]. The special attention is paid to metal-pillared vanadium oxide interface in an aquoues electrolyte of multivalent salts. In that context, the key questions will be adressed: i) Will the vanadium oxide structure be capable of storing a larger amount of multivalent than lithium ions and if so, for what type of specific cation and why?; ii) How to design vanadium-oxide electrode/electrolyte interface to facilitate redox process and what will be the benefit? The results would enable us to make a step forward to a more sustainable and cheaper aqueoes rechargeable systems.

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References:

1. A. Gezović, M. J. Vujković, Miloš Milović, V. Grudić, R. Dominko, S. Mentus, *Energy Storage Materials* **37** (2021) 243.
2. Miloš Milović, Milica Vujković, Dragana Jugović, Miodrag Mitrić, *Ceramics International* **47(12)** 17077-17083.
3. Milica J. Vujković, Dušan Mladenović, Miloš Milović, Tamara Petrović, Danica Bajuk-Bogdnović, Biljana Šljukić Paunković, Slavko Mentus, *Electrochimica Acta* https://doi.org/10.1016/j.electacta.2022.140603.

P.S.I.B.7.

pH-triggered sol-gel synthesis of $Na_4Fe_3(PO_4)_2P_2O_7$ cathode material

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The combination of different structural units in the anionic sublattice (PO_4–SO_4, PO_4–NO_3, PO_4–CO_3, etc.) can provide novel mixed polyanionic structures, which matched properties of Li-ion intercalation materials [1]. Mixed polyanion, $Na_4Fe_3(PO_4)_2P_2O_7$ (NFPP) is of special interest as a cathode for Na-ion batteries [2]. In this study, the simple citric-assisted sol-gel method was used for NFPP/C preparation, with the aim of evaluating its sodium storage capability. When both phosphates and pyrophosphates are used as precursors, the mixed NFPP phase has been successfully obtained, but only if pH is adjusted to the neutral value. Otherwise, when it comes to spontaneous sol-gel reaction (without pH adjustment), the heterostructure $Na_4Fe_3(PO_4)_2P_2O_7/Na_2FeP_2O_7$ was formed. The obtained polyanions have been examined in terms of the structural, thermal and morphological behaviour by XRD, FTIR, TG/DTA and FESEM. Their electrochemical examination in $NaNO_3$, by cyclic voltammetry and chronopotentiometry, reveals the substantial difference in sodium storage properties of synthesized nanocomposites. While the heterestructure delivers the specific capacity of around 90 mAh g^{-1} with a poor rate capability, the mixed phase can rich theoretical capacity of $\approx$ 129 mAh g^{-1} (at a common scan rate), with a high rate capability of $\approx$ 80 C.

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References:

1. Nina V. Kosova, Alexander A. Shindrov, *Energy Storage Materials* **42** (2021) 570–593.
2. A. Gezović, M. J. Vujković, Miloš Milović, V. Grudić, R. Dominko, S. Mentus, *Energy Storage Materials* **37** (2021) 243.

P.S.I.B.8.

Experimental evaluation of mechanical anisotropic material behaviour of carbon reinforced PET-G material

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Carbon reinforced polyethylene terephthalate materials are proposed in additive manufacturing (AM) for the purposes of production of moderately loaded polyester based parts. Scientific papers show that mechanical properties of these materials are substantially influenced by its build orientation regarding printing angle.

In this study, Digital Image Correlation (DIC) was used as an experimental method for evaluating mechanical anisotropic material behaviour of carbon reinforced polyethylene terephthalate with added glycol (PET-G). Experimental evaluation of linear-elastic behaviour of carbon reinforced PET-G test samples with different printing orientation angles was performed. It was confirmed that different printing orientation angles (0^0, 15^0, 30^0, 45^0, 60^0, 75^0, 90^0) strongly influence final mechanical properties of this type of material. For each sample obtained by different printing orientation angle, linear-elastic material behaviour model was determined by modulus of elasticity and yield stress. Obtained results proved that carbon reinforced PET-G material exhibits significant anisotropic material behaviour.

P.S.I.B.9.

Fluidising low temperature thermochemical energy storage materials: degredation and damage assesment

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Within the field of thermal energy storage (TES), thermochemical energy storage (TCES) is has potential to contribute significantly to the ability of TCES materials to store energy for an indefinite period is an advantage over other TES materials that lose energy over time. ‘Salt in porous matrix’, i.e. composite TCES materials, have shown increased performance with respect to energy density and resistance to caking which can increase adsorption [1]. The rate at which this adsorption occurs is directly proportional to the power output of the TCES system, and thus it is clear that composite TCES materials have a highly promising future in TES as a high energy density storage medium. The objectives of this study are to first ascertain whether the use of fluidised beds, which have been shown to further increase the typically low power output of TCES systems, induce degradation of thermochemical energy storage materials. An SEM analysis (Figure 1) of composite TCES material has shown that the act of impregnaton can induce cracking in the surface of the material. General conclusions must be drawn as to the suitability of fluidised bed reactors in adsorption based composite TCES. This could potentially open the door to a new era high-power, high-energy density, long-term TES. This objective will be achieved by impregnating a Zeolite host matrix with magnesium-chloride, and performing and x-ray diffracton analysis prior to and after a typical period of fluidisation cycles, and analysing the level of material degredation and damage occured.

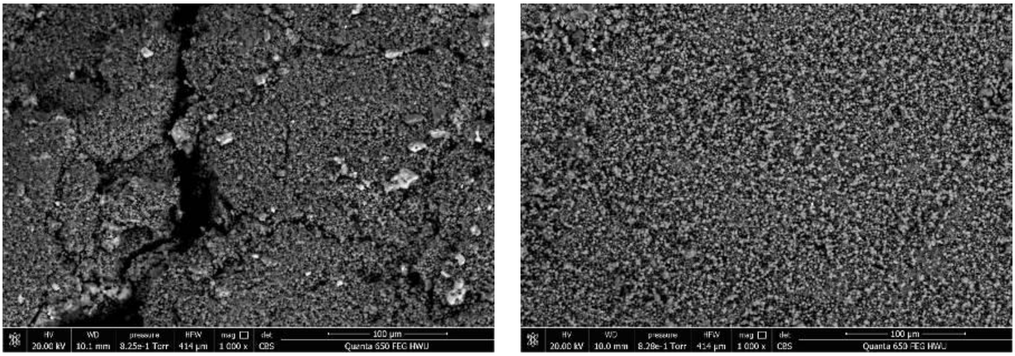

Figure 1: Left, scanning electron microscope image of zeolite after impregnation with MgCl2 salt; Right, zeolite prior to impregnation

1. L. F. Marie *et al.* Advances in Thermochemical Energy Storage and Fluidised Beds for Domestic Heat, *J. Energy Storage*, 2022.

P.S.I.C.1.

Investigation of 3D printing and thermomechanical properties of free-radical resin filled with TiO_2 nanoparticles

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Additive manufacturing provides an easy way to produce prototypes at a small scale with the possibility of complex-shaped 3D prints, which cannot be prepared by conventional subtracting methods. Specifically, stereolithography (SLA) 3D printing uses UV light to cure a photosensitive resin point by point (or layer by layer in case of masked-SLA) to produce a 3D object. The wide commercial availability of 3D printing generally requires further improvements and new technologies implemented in additive manufacturing. For example, SLA 3D prints are usually stiff and very brittle. Therefore, the desire is to make them tougher by either 3D printing using different monomers/oligomers or by mixing other particles/nanoparticles into a free-radical resin.

In our study, we prepared SLA nanocomposites by mixing titanium dioxide (TiO_2) nanoparticles (NPs) in two forms (anatase and rutile) into a free-radical resin. Radical resin prepared at our laboratories was used with varying loadings of NPs. The focus was placed on the investigation of the printing parameters of the mixtures, the comparison of SLA (point-by point) and masked-SLA (layer-by-layer) printing techniques, and the post-curing process that affects the thermal properties and mechanical performance. Jacob's working curves have shown a higher critical energy to cure a layer for resin mixtures with increasing loading of TiO_2 NPs. It has become clear that the nanoparticles in resin interact with UV curing light during 3D printing causing scattering of the UV light and lowering the light penetration depth, which reduces the overall curing degree of the exposed resin. Nanoparticle-curing light interactions have been shown to also be important for post-curing process. 3D prints from pure free-radical resin possessed a higher glass transition temperature and a greater storage modulus with increasing post-curing time. On the other hand, this effect was less pronounced for free-radical resin/TiO_2 nanocomposites.

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P.S.I.C.2.

Thiacarbocyanine dye TCC: features of J-aggregation in aqueous solutions and polymer films

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Some organic luminophores can form high-ordered molecular aggregates. They were discovered by E. Jelley and called in his honor J-aggregates. The unique features of J-aggregates provide their wide applications in various fields, such as photonics, sensorics, photovoltaics, etc.

Due to the strong intermolecular coupling between monomers, the electronic excitations of J-aggregates are the Frenkel excitons delocalized over a certain number of monomers. Depending on the molecular arrangement in the J-aggregates exciton band appear as bathochromically shifted (J-band) or hypsochromically shifted (H-band) relatively monomer band. The J-band appears at "head to tail" molecule packing as the lowest energy state of the exciton band and it accompanied by near-resonant fluorescence.

This work aimed to study the features of J-aggregate formation of thiacarbocyanine dye TCC in aqueous solutions and polymer films. To study the issue of better aggregation, studies were carried out not only on aqueous solutions, but also on electrolyte solutions, solutions with different pH levels at different concentrations of the dye. It was also studied the creation of solid samples with greater photo- and physical stability, where J-aggregates are predominantly formed.

P.S.I.C.3.

Influence of physical cross-linking by montmorillonite on structure and thermostability of hydrogel composites based on polyacrylamide

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The use of clays for physical cross-linking of hydrogel composites for various purposes is a modern trend due to several reasons - namely, it not only reduces the cost of production of such composites and avoids the use of toxic cross-linking agents but also significantly improves some properties, including mechanical strength and swelling. But the effect of clays on the thermostability of such composites has been insufficiently studied. We have examined a series of synthesized hydrogels based on acrylic monomers physically cross-linked by montmorillonite (MMT), which showed enhanced swelling properties: (i) homopolyacrylamide (PAM); (ii) PAM with acrylic acid (PAM-AA). Thermal analysis of the composites (with and without MMT) was performed using the NETZSCH STA 449 F3 Jupiter instrument. The DSC curves, which corresponded to the endothermic reaction of decomposition of xerogels based on acrylic polymers and MMT, have three distinct regions of phase transitions. According to FTIR analysis, in the temperature range of 200-300°C is thermolysis with the predominant release of NO, NO_2, NH_3, as well as H_2O and CO_2, which may be attributed to the thermal decomposition of amide and carboxylate groups of the PAM. In addition, there are two high-temperature regions observed in the range of 345-450 and 468-578°C. The presence of MMT in the gel structure slightly increases the onset temperature of the first stage for PAM and PAM-AA-based gels but reduces the onset temperature of the second and third stages compared with chemically cross-linked composites. Thus, we did not find an increase in thermal stability due to the inclusion of MMT in the gels based on PAM, but all studied hydrogels (both with and without MMT) are relatively thermoresistant, and their thermal decomposition occurs at temperatures above 200 °C, which is higher than for the initial PAM (120 °C). The reduction in thermal stability for composites with MMT is not significant and given the other benefits of using MMT, such as improved swelling.

P.S.I.C.4.

Effect of polymer molecular weight on thermal and surface structural characteristics of MWCNTs/PDMS nanocomposites

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Currently, nanotechnology is rapidly evolving and becoming part of almost every field related to materials chemistry. Well-defined materials composed of polymers (synthetic or natural), nanoparticles, and composites of the two are key components in the fabrication of state-of-the-art nanostructured materials. In particular, the introduction of multi-walled carbon nanotubes (MWCNTs) into the poly(dimethylsiloxane) (PDMS) improves the thermal, mechanical, electrical properties of the resulting composites. MWCNTs has shown large specific surface area, porosity and excellent chemical tunability. PDMS is widely used siloxane polymer due thermal stability over a large temperature range, high flexibility, chemical inertness, biocompatibility, a high degree of water-repellence as well as low cost. It is known about the PDMS–CNTs interfacial interactions, between the methyl groups of the polymer and the π-electron rich surface of the nanotubes, and the so called CH-π interactions.

This work focuses on studying the influence of polymer molecular weight (M_w) on thermal and structural properties of the nanocomposites based on MWCNTs (synthesized by the method of catalytic pyrolysis, CCVD), and linear PDMS with two M_w (PDMS-100 and PDMS-12500, $M_w \approx$ 3410 and 39500 g/mol, respectively). The polymer fluids were physically adsorbed onto nanotubes surfaces in amounts of 5, 10, 20 and 40 wt. %. Thermogravimetric and differential thermal analyses (DTA-TG) were performed in the air to elucidate the thermal stability with increasing weight % addition of PDMS to the pristine MWCNTs (P-MWCNTs). The influence of polymer content and M_w revealed in a shift of characteristic DTG peaks. The mechanism of thermal destruction of the polymer onto the surface of MWCNTs has been evaluated like the degree of conversion of PDMS into SiO_2 and cyclic dimethylsiloxanes. The XRD analysis confirms good graphitization of samples and well-dispersed MWCNTs in the polymer. The surface morphology of P-MWCNTs and fabricated MWCNTs/PDMS nanocomposites was examined employing the TEM and SEM with EDAX methods.

P.S.I.D.1.

Waterborne polyurethanes based on poly(dimethylsiloxane)

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A series of novel waterborne polyurethanes (WBPUs) was synthesized using α,ω-dihydroxypropyl poly(dimethylsiloxane) (PDMS), isophorone diisocyanate (IPDI), 2,2-bis-(hydroxymethyl) propionic acid (DMPA) and triethylamine (TEA). Different DMPA/PDMS and constant –NCO/–OH molar ratio have been applied for the synthesis of six different WBPUs, without the usage of chain extension step. The structure-properties relationship was examined with diverse experimental analyses. ATR-FTIR, ^{1}H and ^{13}C NMR analyses confirmed the incorporation of PDMS parts inside polyurethane backbone and the successful preparation of WBPUs. XRD analysis showed that all WBPUs are amorphous, without any kind of three-dimensional order. According to the conducted TG measurements, the incorporation of PDMS increases thermal stability of WBPUs. DMA results confirmed the existence of microphase separation, which was more pronounced in WBPUs with higher PDMS content. Contact angle measurements with water confirmed good surface hydrophobicity of these WBPUs, which originates from the high percentages of Si atoms present on the surface of WBPU films. Good hydrophobicity originates from PDMS which has known to possess low surface energy and have a high tendency to migrate on the surface of the WBPUs. The synthesis of these WBPUs represents a more efficient and eco-friendly way for preparation of polyurethanes and they are good candidates for application as coatings (1).

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References

1. I.S. Stefanović, J.V. Džunuzović, E.S. Džunuzović, S.J. Brzić, E. Jasiukaitytė-Grojzdek, A. Basagni, C. Marega, Tailoring the properties of waterborne polyurethanes by incorporating different content of poly(dimethylsiloxane), Prog. Org. Coat., 161, 106474 (2021).

P.S.I.D.2.

Structural characterization of geopolymers with the addition of egg shell

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It is well known that alkali-activated materials (AAM) are a newer group of binders that are obtained by alkaline activation of various silicate and aluminosilicate materials and, differ from each other in terms of chemical composition and structure of the binding phase. These materials are usually divided into two subgroups, based on the calcium content in the binding phase. Materials belonging to the AAM subgroup, which is characterized by low calcium content (x) in the binding phase, are called geopolymers.

Geopolymers are formed by the reaction of aluminosilicate materials such as metakaolin and electrofilter ash of thermal power plants (EFP) with alkaline activator solutions. Geopolymer materials based on fly ash are attracting attention in the global research community because of their properties that affect their performance such durability, mechanical properties, physical-chemical properties and reduction of carbon dioxide (CO_2). The present study relates to an economical and ecofriendly method, capable of being implemented in two simples steps. The first step is preparation of solid precursors based on fly ash (Obrenovac, Serbia) rich in silicon (SiO2) and egg shells as waste materials, rich in calcium (Ca). The second step is alkali activation of different mix of fly ash and egg shells and treatment in appropriate laboratory conditions (temperature, relative hummidity, aging). The chemical and physical properties of the prepared geopolymer materials were analyzed by several technics such as DRIFT (*Diffuse Reflectance Infrared Fourier Transform*), XRD (*X-Ray Diffraction*) and SEM (*Scanning electron microscope*). The composition of the sample was determined with XRD, and the results of XRD were confirmed with DRIFT. The morphology of the material was determined with SEM.

P.S.I.D.3.

Sequential extractions and leaching tests as methods for characterization of mine tailings for the purpose of their probable application in eco-friendly geopolymers

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Synthesis of new eco-friendly materials such as geopolymers generally includes utilization of TPP and mine tailings. The environmental assessment of new materials and raw material is performed mainly by leaching tests and sequential fractionalization of heavy metals (metalloids). In the present work samples from Bulgarian tailing dumps were estimated by an algorithm based on sequential extraction approach and study of leaching behavior in different media.
Two methods of sequential extractions were applied to mine tailings. A five- step extraction procedure was applied after modification. On the first stage the exchangeable fraction which contains the most mobile metals was studied. On the second, third and fourth stages Mn, amorphous and crystalline Fe oxides were in the focus due to the fact that they may experience some alterations and can be transformed into mobile phases under certain conditions. And the final fraction meant to determine the residual fraction of metals. The only step which was skipped from the original extracting procedure was the determination of metals bound to organic matter. The obtained results were compared to standard method - Community Bureau of Reference (BCR) three-step sequential extraction for soils and sediments, as follows: (1) exchangeable and bound to carbonates heavy metals; (2) bound to iron and manganese oxides fraction and (3) fraction bound to organic matter. This procedure brings information about the toxicity released under approximately the same conditions as the actual disposal site from leaching tests. In addition to the estimation of leaching characteristics of geopolymer precursors, the developed algorithm for estimation of environmental toxicity provides a powerful tool to study mobilization and encapsulation of heavy metals and metalloids in the structure of newly synthesized materials.

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P.S.I.D.4.

Obtaining and characterising Cu-infused antimicrobial films formed from regenerated cellulose-$CaCO_3$ composite

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Cellulose and cellulose-$CaCO_3$ dopes were prepared by ultrasound dispersion of $CaCO_3$ (0, 0.26, or 0.65 w/w%) and dissolution of cellulose (13 w/w%) in ionic liquid 1-ethyl-3-methylimidazolium acetate at 90 °C. Thereafter, the films were obtained by rode casting over a pre-heated glass plate, together with methanol used as a regeneration agent. Subsequently, the films were washed in hot water (80 °C) to remove the residual ionic liquid solvent - a process that can be extended to recover ionic liquid for re-use. To impart antimicrobial properties to the cellulose-$CaCO_3$ composite films, selected samples of the wet films were treated with 10 mM $CuSO_4$ solution for different times (30, 60, and 120 min). Furthermore, half of these $CuSO_4$ treated films were subsequently treated with ascorbic acid to synthesise in situ Cu-based nanoparticles on the film surface. After drying whilst held under tension at room temperature, the films were characterised in respect to their mechanical properties as well as antimicrobial activity. The results revealed that, in the case of films treated for 30 min with $CuSO_4$ solution, the incorporation of 0.26 w/w% $CaCO_3$ correlated with an increase in the film hardness, while in the case where the treatment with $CuSO_4$ solution was performed for longer (60 min) this hardness trend was reversed. The elastic modulus decreased with increasing content of $CaCO_3$. Only the films treated with $CuSO_4$, and those with Cu-based nanoparticles, possessed excellent antimicrobial activity against the bacteria E. coli, S. aureus, and the fungus C. albicans. However, the results in the case of C. albicans, showed an additional dependence, in that films treated with $CuSO_4$ solution for 60 min demonstrated increasing antimicrobial activity against the fungus specifically with increasing $CaCO_3$ content.

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P.S.I.D.5.

Comparative study of biomass-derived carbon interfacial processes in aluminum-based and conventional acidic electrolyte

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Lately human attention has been focused on the use of clean and renewable energy sources, since there is a major concern about the detrimental impact of traditional fossil fuels. In that regard, electrochemical energy storage and conversion devices have become a central point for further research. Carbon materials found a special place in these energy-related applications.

In this paper, activated carbon (AC_{vs}) was obtained by the carbonization of vine shoots with $ZnCl_2$ as activator. The results of N_2 physisorption revealed its high S_{BET} area of 1494 $m^2\ g^{-1}$ and wide pore size distribution profile. FTIR spectroscopy and TG/DTA analysis have confirmed the high level of purity of prepared AC_{vs} (completely ash-free). To broaden operating voltage of carbon in the aqueous medium, a non-conventional Al-ion based electrolyte was used. In such conditions, prepared AC_{vs} exhibits typical pseudocapacitance behavior of carbon over potential range of 1.8 V, high capacitance of 190 $F\ g^{-1}$ at 5 $mV\ s^{-1}$ (in three-electrode arrangement), 216 $F\ g^{-1}$ and energy density of 24 $Wh\ kg^{-1}$ at 1 $A\ g^{-1}$ (in symmetric supercapacitor configuration). Trasatti & Dunn surface charge distribution models were applied to investigate the nature of Al-ion charge storage of AC_{vs} and to compare it to the acidic one. Density Functional Theory helped further investigate the nature of the interaction between pristine/defective graphene and hydrated Al^{3+} ions.

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References:

1. A. Gezović, J. Mišurović, B. Milovanović, M. Etinski, J. Krstić, V. Grudić, R. Dominko, S. Mentus, M. J. Vujković, High Al-ion storage of vine shoots-derived activated carbon: New concept for affordable and sustainable supercapacitors, *Journal of Power Sources*, **538** (2022) 231561.

P.S.I.E.1.

Laser-induced chemical and mophological changes of the titanium alloy surface under different irradiation parameters

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Titanium alloys are finding increasing use as biomaterials due to their low elastic modulus and high damage tolerance. However, the somewhat inadequate alloy surface performance can impede their biomedical application. Surface modification methods have been therefore developed to improve the alloys' surface bioactivity and osseointegration. Laser treatment allows the alloy surface to be modified, providing it with new functionalized surface chemistry and morphology, without compromising the rest of the material properties. Thus, the aim of the study was to examine the laser-induced alterations generated on the Ti-45Nb alloy surface by an ultrashort pulsed laser. The obtained results reveal that laser beam interaction with the target material led to the formation of significant alterations in surface morphology. Surface craters, microcracks, and surface features in the form of periodic and rippled structures and solidified droplets can be observed in the irradiated area. Also, it was found that the higher damage degree along with the material depth and the higher surface roughness were achieved during the irradiation in the argon atmosphere due to the formation of the more pronounced morphological changes on the alloy surface that are induced by higher laser ablation. Furthermore, obtained results showed that alloy surface modification in air, argon, and nitrogen atmosphere additionally caused changes in the surface chemical composition. Namely, after irradiation, the presence of oxygen was observed in the central irradiated area indicating the formation of bioactive Ti-oxide surface film with content that varies with the irradiation parameters variation. Therefore, laser beam irradiation can be singled out as the surface modification method for efficient inducement of the specific surface characteristics that can provide titanium alloys with enhanced osseointegration properties.

P.S.I.E.2.

Search for "needles" of hydroxyapatite in the "haystack" of ovarian cancer

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Ovarian cancer is one of the leading causes of death among women. Diagnosis in the early stages will reduce mortality and save the lives of many women. Calcification is one of the clinical and morphological features of ovarian cancer. The process of calcification is most common for serous ovarian carcinoma. Histologically the incidence of calcifications in low-grade serous carcinomas is 100%. Nevertheless, their diagnostic and prognostic values are not yet fully understood, despite the relatively high detection rate.

Our work aimed to study the nanocrystalline structure of calcifications of ovarian cancer for use in diagnostics.

We examined 30 samples of ovarian cancer with calcification. Histological study was performed to verify the material and form groups. Scanning electron microscopy (SEM) with energy dispersive X-ray (EDX) microanalysis of the tissue sections from the paraffin blocks of ovarian tumors was performed on SEO-SEM Inspect S50-B (SEO, Sumy, Ukraine) scanning electron microscope with an AZtecOne energy dispersion spectrometer with an X-MaxN20 detector (Oxford Instruments plc, Abingdon, UK). EDX spectra were analyzed with standard software of the microanalysis system. Transmission electron microscopy (TEM) with electron diffraction (ED) was performed on PEM-125K microscope (SELMI, Sumy, Ukraine).

We revealed that calcifications of ovarian cancer are represented by calcium apatite. It was found no signs of other crystalline phases.

The application of TEM with ED is perspective in terms of the effectiveness of high-resolution methods for cancer diagnostics by detection of calcifications. TEM detected that pathological crystalline nanoparticles are polydisperse and their size ranges from 5 to 50 nm.

Consequently, hydroxyapatite is the main mineral that is formed during the calcification of ovarian neoplasms. In a perspective, it could be used for early diagnostics of ovarian cancer.

P.S.I.E.3.

The role of oxalate nanocrystalline for the differential diagnostics of the breast pathology

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Breast microcalcifications mainly consist of calcium oxalate or calcium phosphate with an apatite structure. It was believed that the presence of calcium oxalate is associated with benign breast tumors, whereas the detection of calcium phosphates points out the possible breast malignancy.

This study aims to establish the morphology of oxalate deposits of the breast cancer (BC).

In our study, we have analyzed 30 samples of breast carcer by histology (hematoxylin-eosin staining), scanning electron microscopy (SEM) with EDS and TEM.

We detected amber-colored biomineral deposits in the adjacent intact tissue of tumor samples. They were more transparent and had a complex polygonal structure. The structure of microcalcifications was similar to "bread crumbs" or lumps with small elements. These structures were located in the lumen of the dilated glands or were associated with their lumen (located near the glands). It is important to note that the glands that contained oxalate microcalcifications had a normal histological structure.

We found reddish von Koss staining of the biomineral deposit. This may be due to the deposition of a counterstaining dye (nuclear fast red) on biomineral structures. These intraluminal calcified structures had a propper alizarin red staining.

The SEM showed that mineral deposits had the structure of irregularly shaped particles (30-40 μm) with granulation and growths, not consolidated with the surrounding/adjacent non-neoplastic breast tissue.

However, no oxalate calcifications were found in the tumor tissue. The presence of microcalcifications of oxalate origin in the BC tissue can be explained by the development of malignant tumors on the background of pre-existing benign pathology, which is inherited by calcium oxalate microcalcifications. The simultaneous presence of hydroxyapatite and oxalate biominerals in the tissue of invasive BC complicates the use of crystal-phase difference of pathological biominerals for non-invasive radiological diagnosis.

P.S.I.E.4.

Optimisation of a 3D in vitro model for osteosarcoma cell cultivation

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Osteosarcoma is the most common type of primary bone cancers affecting mostly children and young adults. Evident slow progress in osteosarcoma treatment indicates inadequacy of predominantly used 2D *in vitro* and animal *in vivo* models for antitumor drug testing. These models also failed to bridge the gaps in the knowledge about osteosarcoma in general. Therefore, our aim is to establish a 3D *in vitro* model for osteosarcoma cultivation that has the potential to overcome the inherent weaknesses of the traditional models by imitating the native osteosarcoma cell microenvironment. The model is based on scaffolds, as cell carriers, cultivated under continuous medium flow provided by a perfusion bioreactor system. Two groups of macroporous composite alginate hydrogel scaffolds with incorporated commercial hydroxyapatite (HAp) particles (2% alginate, 2% HAp) were produced using calcium and barium ions as gelation agents in each group separately. Murine osteosarcoma cells (K7M2-wt) are used in this study. In the first step, cell seeding onto scaffolds was optimized and the efficiency achieved was >80%. Also, histological analysis of scaffold cross-sections confirmed cell distribution within the scaffold pores. In the next step, the cell-seeded scaffolds were cultivated in short-term cultures up to 7 days under continuous medium flow (superficial velocity 40 µm/s) in perfusion bioreactors (3D Perfuse, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia), while static 3D cultures served as controls. The results revealed beneficial effects of the perfusion on the cells. Cells subjected to the perfusion conditions exhibited increased metabolic activity and proliferation rate in comparison to the static controls, which was attributed to the more efficient convective mass transport in contrast to diffusion only in the latter system. These studies indicate potentials of the biomimetic 3D model for osteosarcoma cell culture and further use to engineer this aggressive tumor in vitro.

P.S.I.E.5.

Development of a 3D in vitro model based on alginate microfibers with immobilized cancer cells for cancer research and anticancer drug testing

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Anticancer drug development is a very slow and complicated process mainly due to the lack of adequate cancer model systems that can mimic the complex structure of cancers in vivo. Tumor engineering tries to address this problem by adopting some of the tissue engineering strategies such as application of biomaterials as cell carriers imitating the extracellular matrix and providing cells with a three-dimensional (3D) structural support. In this work we have applied alginate hydrogel in the form of microfibers and investigated immobilization of three different cancer cell lines: rat glioma C6, human non-small cell lung carcinoma NCI-H460, and murine osteosarcoma K7M2-wt. Cell immobilization was achieved by simple manual extrusion of cell suspension in Na-alginate solution (2-8×10^6 cells/ml, 2.8% Na-alginate) into the gelling bath containing 0.18 M Ca^{2+} through a blunt edge stainless steel needle (22-25 G). It was shown that the immobilization process had to be optimized for each cancer cell line in terms of initial cell concentration, needle size and time of gelation. The obtained alginate microfibers with uniformly distributed viable cells were further cultivated under static conditions and cell viability over different cultivation periods was determined by MTT assay. In order to evaluate this biomimetic 3D system as a model for anticancer drug testing, oncology drugs cisplatin and doxorubicin have been used and the response to the treatment of cells in alginate microfibers was compared with the response of cells in 2D cultures. The results showed altered sensitivity of the cells to the treatments in 3D cultures compared to 2D cultures, thus confirming potentials of the described system for anticancer drug research and development.

P.S.I.E.6.

PCL-MXene composite electrospun membrane for nerve regeneration: structural and biological assessment

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Despite promising results reported in the literature, all materials for conductive scaffolds have some drawbacks that limit their translation to clinical practice. The new family of 2D nanomaterials – MXenes, demonstrate promise to biomedical application, including conductive materials for nerve, cardiac and muscular tissues regeneration. Electrospinning is a unique technology for development of porous high biocompatible materials that could be modified with various nanomaterials. The purpose of current research was a development of composite Polycaprolactone (PCL)-MXene electrospun membranes for conductive tissue regeneration.

PCL membranes was made using conventional electrospinning technology with following loading with Ti_3C_2 MXenes in different concentrations. Scanning electron microscopy (SEM) with EDS, Transmission electron microscopy (TEM) and Raman were used to evaluate structural and chemical composition of PCL-Mxene composite membranes. Biocompatibility and cell proliferation assays applied to assess biological response.

We demonstrate the formation of high porous electrospun membranes with fiber diameter ranges from 20 to 200 nm. After MXene immobilization we detected links between PCL fibred and nanolaminates that increase the surface ration and affect wettability. Cell culture experiment (using primary human fibroblast cells) show significant higher cell attachment compare to as-spun membrane due to increasing of hydrophilic properties. We also demonstrate adequate cell proliferation from day 1 to day 7. Based on preliminary structural, chemical and biological study, PCL-MXene electrospun composite materials should be used for development of the substitutes for conductive tissues.

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P.S.I.E.7.

3D Printed calcium phosphate cement scaffolds loaded with liposomal antibacterial enzymes for the prevention of osteomyelitis

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To treat large-scale bone defects, three-dimensional (3D) printing has been in focus in recent years due to the possibility of fabricating patient-specific bioactive and porous scaffolds[1]. When the 3D printed implant begins to resorb, the osteointegration process is often accompanied by several microorganisms that cause a bone infection known as osteomyelitis[2]. By combining the ceramic phosphate powder, thermosensitive copolymer, and **enzymes**, we obtain the bio-ink suitable for 3D printing of bone implants with controllable degradation rate, mechanical properties, pore size, and antibacterial activity. Therefore, as the calcium phosphate cement (CPC) implant resorbs, it suppresses the growth of undesirable microorganisms.

Our previous study discovered that antibacterial enzymes incorporated into the bio-ink do not release from the implants in more significant amounts than expected. This probably results from the CPC structure as the enzymes are “locked” within the CPC structure. In this project, the antibacterial enzyme Lysozyme is encapsulated into liposomes with diameters around 100 nm, providing additional chemical and physical protection to the enzyme during the implant preparation and curing. Liposomes prepared by an optimized “heating method” exhibit a low polydispersity index and diameters around 97.8±4.8 nm and zeta potential of -15.2±3.2 mV (n=3). The encapsulation efficiency of Lysozyme in these formulas is around 64 %. It was determined that Lysozyme is released from such liposomes in a first-order release mechanism. The release of the liposome-Lysozyme system from the CPC scaffolds is currently being evaluated.

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1. Bisht, B. et al., **2021**. Advances in the Fabrication of Scaffold and 3D Printing of Biomimetic Bone Graft. *Annals of Biomedical Engineering.* 49(4): 1128-50.
2. GOGIA, J. et al., 2009. Local Antibiotic Therapy in Osteomyelitis. *Seminars in Plastic Surgery.* 20(02), 100-107.

P.S.I.E.8.

Hydrogel dressings for phage therapy of chronic wounds

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Chronic wounds affect about 1-2% of the developed countries population, thereby becoming a worldwide financial threat to the healthcare system, significantly affecting the patients' lifestyle. Chronic wounds tend to have a slow healing process; they can be easily infected with a biofilm-forming multidrug-resistant bacteria. To overcome such a burden, bacteriophages (phages) therapy can combat resistant bacterial infections as an alternative to conventional antibiotics, infecting a specific bacterial strain and leading to their destruction without affecting eucaryotic cells. For effective topical phage application, hydrogels can be used to ensure phage delivery, stability, and controlled release in the wound site. This work describes hydrogel preparation and modification with phages via a freeze-drying technique of polymer blend composed of natural polysaccharide gum Karaya (GK) with synthetic polymers acting as surfactants. Physicochemical characterization shows that the ratio between GK/PVA strongly influences visual appearance, water swelling (60- 70% of original weight), retention, and degradation (stable after 28 days, weight loss of 55%). Then the polyvalent phage JK2(=812K1/420) was coated on the surface of the hydrogel. This phage was used as it interacts specifically with Staphylococcus aureus family stains that are frequently present in chronic wounds. The release from hydrogel coated with phages was tested by double agar method with over 90% of released phages, and the antimicrobial activity against Staphylococcus aureus ATCC 43300 (CCM 4750) proved to be effective in 12 hours. Gum Karaya-based hydrogel coated with phages shows the potential to become a suitable carrier for the phage therapy of chronic wounds based on antibacterial tests against strains of Staphylococcus aureus. This work was supported by the Ministry of Health of the Czech Republic under project no NU20-05-00166. All rights reserved.

P.S.I.E.9.

Biomechanical DMA characterization of calcium and barium alginate hydrogel scaffolds

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Objectives: Design of bone tissue engineering scaffolds imposes a number of requirements for their physical properties, in particular porosity and mechanical behavior. Alginates are known as a potential material for such purposes, usually deploying calcium as a cross-linker. Calcium over-expression was reported having proinflammatory effect, which is not always desirable. Contrary to this, barium has better immunomodulatory outcome but data for barium as a cross-linker are scarce. In this work the objective was to study if DMA is a suitable method to measure Ba- and Ca-linked alginates and to compare their viscoelastic properties in vitro.

Methods: Sodium alginate aqueous solution (1 wt%) with 0.03 wt.% CaCl2 was gelled in dialysis tubing immersed in 27 mM CaCl2 (controls) or BaCl2, for 48 h, followed by freeze-drying and rehydration (with 0.3 wt.% CaCl2 and 0.8 wt.% NaCl). Hydrogel discs (diameter 8-10 mm, thickness 4-6 mm) were assessed in dry and wet (DMEM immersed) states by dynamic mechanical analysis (DMA) under compressive creep conditions with increased loads, frequency scans and strain-controlled sweeps in physiological range (0.1-20 Hz) at 25°C and 37°C. Resulting data were analyzed by conventional methods and by a model-free BEST (Biomaterials Enhanced Simulation Testing) to extract invariant values and material functions.

Results: DMA was able to detect significant differences in properties between Ba-linked hydrogel scaffolds vs. Ca-linked controls. Specifically, for the similar porosity Ba-samples exhibited lower creep compliance, substantially higher dynamical stiffness, and lower loss factor in the whole studied range. Invariant modulus exhibited a non-linear decay vs. applied stress. These differences were observed in both dry and wet states and temperatures.

Conclusions: Use of DMA is a suitable method for studying barium as a cross-linker for alginate scaffolds. This allows further modification of biomechanical properties of the scaffolds for better compliancy to the application. Barium release might have an immunomodulating effect but also promote ion exchange for osteogenesis due to additional Ca/Ba concentration gradient.

P.S.I.E.10.

Hydroxyl radical scavenging activity of titanium oxide nanocrystals

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Titanium oxide nanocrystals (TiO_{2-x}) are well-known material due to its excellent photocatalytic properties. During the last years, some researchers have accidentally reported on the strong antioxidant activity of titanium oxide nanoparticles. However, the general role of titanium oxide surface defect structure in its redox activity is still a subject of discussions. In this report, we consider the role of the defect structure on redox properties of TiO_{2-x}.

Changing the amount of nitric acid as a catalyst and peptizing agent, we obtained two different types of titanium oxide nanocrystals with the same size, but different Ti^{3+}/Ti^{4+} ratio in the crystal lattice (which were confirmed by XPS measurements), and so, different reactive oxygen species scavenging properties. Both types of titanium oxide nanocrystals are characterized by quite good biocompatibility against red blood cells even at high concentration.

Electron donating properties and reactive oxygen species scavenging action of both types of titanium oxide nanocrystals against hydroxyl radicals (·OH) have been studied. Hydroxyl radicals are formed at water radiolysis during X-ray irradiation of the cell. Extremely high reactivity of ·OH radicals (average ·OH lifetime in the biological environment of only few nanoseconds) makes the task of its effective elimination by the internal systems of the living cell rather difficult. Hydroxyl radicals scavenging properties of obtained titanium oxide nanocrystals have been revealed to be directly related to Ti^{3+}/Ti^{4+} ratio being higher for the samples with higher Ti^{3+} content.

The efficiency of reactive oxygen species scavenging by titanium oxide nanocrystals in water solutions is close to that of nanoceria (CeO_{2-x} nanocrystals) of the same size suggesting that titanium oxide nanoparticles can be effective as an antioxidant in living cells as well. Moreover high biocompatibility of synthesized nanocrystals could be associated with their reactive oxygen species scavenging ability, which make them a prospective material for biomedical applications.

P.S.I.E.11

Magnesium alloy with yttrium, gadolinium and calcium alloying elements designed for aviation applications

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Magnesium alloys with low density and high specific strength are suitable candidates for the use in weight-saving industries, such as the aerospace industry. The use of magnesium alloys in the aerospace industry is limited because of their low flammability resistance. Flammability resistance of magnesium alloys can be affected by alloying elements. It has been proven that rare earth metals and calcium increase resistance to ignition.

Magnesium alloy containing yttrium, gadolinium and calcium was designed for use in the aerospace industry. In order to obtain a fine-grained microstructure, alloy was processed by extrusion and also eight passes of Equal Channel Angular Pressing (ECAP). The microstructure after extrusion was bimodal. The grain size and the degree of recrystallization depended on the parameters of extrusion. ECAP processing led to homogenous microstructure with mean grain size less than 1 μm, which meets the parameters of ultrafine-grained alloys. The mechanical properties corresponded to the observed microstructure. The alloy is also characterized by a high ignition temperature and is therefore promising for use in the aerospace industry.

The microstructure was observed using transmission and scanning electron microscopy, including electron backscatter diffraction (EBSD). Mechanical properties were studied using tensile/compressive deformation tests and microhardness measurements.

P.S.I.E.12

Resonance ultrasound spectroscopy measurements of elastic modulus of biomedical Ti-based alloys prepared by SPS

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Various Ti-Nb-Zr-O based biomedical alloys were prepared from elemental powders and titanium dioxide by spark plasma sintering (SPS). Four layered samples covering together 24 chemical compositions were prepared. Elastic constants for each layer (the shear modulus G and the Young's modulus E) were determined using resonant ultrasound spectroscopy. The ultrasonic measurements were complemented by detailed SEM and XRD analysis. The results show that in the considered compositional space, elastic constants exhibit a dependence on the volume fraction of beta stabilizing Nb and interstitial oxygen. Minimum elastic modulus was achieved for the compositions close to the stability limit between parent beta matrix and alpha double-prime martensitic phase.

P.S.II.A.1.

Synthesis and characterization of glass-ceramic-metal composite materials obtained by sintering

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The industry's progress is closely connected with the development of new materials. Complex industrial systems, such as thermal power plants, pose a significant challenge in terms of maintenance as well as achieving high performance of machine elements and structures that operate under conditions of different damage mechanisms. For that reason, new materials are constantly being developed, which, in addition to good physical and mechanical properties, today must also meet ecological criteria, and economic viability. The aim of this paper is the synthesis of new glass-ceramic-metal composite materials and their characterization.

Andesite basalt rock from the deposit site "Donje Jarinje", Serbia, was used as a starting material for obtaining a glass-ceramic matrix of composite materials. The rock was milled in a tungsten-carbide vibrating cup mill to obtain the fine powder suitable for synthesis. Commercial austenitic stainless steel 316L, spherical shape, was used as reinforcement in composite materials. The diameter of 316L powder is in the range from 45 to 90 μm.

The composite materials were manufactured by mechanical mixing andesite basalt powder with 316L powder in the contents of 10, 20, and 30 wt.%. Paraffin wax was used as a binder in the content of 0.6 wt.%. After homogenization of the powders and binder, the green compacts were obtained by single-side pressing about 50 MPa, a then cold isostatic pressing about 230 MPa to increase the density of the green compacts. Sintering was performed at 1060 °C for 60 min in the air.

The starting powders, and the sintered composite materials were characterized by the X-ray diffraction method (XRD). Morphology of the powders and microstructure of the sintered samples were observed by a scanning electron microscope (SEM) and a light optical microscope (LOM). After the characterization, the obtained glass-ceramic-metal composite materials were confirmed.

P.S.II.A.2.

Positronics science in the contemporary nanocomposites engineering: towards guided functionality of PVP-nanosized glassy arsenoselenides

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Mechanochemistry-guided nanostructurization effects are studied in glassy arsenoselenides g-As-Se subjected to nanomilling in polyvinylpyrrolidone (PVP) water solution employing Positronics, an advanced characterization tool tracing free-volume entities in solids based on positron annihilation lifetime (PAL) spectroscopy. Nanomilling is shown to be ineffective in under-stoichiometric g-As-Se possessing network structures, while causes reamorphization in over-stoichiometric glass due to molecular-to-network transition. Compositional changes in the PAL spectra reconstructed under unconstrained three-component fitting are revealed in under-stoichiometric g-As-Se/PVP nanocomposites, showing depressing trend in positionally-invariant PAL spectrum peaks supplemented by widely expanded tails composed of accumulated long-lived annihilation events, while these changes are suppressed in over-stoichiometric composites. Preliminary analysis within two-state simple trapping model, testifies that positron trapping occurs in intrinsic voids of g-As-Se enlarged to the character volumes of multiatomic vacancies, while bound positron-electron (positronium, Ps) states decay merely in the PVP environment. Formalism of x3-x2-CDA (coupling decomposition algorithm) describing conversion of Ps-related states into positron traps (and vise-versa) is applied to identify volumetric changes in non-stoichiometric nanocomposites in respect to stoichiometric. The governing process in under-stoichiometric nanocomposites is recognized as unified positron-to-Ps trapping conversion, disappearing positron traps being PVP-nanosized vacancies character for g-As-Se. But there is no alone modification process governing such effects in over-stoichiometric nanocomposites, possessing molecular-network structure with principally different trapping sites.

P.S.II.A.3.

Novel technology for production of nanopowders by electroerosion dispersion method

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An energy efficient process is proposed for the synthesis of magnetic nanopowders (5 - 500 nm) of iron or aluminium oxides. For this purpose the method of electroerosion dispersion of iron low-alloyed steel or aluminum granules or chips with metal evaporation in plasma and further condensation in water was developed. The EED method allows the generation of temperature gradients up to ± 10^6 K/mm, as a result, micrograins form in distinctly no-equilibrium conditions. The metal vapour in 10^{-6} s solidify in the cold zone. The formation conditions of such particles result in many unique properties of the powder, such as deformation of crystalline lattices and high specific surface of the grains. The technological equipment for implementation of this approach was also designed and manufactured. The installation incorporate disintegration reactors and pulse generators, allowing varying discharge frequency and voltage in broad ranges: 100-500 Hz and 100-500 V, respectively. Varying these parameters it is possible to control the powders quality: composition, size of grains (from nanometers till microns), their shape with highly developed surfaces, phase state (amorphous or crystalline).

Phase analysis of the iron oxide powder were carried out with the Siemens/Bruker D-5000 XRD system revealed that the main phase is magnetite Fe_3O_4. The material demonstrated magnetic properties: the saturation magnetization of 301.0 kA/m. The powder is agglomerated and particles about 7-10 nm can be observed. The powder of aluminium oxide was analyzed by Quantrachrome ASiQwin Gas Sorbtion Instruments: surface area of 140 m^2/g, pore volume of 0.1650 cc/g, pore size of 2.50 nm.

The nanopowders produced are efficient sorbents for wastewater contaminants, in particular for ions of heavy metals and can be used for industrial wastewater treatment. The advantages of the treatments by the nanosorbents include their large activity, high degree of removal for heavy metals from liquids (up to 98,5 %), while the resulting sediments may be reliably utilised. The application of the sediments can be accomplished in metallurgy (by melting). In the iron oxide case the sediments may be used for production of ferromagnetic materials and pigments.

The method is environmentally friendly, generates no water and air pollution, has low expenses of energy.

P.S.II.A.4.

New directions of arylamines oxidation with H_2O_2: polymerization of aniline in the presence of para-aminodiphenylamine

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Conductive polymers are a special group of organic synthetic polymers that have attracted significant interest over the past few decades because they synergize the advantageous features of conventional polymeric materials and metals. Among their many applications, they have gained much attention as electrodes for charge storage, especially in supercapacitors. Current research focus is on properties – charge storage interrelation, since their electrochemical behavior is strongly dependent on their physicochemical properties, which are directly controlled by the synthesis routes.

We have recently developed a simple and ecologically improved method for the oxidation of arylamines employing H_2O_2 as an oxidant and Fe_3O_4 nanoparticles (NPs) as a catalyst [1,2]. Knowing that various aromatic molecules, radical cations, oligomers, and even PANI itself present in a very small percentage in the processes of oxidation of aniline can serve as initiators that significantly accelerate the polymerization process, here we investigated the influence of a small amount of para-aminodiphenylamine (p-ADPA) on the rate of aniline oxidation reaction, as well as on the molecular structure, yield and electrical conductivity of products synthesized using H_2O_2/Fe_3O_4 NPs oxidant/catalyst system. It was confirmed that p-ADPA significantly speeds up the oxidation reacition of aniline in applied conditions. FTIR and Raman spectra indicated the presence of a highly conductive PANI-ES form in all the products.

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References:

1. J. Mišurović, M. Mojović, B. Marjanović, P. Vulić, G. Ćirić-Marjanović, Magnetite nanoparticles-catalysed synthesis of conductive polyaniline, Synth. Met. 257 (2019).
2. J. Mišurović, M. Mojović, B. Marjanović, P. Vulić, G. Ćirić-Marjanović, Magnetite nanoparticles-catalyzed synthesis of conductive poly(p-aminodiphenylamine), Synth. Met. 269 (2020) 116577.

P.S.II.A.5.

Laser processing structure optimization of the metal materials created using additive technologies

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In this work, the authors investigated the physical regularities of the structural-phase and chemical state formation in the volume of 3D printed titanium products consisting of several layers (surface layers of 3D printed alloys in the original and modified state and transition zonessurface layers of 3D printed alloys in the original and modified state and transition zones) depending on the applied methods and regimes of obtaining and high-energy processing. The authors of the method provided a physical justification of the effectiveness of the combination of electron beam 3D printing with surface treatment by means of precision gas dynamic 3D printing and laser treatment. It has been established that this approach makes it possible to eliminate the main disadvantages of 3D-printed alloys, which are their structural imperfection, which causes low plasticity, fatigue strength and corrosion resistance. From a fundamental point of view, it allows to give a complete physical picture of the process of forming the structure and physical and mechanical properties of metal materials during 3D printing and to find ways of "managing" this process.

The investigations were performed in the frames of the Project No. 3-A-2022 "Physical principles of optimization of the structure and complex of physical and mechanical properties of metal materials created using additive technologies"

P.S.II.B.1.

Reduced mobility for H3 + in n-butanol gas

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n- Butanol (C_4H_9OH) also known as 1-butanol or bio-butanol has a 4 carbon straight-chain structure, with the –OH at the terminal carbon. It is an important chemical feedstock used to produce solvents (butyl acetate, butyl glycol ethers) [1, 2], polymers (butyl acrylate, butyl methacrylate) [3] and plastics. But the recent interest in n-Butanol is mostly due to its application as a biofuel for use in engines, as an alternative to conventional gasoline and diesel fuels [4-7]. In this paper we show predictions for the low energy cross sections and transport properties specially reduced mobility for the H3 + in n-Butanol gas. These data are needed for modelling in numerous applications of technologically important. Appropriate gas phase enthalpies of formation for the products were used to calculate scattering cross section as a function of kinetic energy. Calculated cross sections can be used to obtain transport parameters as a function of E/N (E -electric field; N-gas density) for H2 + in n-Butanol gas.

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1. H. Xu, C. He, Sep. Purif. Technol. 56, 85-89 (2007).
2. M. Johnson, S. Barnes, R. Diasio, Anal. Biochem. 182, 360-365 (1989).
3. H. Jiang, S. Lu, X. Zhang, H. Peng, W. Dai, J. Qiao, Catal. Sci. Technol. 4, 2499-2503 (2014).
4. Z. Sahin, O. Aksu, Renew. Energy 77, 279-290 (2015).
5. N. Yilmaz, F. Vigil, K. Benali, S. Davis, A. Calva, Fuel 135, 46-50 (2014).
6. H. Liu, S. Li, Z. Zheng, J. Xu, M. Yao, Applied Energy 112, 246-256 (2013).
7. D. Rakopoulos, Fuel 105, 603-613 (2013).

P.S.II.B.2.

Intrinsic magnetic properties of the $RFe_{11}Ti$ (R = Y, Gd and Pr) by Zr, Co and C doping

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We present theoretical investigations on the electronic and magnetic properties of the $RFe_{11-x}Co_xTiC_z$ and $R_{1-y}Zr_yFe_{11}Ti$ (R = Y and Gd; x = 0 – 3, y = 0 - 0.1, z = 0 and 1) alloys describing the dependence of the magnetic properties (magnetic moments, magneto-crystalline anisotropy, exchange-coupling parameters and Curie temperatures) on the R/Zr and Fe/Co ratios and by C addition. According to our calculations for $YFe_{11-x}Co_xTi$, the total magnetic moment and magnetocrystalline anisotropy energy (MAE) are maximized for x = 1. On the other hand, Co doping enhances the MAE but reduces the total magnetic moment in $GdFe_{11-x}Co_xTi$ alloys. The C doping adding one C atom to the near-neighbour environment of Fe 8j site affects the magnetic moments of Fe atoms more pronounced as the Zr for R (R = Y, Gd) substitution. Also, Zr for R substitution and C addition have lower impact on MAE, compared with Co for Fe substitution in $RFe_{11}Ti$- type alloys. The calculated exchange-coupling parameters show highest values between Fe 8i spins, followed by Fe 8i – Fe 8j spins for all investigated alloys. The corresponding mean-field approach estimated Curie temperatures show qualitative agreement with available experimental data.

P.S.II.B.3.

Lanthanides-doped tellurite glasses: A new screen material candidate for volumetric 3D display applications

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The world is perceived in three dimensions by human vision. Commercially available displays, on the other hand, can only display two-dimensional images. Virtual reality and stereoscopic displays are two ways that have been proposed to overcome the fundamental restrictions of two-dimensional displays. However, these technologies have major limitations that prevent them from being used by the general population, such as a small viewing angle, single-user access, and/or the necessity to wear unpleasant gear. To address the aforementioned problems, laser-based volumetric display concept has been recently created. However, none of the proposed screen materials has so far met the parameters required for a successful volumetric display. Because of their unique set of physico-chemical properties tellurite glasses are promising materials for photonic applications in the visible and infrared regions. As we previously reported, the primary color components of red, green, and blue emissions can be generated by frequency modulating the 980 nm laser excitation source in a specified tellurite glass composition [1]. This phenomenon paves the possibility for volumetric display applications using tellurite glasses. Hence, in this study, Ce^{3+} and/or Nd^{3+} ions are combined with $Ho^{3+}/Tm^{3+}/Yb^{3+}$ ions in a robust tellurite glass matrix to obtain full-color tunable emission by varying power density, pulse width, and frequency parameters. To quantify the color gamut upon excitation modulated single beam irradiation and to evaluate the viability of such materials for 3D displays, color space coordinates and purities of the resulting emissions are determined. Consequently, a concept of the 3D display system is tested by visualizing simple shapes such as cross, circle, and lissajous figures via scanning a 3.0 cm^3 lanthanides-doped tellurite glass cube using dual-axis galvanometer and a NIR laser setup. The dimensions of the shapes are successfully controlled by modifying the flickering speed of the galvanometer's mirrors.

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1. O. Kıbrıslı, N. Vahedigharehchopogh, A.E. Ersundu, M. Çelikbilek Ersundu, Instantaneous color tuning of up-conversion emission in a novel lanthanide doped monolithic glass via excitation modulation, J. Phys. Chem. C (2020)

P.S.II.B.4.

Phosphorescence decay kinetics of the Becquerel type in YAP:Mn

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The phosphorescence glow decay kinetics in solids was studied in a significant number of materials under the different types of excitation. It gets especial interest in last decades with growing interest to phosphors with so called persistent luminescence (PersL) and their application in many fields. It was found even in the middle of the 19th century, that the afterglow decay kinetics of many of irradiated phosphors is well described by the empirical Becquerel decay function $I(t) = I_0(1+\mathrm{w}t)^{-\alpha}$, where parameter w and α can be found from the approximation of experimental dependence. The integral glow intensity $\int_0^{\propto} I(t)\mathrm{d}t$ of the afterglow light corresponds to the net amount of stored energy (or dose of irradiation) in storage phosphor. But sometimes the power α becomes less than one and the Becquerel decay function becomes non-integrable which means formally that the light sum of phosphorescence becomes infinite that, of course, has no physical meaning. It is exactly the case of YAP:Mn crystal being studied as storage phosphor for luminescence dosimetry which demonstrates the kinetics of the Becquerel type in phosphorescence glow and optically stimulated luminescence [1]. Similar phosphorescence decay kinetics is observed in some other phosphors studied before [2]. Several approaches are known to explain the hyperbola-like kinetics with $\alpha < 1$ [2-5], but till now there is no general understanding of this phenomenon. The present work is devoted to analysis of theoretical models of processes occurring during the phosphorescence and to searching of their consistency with observed kinetics described empirically by non-integrable Becquerel function.

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1. S. Ubizskii1, O. Poshyvak, D. Afanassyev et al., Acta Phys. Polon. A, to be published.
2. V. Degoda, A. Gumenyuk, I. Zakharchenko, O. Svechnikova, J. Phys. Stud., 2011, 15, 3301.
3. E.I. Adirovich, Some problems in the theory of luminescence of crystals, Gostekhizdat, Moscow-Leningrad, 1956.
4. D.J. Huntley, J. Phys.: Condens. Mat., 2006, 18, 1359.
5. M.K. Sahai, A.K. Bakshi, D. Datta, J. Lumin., 2018, 195, 240.

P.S.II.B.5.

Organic and perovskite solar cells – Which wet will win the bet?

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Although the photovoltaic market is still dominated by crystalline Si solar cells, there is a rising demand for thin film devices which has sparked extensive research in the field of third generation (3G) solar cells, most notably organic based as well as hybrid organic-inorganic (perovskite) based. These cells present a very attractive area of research because of their ability to overcome the Shockley-Queisser limit of power efficiency for single bandgap solar cells (SC) as well as to fulfill industry demands like flexibility, scalability and simple/cost effective processing.

P.S.II.B.6.

Synthesis and properties of stable nitrogen-doped MWCNTs for thermoelectric applications

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Thermoelectric materials and technologies based on them allow the direct conversion of heat into electricity. Such devices are expected to play an important role in solving one of the biggest global challenges, which is improving the energy efficiency of domestic and industrial processes by capturing waste heat and converting it into useful energy.

Carbon nanotubes (CNT) in networks create good electrically but not thermally conductive connections, making them favorable for thermoelectric applications. Semiconductor electronics require the use of both p- and n-type semiconductors. While p-type CNT doping is easy, n-type CNT doping is more difficult in terms of its stability and efficiency.

We describe a method for obtaining nitrogen-containing multiwalled carbon nanotubes (N-MWCNTs) under chemical vapor deposition conditions. The thermoelectric sensitivity measurements show that doping by this method is effective and stable at elevated temperatures (500 °C) with an n-type behavior persisting through a long period of time. Due to their semiconducting abilities N-MWCNTs are seen as promising thermoelectric materials especially in case of flexible heterostructures formation at high temperatures.

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P.S.II.B.7.

Fabrication and characterization of high entropy pyrochlore ceramics

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High-entropy rare-earth (RE) zirconates with pyrochlore structure were successfully fabricated by pressureless and spark plasma sintering. $RE_2Zr_2O_7$ compound with nominal composition $(La_{0.2}Y_{0.2}Gd_{0.2}Nd_{0.2}Sm_{0.2})Zr_2O_7$ was prepared by simple glycine nitrate procedure (GNP). GNP process yielded powders with low crystallinity and after subsequent calcination, well crystalline ceramics were formed. During calcination defective fluorite (F-$RE_2Zr_2O_7$) and crystal pyrochlore (Py-$RE_2Zr_2O_7$) structures coexist. Formation of pure crystalline pyrochlore occurs after sintering at 1450 °C. High-density ceramics, free of any additives, were obtained after powders compaction and pressureless (PS), as well as Field Assisted Sintering Technique (FAST) at 1450 °C. Theoretical investigations of the high-entropy $RE_2Zr_2O_7$ pyrochlore systems were performed. Unit cell parameter of the obtained Py-$RE_2Zr_2O_7$ is 10.5892(2) Å and 10.5999(2) Å for PS and FAST sintering, respectively, which is in good agreement with the results of Density Functional Theory (DFT) calculations. The thermal diffusivity of sintered samples at room temperature was ~0.7 mm^2/s for both sintering methods.

P.S.II.B.8.

Discrimination of the exhaled compound of lung cancer patients and healthy subjects by a biosensor based on essential 20 amino acids

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Treatment and diagnosis of lung cancer, which ranks first in cancer mortality in Korea, is a very important matter for the health of the people. In particular, in the case of cancer treatment, early diagnosis is even more important because it determines life. For this reason, there is a need for a diagnostic technology equipped with quickness, easy access, and accuracy. Here, we investigated to develop an appropriate sensor to satisfy the needs of diagnostic technology for lung cancer. We generate essential 20 amino acids expressed the M13 bacteriophage-based color sensor. M13 bacteriophage engineered genetically was used as a biomaterial to fabricate colorimetric bio-sensors where the M13 bacteriophage coating film by the pulling method was used. We exposed the colorimetric bio-sensors to gas samples that were collected from the breath of lung cancer patients and non-patients. We checked the color changes of coated films according to the exposure which is caused by changing bundle structure of the M13 bacteriophage. The changing color had a quick response to the exposure and had a correlation to lung cancer. Additionally, we confirmed that the diagnostic accuracy can be improved using the machine learning application with combined colorimetric bio-sensors. We expect that our M13 bacteriophage-based colorimetric bio-sensors will contribute to saving the life by assisting early diagnosis of lung cancer easier. Moreover, it is anticipated to be applicable to other respiratory diseases as well.

P.S.II.B.9.

Three-dimensional plasmonic nanoclusters for high sensitivity SERS platform development

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Plasmonic nanoparticle clusters, due to their excellent electromagnetic response properties, offer the potential to create a new concept of devices for nanophoton applications. It is difficult to localize the target material in surface nanostructure-based SERS. This requires a wide beam width and time to scan the area. Here, we propose a three-dimensional superstructure based on packed nanoparticles. Super structures are fabricated by a simple three-dimensional assembly process. Dispersed nanoparticles self-assemble by meniscus contact in the dispersion state. With rapid evaporation of the solvent, the particles are strongly packed. Packed nanoparticle clusters constitute a high-density nanogap and force the target material into the nanogap. The electromagnetic field amplification between nanoparticles strongly amplifies the optical signal of the target material. The femtolith volume superstructure with the target material has succeeded in overcoming the limitations of the existing substrate-based SERS. The superstructure-based platform can make a great contribution to the development of diagnostic equipment for effective detection of pathogens.

P.S.II.B.10.

Dielectric properties of polyvinyl alcohol composites with improved ionic conductivity

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All in printed micro-supercapacitors (MSC) may represent the solution for ensuring optimal powering and large-scale deployment of wearable bio-medical flexible electronics. In order to foster the emergence of this category of commercial devices, an outstanding solid electrolyte easy printable may represent the solution for fabricating self-powered electrochemical and electrical disposable biosensors. In spite of the multiple attempts reported within the literature, a convenient solid electrolyte is not yet ready to be launch on the market. In line with the aforementioned desideratum, fire resistant polymer composites were prepared based on polyvinyl alcohol (PVA) as polymer matrix and a polyphosphonate as flame retardant. $LiClO_4$, $BaTiO_3$ and graphene oxide were also incorporated into PVA matrix to increase the ionic conductivity. Oxalic acid was used as crosslinking agent. The composites were investigated by infrared spectroscopy, scanning electron microscopy, thermogravimetric analysis, differential scanning calorimetry and microscale combustion tests.
The dielectric behaviour of the samples was analysed based on evolution of real permittivity and dielectric losses in a frequency domain from 10 Hz up to 10 MHz. The ionic conductivities of the samples under test were determined and discussed in relation to $LiClO_4$ content.

References:

1. G. Hirankumar, N. Mehta, "Effect of incorporation of different plasticizers on structural and ion transport properties of PVA-LiClO4 based electrolytes", Heliyon 4, e00992 (2018);
2. M. Wak, R. Gul, "Conductivity, Structural and Thermal Studies on Electrospun PVA-PANI-LiClO4-Sb2O3 Composite Nanofibers Polymer Electrolytes for Battery Applications", J Material Sci Eng 8: 529 (2019);
3. K. Sundaramahalingam, M. Muthuvinayagam, N. Nallamuthu, et al. "Investigations on lithium acetate-doped PVA/PVP solid polymer blend electrolytes", Polym. Bull. 76, 5577–5602 (2019).

P.S.II.B.11.

Synthesis and characterization of iridium oxide based films

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Electrochemical synthesis of Iridium oxide films at the Ti_2AlC support was performed by two procedures: I) by anodic electrodeposition from the solution containing: $IrCl_3xH_2O$, H_2O_2, $H_2C_2O_4$ and K_2CO_3, pH 10; II) by cycling the layer of previously electrodeposited pure metallic iridium in the 0.5 M H_2SO_4. During anodic electrodeposition of iridium oxide columbic efficiency decreased with potential increase, remaining only several percent (~4%) at the potential of 0.7 V vs SCE. Only one pair of peaks corresponding to the transition Ir_2O_3/IrO_2 was observed on the cyclic voltammograms recorded in the same acid electrolyte. On the other hand, cycling pure metallic Ir layer in the potential range from -0.25 V to 1.20 V (vs SCE, up to 100 cycles) typical cyclic voltammogram response was characterized with the one pre-peak and a pair of peaks corresponding to the above mentioned Ir(III)/Ir(IV)-oxide transition.

The oxygen evolution at both iridium oxide based films was studied by electrochemical techniques – polarisation measurements and cyclic voltammetry. The typical Tafel slope value for this anode reaction close to 40 mV dec-^{1} has been obtained, indicating that the rate determining step (RDS) was the first oxygen atom adsorption, in accordance to earlier reffered data in the literature. After repetitive cycling in the potential range of the oxygen evolution, the decrease of activity of both oxide films was observed, indicating dissolution reaction of iridium oxides taking place paralel with the OER, unlike many other earlier literature findings. These facts were experimentally proven by physical-chemical characterization - by applying XPS, SEM and EDS techniques, as well.

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P.S.II.B.12.

3D printed auxetic structures with enhanced energy absorption

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Presented study focuses on the 3D printed auxetic structures with gradient porosity as a way to increase the effective energy dissipation through engineering their architecture. Auxetic structures, considered as one of the 16 smart materials in 21st century, exhibit several enhanced mechanical properties due to the negative Poisson's ratio. In this study, we proposed several auxetic lattices in order to enhance an energy absorption under compression by varying their topology, porosity and gradient. The lattice structures were 3D printed by stereolithography from both flexible and rigid polymeric resin, while paying attention to their chemical nature, crosslink behaviour, printing and post-processing parameters. The experimental compression test results were compared with finite element analysis and the results show that properly chosen graded system significantly enhances the mechanical performance such as stiffness and energy absorption capacity at high compressive strains. Also, the number of the unit cells as well as the porosity of the auxetic structure show large effect on studied parameters. Based on these results, there is a possibility to design a lattice which exhibit outstanding energy absorption properties while being lightweight and easily scalable by additive manufacturing. Thus, fully use the large potential of auxetic structures.

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P.S.II.B.13.

Effect of molten salts and high temperatures on the corrosion resistance of materials

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Molten salts are a promising working environment for many industries operating in high-temperature chemical regimes. However, salts can be highly corrosive at high temperatures, making this difficult to select construction materials. This work is devoted to comparing the state of exposed materials at high temperatures in an inert environment and at high temperatures in molten salts.

Two sets of material samples were produced for high-temperature exposures: Inconel 601, 617, 625, Hastelloy C22, and alloy MoNiCr. The first exposure took place in argon at 600°C, and the second exposure at 440°C in molten salts (LiCl – KCl). After exposure, the surfaces and cross-sections of the samples were analyzed by scanning electron microscopy and their corrosion rates were compared.

P.S.II.B.14.

Surface characterization of chromium nickel alloys in molten salts using X-ray photoelectron spectroscopy

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High-temperature chromium-nickel alloys that could be suitable as construction materials for reactor components IV. generations were exposed in an argon atmosphere without and using molten alkali chloride salts (440-660 °C, eutectic mixtures of LiCl-KCl salts, 0.2 MPa). High-temperature and chloride mixtures can have a major impact on corrosion and material life. The samples were analyzed by XPS without and after argon-ion sputtering.

Tenuous oxide layers formed on the surface of the samples after exposure. After exposition without salts, the layers were mainly composed of chromium oxides and, in all cases, Mo was also detected. Ni was also found for the 601, C-22, and MoNiCr alloys, and Ti was detected for Inconel 601 and 617. In contrast, in the case of exposure to salts, the surfaces of all materials were mainly composed of NiO oxide and Cr_2O_3. Fe (except alloy MoNiCr) and Mo (except alloy 601) were also detected.

P.S.II.B.15.

Selection of container materials for deep repositories of radioactive waste in connection with microbial corrosion

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Construction materials for deep radioactive waste repositories must withstand many physical and chemical parameters, and the question of the influence of microorganisms present in underground environments must be considered.
This work summarizes the basic conditions of the storage in the granite subsoil of Central Europe and the possible effects of microorganisms on the corrosion processes of construction materials. Solutions from long-term exposures of two alloy samples in a model groundwater environment were analyzed, and the presence of microorganisms was verified.

P.S.II.C.1.

Photocatalytic activity of g- and n-C_3N_4 in phodegradation of textile dye Acid orange 7

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In pursuit for photocatalyst responsive on visible light activation, "graphitic" carbon nitride (g-C_3N_4) emerged as good candidate. Constituted only from carbon and nitrogen atoms, it is considered as a very „green "semiconductor, which can be easily synthesized by thermal treatment of urea or another organic amide.

Carbon nitride has 2D layered structure similar to graphene, which is why it is usually denoted as "graphitic". It is pale yellow material with the bulk band-gap energy of about 2.7 eV [1] and suitably positioned potentials of valance (~ +1.4 eV *vs.* NHE) and conduction band (~-1.3 eV vs.NHE) [1] for generation of OH and superoxide radicals, main oxidative species involved in any successful photodegradation process.

However, it suffers from fast recombination of photogenerated charges, which leads to lowering of its photodegradation efficacy. It is proposed that addition exfoliation process of g-C_3N_4 to so-called nano (n-) C_3N_4 can suppress process of charge recombination.[2] n-C_3N_4 has slightly higher value of band gap energy, but, also, higher activity in photodegradation of some organic molecules.[3]

Here, differences in optical properties, structure and photocatalytic efficiency in photodegradation of organic textile dye Acid Orange 7 will be presented. Mechanism of photogeneration of oxidative species, as well as their role in degradation of AO7 will be discussed.

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References:

1. X. Wang et al., ACS Catal. 2012, **2**, 1596−1606.
2. P. Niu et al., Adv. Funct. Mater. 2012, **22**, 4763–4770.
3. F. Dong et al., J Colloid Interf. Sci. 2013, **401**, 70–79.

P.S.II.C.2.

Band gap engineering in novel fluorite-type rare earth high-entropy oxides (RE-HEOs) with computational and experimental validation for photocatalytic water splitting applications

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Five different rare-earth-based nanocrystalline high entropy oxides (HEOs) with fluorite type of structure and average crystallite sizes between 6 and 8 nm were prepared and their photocatalytic behaviour towards AZO dye degradation and photoelectrochemical water splitting for hydrogen generation was examined. The cationic site in the fluorite lattice consists of five equimolar elements selected from the group of rare-earth elements including La, Ce, Pr, Eu, and Gd and second-row transition metals, Y and Zr. Studied HEOs exhibit bandgaps in the range from 1.91 eV to 3.0 eV and appropriate valence and conduction bands for water splitting. They reveal high photocatalytic activity that is mostly attributed to the accessibility of more photocatalytic active sites which provided radicals responsible for the AZO dye degradation. The materials successfully produce hydrogen by photocatalytic water splitting, suggesting the potential of HEOs as new photocatalysts. The photocatalytic performances of all studied HEOs outperform the single fluorite oxides or equivalent mixed oxides. The $Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Y_{0.2}O_2$ (CZLPY) engender hydrogen in 9.2 $\mu molmg^{-1}$ per hour that is much higher content than for pristine CeO_2 material which amounts to 0.8 $\mu molmg^{-1}$ per hour. The density of states (DOS) and the projected DOS after high-entropy equimolar doping (CZLPY) of starting pristine CeO_2 indicated that the bandgap is significantly reduced from 3.48 to 2.71 eV due to Pr 4f and O 2p orbital mixing. DFT calculation also disclose that a strong interaction between AZO dye methylene blue (MB) and CZLPY(111) is responsible for observed higher photodegradation of MB by CZLPY compared to pristine CeO_2. This occurs due to the existence of three solid bondings of MB with the surface of CZLPY(111) compared to only one solid bonding with the surface of CeO_2 (111).

P.S.II.C.3.

Influence of different synthesis methods on morphological and optical properties of the rare earth doped fluorides

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Over the last few years there has been a great interest in developing the efficient methodologies for the preparation of rare earth doped up-converting nanoparticles (UCNPs), which exhibit emission in visible part of spectra when excited by the near infrared (NIR) radiation. Due to this unique optical property, as well as the high chemical stability they could be used either as security or fluorescent biological labels. Depending on the host crystal structure and choice of the dopant, these could exhibit different luminescence response. In this work we represent the effect which hydro/solvo thermal treatment and simple co-precipitation have on structural, morphological and optical properties of $NaYF_4$:Yb,Er UCNPs. We showed that pure cubic phase crystallizes in monodisperse spherical nanoparticles obtained through hydro/solvothermal synthesis, while co-precipitation and annealing at 500°C for 5 hours leads to the obtaining of agglomerated microparticles with hexagonal phase. Due to the difference in size and morphology of the samples, the different up-conversion mechanisms are established upon the excitation by the infrared light (λ = 978 nm), intensifying green emission ($^2H_{11/2}, ^4S_{3/2} \rightarrow ^4I_{15/2}$) in sample obtained through hydro/solvo thermal synthesis.

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P.S.II.C.4.

Possibilities of application of green's function methods to research of nanoscopic crystal structures

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The method of Green's functions is one of the most powerful and reliable quantum statistical methods of theoretical research in solid-state physics because it consists of a completely closed formalism within which problems of particle and quasiparticle systems can be completely solved, and the energy and lifetime of elementary excitations, as well as statistical mean values of the corresponding physical quantities, can be calculated. Green's functions depend on both spatial and temporal variables, so this method can be successfully applied to study very specific properties of nanoscopic structures. In this paper, we presented the general procedure for defining Green's functions and the manner of their use to calculate the microscopic and macroscopic properties of the observed physical system. In the second part, this procedure is illustrated by determining the thermodynamics of phonons, and by analyzing the general properties of ultrathin crystalline films.

P.S.II.C.5.

Characterization of magnetron sputtered Ti-Al-N thin films

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Ti2AlN thin film could be employed in various fields of application, such as protective wear coating of high speed machining tools and diffusion barriors in microelectronic devices etc.. In this study three types of Ti-Al-N thin film with different phase structure (armorphous, polycrystalline fcc and MAX(Mn+1AXn) phase) were fabricated on the route of magnetron sputtering process. Thermomechanical and tribological properties of the Ti-Al-N films were investigated. Phase structure of thin films were analyzed with HR-TEM, SAED patterns and fast Fourier transforms(FFT). Comparing to amorphous and polycrystalline Ti–Al–N thin films, MAX-phase Ti2AlN film exhibited higher hardness value and H/E(hardness/elastic moudulus) ratio. MAX-phase Ti2AlN film also revealed superior toughness. All these enhanced properties were found to be attributed to the unique nanolaminated microstructure of MAX phase Ti2AlN film. Therefore MAX-phase Ti2AlN film exhibited better nano wear resistance due to higher toughness, hardness, and H/E values.

P.S.II.C.6.

Characterization of adsorption site heterogeneity in gas sensors based on LPE graphene by using sensor noise analysis

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In adsorption-based gas sensors adsorption properties of the sensing material inherently influence the sensor performance (e.g. sensitivity, selectivity, response rate and magnitude), as well as the ability of efficient sensing surface regeneration, which is necessary for sensor reusability. Sensing layers are often heterogeneous, which means that they contain different types of adsorption sites with different adsorption/desorption energies. Characterization of an adsorption surface includes the determination of relative abundances of different binding sites, their numbers and surface densities, and binding energies. It reveals the dominant sensor response generation mechanism, and it is important for designing and optimization of sensors with either spontaneously occurring or intentionally introduced surface heterogeneity. Liquid-phase exfoliated (LPE) graphene is a promising material for gas sensing due to its defect-rich structure. It consists of flakes with edges where highly reactive adsorption sites are located, while another type of adsorption sites exists on basal planes of the flakes, making LPE graphene a heterogeneous sensing material. Here we present a method for characterization of LPE graphene surfaces based on the analysis of sensor noise in the frequency domain, and the underlying theoretical noise model. We consider the case in which there are three types of adsorption sites for binding of target gas particles. The presented theoretical model encompasses analytical expressions for all characteristic noise spectrum features (five characteristic frequencies) that can provide information about the numbers of adsorption sites and their surface densities. Apart from the already mentioned two types of adsorption sites, we introduce as the third type of sites those that are already occupied by particles of highly reactive species from the environment. This brings our model even closer to real gas sensing applications. The presented method and the theoretical model have proven to be useful for characterization of adsorption sites heterogeneity in gas sensors based on LPE graphene.

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P.S.II.C.7.

Impact of TiO_2 nanoparticles on the kinetics of free-radical and cationic photopolymerization in Vat 3D printing

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Photopolymerization, which is a light-induced reaction, can be distinguished as a free-radical and cationic, based on the photoinitiation mechanism. The commonly used radical resins typically utilize acrylate and methacrylate monomers and oligomers, which react with free radicals upon photoinitiation. On the other hand, cationic resins are usually based on epoxy monomers, where a cation is formed to ring-open the epoxy groups.

Photopolymerization reactions are the basis of Vat 3D printing technology, in which the liquid monomer mixture is converted into solid polymer upon the exposure to light. Vat 3D printing can be used not only for preparation of pure polymer samples but also for polymer nanocomposites. In this case, the overall photopolymerization kinetics depends on the monomers used, the processing parameters (wavelength of light, light intensity, and curing time), and the presence of nanoparticles in the monomer mixture.

The growing demand for the preparation of nanocomposites using Vat 3D printing technology requires further study of the photopolymerization kinetics. The present nanoparticles interact with the incident light via scattering or absorption. Some of the nanoparticles, e.g., metal oxides, can even exhibit a photoinitiating effect after light irradiation. In addition, the nanoparticles interact chemically with the surrounding photopolymerizable resin, which can also affect the kinetics.

This study investigates the photopolymerization kinetics of free-radical and cationic photopolymerizable resins filled with different content of titania (TiO_2) nanoparticles in both anatase and rutile form. Photolysis measurements, real-time FTIR, and photo-DSC revealed that photoactive anatase and rutile nanoparticles can accelerate the photopolymerization kinetics, whereas the higher effect was observed via a free-radical photopolymerization mechanism. The results were compared to those of an unfilled matrix to judge the effect caused by the present nanoparticles.

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P.S.II.C.8.

Study of influence of Mn dopant on dielectric response of $SrTiO_3$ ceramics

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The influence of Mn incorporation into the Sr and Ti sites of $SrTiO_3$ ceramics on the structure, microstructure and dielectric tunability was studied. Manganese doped $SrTiO_3$ ceramics with various manganese dioxide weight percentages (1.5, 3 and 6 wt %) were prepared by a solid-state method in the presence of mechanical activation (10, 30 and 120 minutes). According to Ritveld's analysis it was found that the size of the crystallite in doped activated $SrTiO_3$ ceramics is smaller than the size of the crystallite in undoped ceramics. This lower degree of crystallinity is a consequence of additional distortion of the crystal structure due to ion substitution. SEM analysis showed that with increasing dopant concentration in the sample, at the same time as a time of mechanical activation, the grain size decreases, which is explained by the increasingly dominant incorporation of Mn^{4+} ions at sites of Ti^{4+} ions. On the Raman spectra of doped ceramic samples, the appearance of a peak at ~750 cm^{-1} was observed, its change in intensity with the increase of dopant concentration indicates the incorporation of dopant in the $SrTiO_3$ lattice. It was stated that mechanical activation leads to a more pronounced increase in the intensity of the mentioned peak, i.e. that activation leads to effectively higher incorporation of dopant into the strontium-titanate lattice. Higher values of relative dielectric permittivity of doped $SrTiO_3$ ceramics were observed for 1.5 wt %, in relation to inactivated and activated undoped ceramics. Based on all previous analysis, it is estimated that this can be related not only to higher sample densities but also to the contribution of Mn^{2+} ion incorporation at Sr^{2+} ion positions in the lattice. Based on all the above, the optimal electrical properties of $SrTiO_3$ ceramics can be achieved by the appropriate choice of mechanical activation time and dopant concentration.

P.S.II.C.9.

Physicochemical properties of copper-doped bismuth vanadate nanoparticles

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Environmentaly friendly photoelectrochemical (PEC) materals are in the center of the research interest for sustainable solar-to-chemical energy conversion. Lately, bismuth vanadate ($BiVO_4$) has attracted attention due to its visible light harvesting properties, band edge positions and low-cost synthesis method. However, $BiVO_4$ has poor charge transfer properties due to the high rate of electron-hole recombination. It has been shown that metal doping efficiently boosts charge separation and hence increases PEC water splitting activity. Herein, we report physicochemical properties of hydrothermaly sinthesized 1%-, 2.5%- and 5%- Cu-doped $BiVO_4$ powders for 8 h and 20 h. X-ray diffraction (XRD) study indicates that, depending on the degree of doping and synthesis time, material exists in monoclinic or tetragonal scheelite phase, but mixed phase composition was also possible. Monoclinic phase was formed in a case of pristine samples (synthesized for 8 h and 20 h) and 1% and 2.5% doped samples synthesized for 8 h. Tetragonal phase was observed in case of 5% and 1% doped samples synthesized for 8 h and 20 h, respectively. In the samples synthesized for 20 h and doped with 2.5% and 5% mixed phase was noticed. Scanning electron microscopy (SEM) reveals that samples with monoclinic phase consists of combination of worm-like and prismatic structures while tetragonal samples showed spherical shape. In case of samples with mixed phase a combination of prismatic and spherical shape was observed. Local structure was examined with Raman and Fourier Transformed Infrared (FTIR) spectroscopy. Optical properties were characterized with UV-Vis Diffuse Reflectance Spectroscopy (DRS) and Photoluminescence (PL) spectroscopy. Monoclinic phase has band gap in range 2.35 – 2.52 eV while samples with tetragonal phase has band gap in range 2.8 – 3 eV. Based on the results it can be concluded that band gap is dependent on the phase composition of samples. PL results indicate that monoclinic samples possess better recombination features than tetragonal ones. Preliminary measurements confirmed considerable higher PEC activity of light-irradiated samples.

P.S.II.C.10.

The effect of heat treatment and pulsed laser treatment on the morphology of Au and Ag nanoparticles and nanowires

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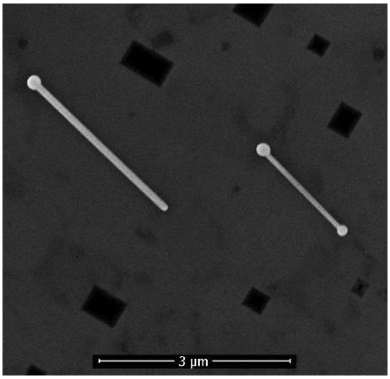

We investigated the effect of heat treatment and pulsed laser irradiation on the geometry of Au and Ag nanoparticles (NPs) and nanowires (NWs). Chemically synthesized Au NPs and NWs, as well as Ag NWs deposited on oxidized Si wafer were were annealed at temperatures ranging from 200 to 800 °C [1,2] or treated by pulsed nanosecond 532 nm laser at RT [3,4,5]. In both cases for spherical NPs a change in the geometry from faceted to more rounded shapes were observed with increasing annealing temperature. Effect of NWs treatment was different for heat or laser processing. Thermal treatment evenly increase thermal diffusion of metal atoms of every region of a nanowire, while thermal effect of laser irradiation is mediated by surface plasmons, which heat up the ends of NWs much more effectively than other NWs parts. This nonhomogeneous heating cause "bulb"-like formations on NWs ends (see figure).

1. Sven Oras et al., Beilstein J. Nanotechnol. (2020) 11, 61–67. doi:10.3762/bjnano.11.6
2. Simon Vigonski et al., Nanotechnology (2018) 29 015704. doi:10.1088/1361-6528/aa9a1b
3. Boris Polyakov et al., Phys. Scr. 90 (2015) 094007. doi:10.1088/0031-8949/90/9/094007
4. Boris Polyakov et al., Beilstein J. Nanotechnol. (2014) 5, 133–140. doi:10.3762/bjnano.5.13
5. Sergei Vlassov et al., Nanotechnology (2018) 29, 195707. doi:10.1088/1361-6528/aab163

P.S.II.C.11.

Structural chemistry, electrical and X-ray spectroscopic properties of the ternary Ce-Ni-P compounds

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In rare earth compounds, where 4f levels are relatively close to the Fermi energy, various anomalous phenomena frequently appear. Most of them can be attributed to the hybridization between the 4f states and conduction bands. A mixed-valence (MV) state is one of these phenomena. The MV phenomenon has attracted a great deal of interest during the last several decades in connection with valence fluctuations. We have studied experimentally and theoretically the electronic structure and x-ray absorption spectrum at the Ce L_{III} -edge and x-ray emission spectra of Ni and P at the K- and L_{III}-edges in the mixed valence compound $Ce_{20}Ni_{42}P_{30}$, $Ce_2Ni_{12}P_5$ and $Ce_2Ni_{12}P_7$ compounds. The theoretical calculations have been carried out by means of the *ab initio* fully relativistic spin-polarized Dirac linear muffin-tin orbital method. The calculations show good agreement with the experimental measurements. The Ni K X-ray emission spectrum is much wider than the L_{III} spectrum and possesses two fine structures: the major peak at −3.2 eV and low energy shoulder at around −6.0 eV to −11 eV. Because dipole allowed transitions dominate the X-ray emission the Ni K spectrum reflects primarily the partial DOS of occupied 4p-like states Np(E) of Ni below the Fermi level. The occupied Ni 3d partial DOSs are located mostly at the −4.8 eV to 0.0 eV and almost do not hybridize with the P 2p states. We present occupied part of the partial Np(E) DOS at the Ni site. Compare the XES and Np(E) we can conclude that influence of the dipole matrix elements is minor and already Np(E) partial DOS well describe the shape of the Ni K emission spectrum. The x-ray absorption experiments prove the f-d hybridization effects at low temperatures. The magnetic and electrical resistivity measurements, together with the analysis of the Xray absorption spectra, prove the ambivalent character of the cerium atom in these compounds.

P.S.III.C.12.

Electrochemical properties of composites of graphene oxide and cobalt ferrite doped with zink and gallium

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The possibility of surface functionalization and formation of stable aqueous suspensions make graphene oxide (GO) suitable as base for composite materials, especially with nanoparticles. Cobalt ferrite (CFO) has attracted attention due to its unique properties such as large magnetic anisotropy, high coercivity, moderate saturation magnetization, excellent chemical stability, mechanical hardness, etc. This study presents the electrochemical properties of GO and CFO composites, as well as CFO doped with zinc (CFO_Zn) and gallium (CFO_Ga). Magnetic nanoparticles were synthesized using the solvothermal method, after which the oleic acid was exchanged with dihydrocaffeic acid to obtain the hydrophilic material. GO was synthesized using a modified Hummer's method. Composites of GO and magnetic nanoparticles were synthesized by the hydrothermal method ($T = 120$ °C, $t = 3$ h), with nominal fractions of 5 and 15 wt.% of magnetic nanoparticles. X-ray structural diffraction, as well as FTIR analysis, confirmed the complete oxidation of graphene layers. SEM and TEM images showed deposition of magnetic nanoparticles on GO layer with the different distribution density between 5 wt.% and 15 wt.% composites. Also, shape and size of magnetic nanoparticles remained unchanged. Based on FTIR analysis of hydrothermally treated GO and composites a partial reduction of epoxy groups was found along with hydrogen bond established between the components of the composite. The electrochemical charge storage of composites is mainly of pseudocapacitive nature, which originates from the oxidoreduction reactions of H^+ ions from electrolytes and surface functional groups of GO. The best electrochemical properties, in terms of the highest specific capacity, were shown by the composite which contains 15 wt.% CFO, which value is 36.86 F g^{-1} at a polarization rate of 5 mV s^{-1}.

P.S.III.C.13.

Electrochemical charge storage properties of thermally treated and ion-beam irradiated graphene oxide/12-tungstophosphoric acid nanocomposites

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In recent years the 2D carbon nanomaterials have found a wide application in energy storage devices. Among them, graphene oxide (GO) has distinguished itself as a material with interesting surface chemistry and structural properties that can be modified. Surface chemistry has a twofold influence on GO charge storage properties: basal plane groups decrease conductivity of material while some edge groups can improve wetting and can contribute to increased capacity thanks to redox reactions. Mixture of oxidized and sp^2 hybridized parts as well as high specific surface area are favorable for introduction of different additive materials which can potentially improve the capacity. In this work composites of graphene oxide and 12-tungstophosphoric acid (WPA) with 6 and 13 wt.% of 12-tungstophosphoric acid were synthesized and modified with thermal treatment up to 400 °C in argon atmosphere and ion beam irradiation (H^+, 15 keV; N^{5+}, 75 keV). Resistivity of the pristine and modified samples was investigated with solid state electrochemical impedance spectroscopy. The results showed that the resistivity of the samples irradiated with hydrogen ions decreased up to fluence of 1×10^{16} ions/cm^2 after which the increasing structural damage caused the increase in resistivity. Thermally treated samples of GO showed substantially lower resistivity that was even lower in the case of composites showing the beneficial influence of WPA on electric properties of GO. Galvanostatic charge-discharge was used for assessment of applicability of samples in supercapacitors. Capacity of pristine and irradiated samples was quite low which was connected to low conductivity of these samples and low penetration depth of used ions. Thermal treatment in inert atmosphere was again proven beneficial, with much higher capacity of treated samples as compared to the pristine ones while also incorporation of WPA caused substantial increase of GO capacity.

P.S.III.C.14.

Mechanochemical synthesis of MgH_2-V nanocomposistes

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The future role of hydrogen as an energy vector is inevitable, especially as a basic tool for the decarbonisation of the energy sector. However, in order for hydrogen to gain its full commercial role, challenges such as cost-effective production as well as security of storage must be addressed Until now, hydrogen was usually stored under pressure (350-700 bar), which poses a significant safety risk or in the liquid state by liquefaction at cryogenic temperatures (-253.15 ºC), which implies a high cost of maintaining such low temperatures and the risk of hydrogen leakag. From this point of view, solid state hydrogen storage offers a promising solution both in terms of safety and cost, especially if light metal hydrides are chosen for storage materials. The chemical bond between hydrogen and metals in metal hydrides is usually strong, which in turn leads to slow kinetics and high dehydration temperatures, and it is necessary to cause destabilization of the structure. In this paper, the influence of destabilizing the structure of magnesium hydride using vanadium as an additive and the method of mechanical grinding in a high energy ball mill is investigated.

The influence on the morphological and microstructural changes in structure was monitored by X-ray diffraction, scanning electron microscopy, particle size analysis and Fourier transform infrared spectroscopy attenuated total reflection. Due to the correlation between changes in dehydration temperature and hydrogen desorption kinetics, DSC analysis followed. After applied destabilization methods to pure magnesium hydride, a significant improvement in the performance of the test material is observed.

P.S.III.C.15.

Structural, optical and mechanical characterization of the PMMA- ZrO_2 nanocomposites

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The aim of this research was to investigate the impact of functionalization of the ZrO_2 (zirconia) nanoparticles with γ-methacryloxypropyltrimethoxy (MEMO) silane on the structure, thermal, mechanical and optical properties of nanocomposites with pure and MEMO silane modified ZrO_2 nanoparticles. Morphology of nanocomposites was observed through SEM analysis. Fourier transform infrared spectroscopy (FTIR) confirmed the formation of the chemical bond between ZrO_2 nanoparticles and MEMO silane. The results of the tensile test showed that the addition of modified nanoparticles leads to an increase in Young's modulus. DSC analysis revealed an increase of glass transition temperature with the embedding of modified nano zirconia. Furthermore, time-resolved laser-induced fluorescence measurements were employed to characterise the optical properties of the pure PMMA and nanocomposites.

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P.S.III.D.1.

Synthesis and characterization of thermally treated geopolymer composite materials

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In this paper, the influence of thermal treatment on the mechanical properties of composite geopolymer materials was investigated. Geopolymer composite materials were synthesized using brushite ($CaPO_4 \cdot 2H_2O$) and raw abandoned kaolinite ($Al_2Si_2O_5(OH)_4$) clay which is previously thermally transformed into metakaolin. The geopolymer composites were made by mixing metakaolin with the addition of 2, 4, 6, 8, and $10\%_{w.t.}$ of brushite and activated using an alkaline activator with 8M NaOH. After a synthesis and aging period, the samples were thermally treated for one hour at two temperature ranges of 800 °C and 900 °C in air. X-ray powder diffraction and Fourier transform infrared spectroscopy were used to obtain the phase composition and structural vibrations of molecules in synthesized materials. Microstructural properties and also semi-quantitative analysis was performed using SEM-EDS analysis. Based on obtained results the pore-filling effect as a consequence of calcium ions incorporation into the geopolymer composite networks improved the compressive strength of thermally untreated geopolymer materials. On the other hand, the chosen sintering temperatures at 800°C and 900°C in an air atmosphere for one hour caused the phase transformation of brushite into calcium pyrophosphate phases which negatively affected the compressive strength of thermally treated geopolymer composite materials.

P.S.III.D.2.

Photocatalytic activity of N-TiO_2 nanotubes decorated with CdS QD

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The negative consequences of the modern world are environmental pollution. To decrease it, a lot of research is focused on finding solution for its remediation. Photoactive materials have ability to utilize solar energy for the degradation of organic and inorganic pollutants. Among different photoactive material TiO_2 has advantages due to its non-toxicity, chemical stability and corrosion resistance. The aim of this study was to investigate the synergetic effect of nitrogen incorporation into crystal structure of TiO_2 and deposition of CdS onto amelioration of the photocatalytic degradation of methylen orange compared to the pristine TiO_2. For that purpose TiO_2 nanotubes were obtained by anodization of titanium foil in HF containing electrolyte. To achieve crystal structure and at the same time to introduce nitrogen in TiO_2, the samples were annealed in ammonia atmosphere at 450 °C, for different time of annealing. The highest amount of nitrogen was achieved for the shortest time of annealing (30 min). Beside that, it was observed that the highest level of interstitial nitrogen was also achieved for the shortest time of annealing. Further, CdS quantum dots (QDs) were deposited on the nitrogen doped TiO_2 nanotubes via an ex-situ method (using binding reagent). According to the FESEM micrographs, a partial agglomeration of CdS QDs on some domaines on top of the nanotubes was observed. By performing the DRS, the improvement of the optical response after nitrogen doping and deposition of CdS was demonstrated. The sample with the highest amount of total nitrogen and interstitial nitrogen in combination with deposition CdS QDs exhibited the highest photocatalytic efficiency.

P.S.III.D.3.

Study of oil type pollutant adsorption on Vrbas river sediments (Bosnia and Herzegovina)

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Samples of coastal river sediments of the Vrbas River were examined in this paper. Samples were taken at 18 locations in a 250 km long river course. They were collected during October and November 2021: five samples were taken in the upper part of the stream from the spring to the city of Banja Luka. Six samples were taken from the coast that belongs to the city itself, and seven samples belong to the part of the flow from Banja Luka to the confluence of the Vrbas and the Sava River. Samples were taken from the surface (up to a depth of 10 cm). Organic substance was isolated in all sediments and its content was determined. It was analyzed in detail using column chromatography, followed by gas chromatographic mass spectrometric (GC-MS) analysis of alkanes and aromatic fraction (n-alkanes, isporenoid aliphatic alkanes, polycyclic alkanes and aromatic hydrocarbons of naphthalene and phenanthrene type). On the other hand, the mineralogical composition of the samples was defined using X - ray fluorescence analysis (XRF). The obtained results made it possible to assess the extent to which the inorganic composition of sediment affects the adsorption of organic pollutants of petroleum type (some of its compounds, as well as the corresponding structural and stereochemical isomers), and how much it affects retention of petroleum pollutants in coastal areas.

P.S.III.D.4.

Evaluation of photocatalytic activity of $Sr_{0.9}La_{0.1}TiO_3$ and $Sr_{0.25}Ca_{0.25}Na_{0.25}Pr_{0.25}TiO_3$ nano-sized ceramic powders for water treatment

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Water pollution is a significant issue nowadays. Among many different technologies for water purification, photocatalysis is a very promising environmental-friendly approach [1]. In this study, a photocatalytic activity of $Sr_{0.9}La_{0.1}TiO_3$ and $Sr_{0.25}Ca_{0.25}Na_{0.25}Pr_{0.25}TiO_3$ nano-sized powders were evaluated by degradation of metoprolol (MET) and pindolol in water. MET is a widely detected in rivers in a concentration varying from 3 ng/cm^3 to 4.9 µg/cm^3 [2], while pindolol is almost entirely insoluble in water due to its lipophilic properties.

The synthesis of $Sr_{0.25}Ca_{0.25}Na_{0.25}Pr_{0.25}TiO_3$ (SCNPTO) was performed by reverse co-precipitation (RCP) method using nitrate precursors, whereas $Sr_{0.9}La_{0.1}TiO_3$ (SLTO) was produced by spray pyrolysis (CerPoTech). The phase purity of synthesized powders was validated by XRD, while particle size about 80 nm by HR-SEM. The obtained powders were agglomerated and they possess a similar specific surface area of about 30 m^2/g. The energy band gaps of SCNPTO and SLTO were calculated (DFT) to be about 2.69 and 3.05 eV, respectively.

Photocatalytic performances of the materials were examined by removing MET and pindolol from polluted water under simulated solar irradiation (SSI), UV, and LED irradiation. Kinetics of MET and pindolol degradation was monitored by Ultra-Fast Liquid Chromatography with Diode Array Detection (UFLC–DAD) [3].

Concentration of MET in water decreases in the first 240 min up to 17 and 20 % under SSI and up to 30 % under UV irradiation when SCNPTO and SLTO were used, respectively. On the other hand, SLTO removed 68%, 94% and 100% of pindolol after 240 min under SSI, UV-Led and UV irradiation, respectively. Somewhat lower photocatalytic activity was obtained with SCNPTO under identical conditions, resulting in 65%, 84%, and 93% degradation of pindolol, respectively. The obtained results indicate a significant potential for future practical applications.

1. J. Shi, L. Guo, ABO_3-based photocatalysts for water splitting, Progress in Natural Science: Materials International, **22**, 592-615, (2012).
2. E-J Van den Brandhof, M. Montforts, Fish embryo toxicity of carbamazepine, diclofenac and metoprolol, Ecotoxicology and Environmental Safety, **73**, 1862-1866, (2010).
3. S.J. Armaković, M. Grujić-Brojčin, M. Šćepanović at al. Efficiency of La-doped TiO_2 calcined at different temperatures in photocatalytic degradation of β-blockers, Arabian Journal of Chemistry, **12**, 5355-5369, (2019).

P.S.III.D.5.

Performance of ternary cement binders containing high volume of fly ash and fluid catalytic cracking catalyst residue

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The use of binders based on waste materials in construction industry has both ecological and economic advantages over the use of commercial Portland cements (PC). Preserving the natural resources needed for PC production, as well as reusing waste materials instead of disposing them in landfills, contributes significantly to the protection of the environment. Also, the price of waste materials is usually much lower than the price of raw materials used for production of PC.

Coal combustion in thermal power plants produces huge amounts of fly ash (FA). It is estimated that 500-750 million tonnes of FA are generated worldwide annually, with a global utilization rate of only 25 %. Due to pozzolanic properties of this aluminosilicate waste material, FA has been used as PC component for decades. However, the broad use of binders made of high volume of FA (>50%) is limited by their relatively long setting time and low early strength.

The other waste material of interest in this work was fluid catalytic cracking catalyst residue (FC3R), a by-product from petrol refineries, which primarily consists of zeolite and amorphous aluminosilicates and also shows pozzolanic activity. Due to relatively small quantities of FC3R produced (~160000 tonnes per year globally), landfilling is usually considered as the most economical option for its disposal.

The aim of this work was to investigate the performance properties of ternary binder containing high volume of the two different waste materials, FA and FC3R. The binder consisted of FA, FC3R, and PC (commercial CEM I) mixed in a 49:21:30 mass ratio. Both waste materials were mechanically activated prior to the binder synthesis. Characterization of raw and mechanically activated waste materials via determination of particle size distribution, morphology and mineral composition, was conducted. Analyses of the ternary binder properties showed that using FC3R as the binder component resulted in acceleration of cement hydration and pozzolanic reaction. The ternary binder had shorter setting time and higher early strength than the control binder synthesized with 70 mass% of FA and 30 mass% of PC.

P.S.III.D.6.

Comparative assessment of chemically and 'green' synthesized magnetic nanoparticles and their use for removal of pollutants

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The ever-growing needs of modern science and technology in new materials with specific properties increase the interest of the world industrial and scientific community in nanomaterials. The magnetic nanomaterials have attracted perspective in biomedical and environmental applications because of their effective and low toxicity for human cells.

This work aimed to evaluate the toxicity and environmental application of magnetite-based magnetic nanoparticles (MNPs) synthesized by biogenic (Bio) and chemical (Ch) routes. Ch-MNPs and Bio-MNPs samples were prepared using chemical co-precipitation method or ethanolic extract of Artemisia vulgaris L 'hairy' roots without any additive, respectively. The nanoparticles were characterized by X-ray diffraction (XRD), vibrating-sample magnetometry (VSM), Fourier-transform infrared spectroscopy (FTIR), electron microscopies (SEM and TEM), etc. The ecotoxicity of MNPs was evaluated using Lactuca sativa and Cichoriun intybus as model plants.

The XRD data indicated that MNPs obtained by "green" and chemical technologies were Fe_3O_4 (JCPDS No. 98-015-9975) with a face-centered cubic spinel crystalline structure. The formation of spherical nanoparticles (9-12 nm) Ch-MNPs was confirmed. The TEM data revealed that the Bio-MNPs differed in morphology (spherical, cubic and nanorods) and size (10-23 nm). VSM demonstrated the superparamagnetic behavior of Ch-MNPs, and FTIR provided evidence of the differences in the surface of MNPs, suggesting the presence of phenolic compounds on the surface of Bio-MNPs. Thus, according to FTIR data, Bio-MNPs had a magnetic core and the shell formed by bioactive molecules from the plant extracts. The Cu^{2+} ions adsorption assay tests showed that Bio-MNPs demonstrated the adsorption capacity as adsorbents compared to Ch-MNPs, making these nanoparticles potentially useful for environmental remediation. It should be emphasized that Bio-MNPs demonstrated negative ecotoxicological activity on all tested plant.

In conclusion, although Bio-MNPs and Ch-MNPs present similar composition and structures, their characteristics of magnetic saturation and surface structure, providing diversity in their biological and chemical activity.

P.S.III.D.7.

Environmentally friendly hybrid poly(methyl methacrylate)-wood-poly(ethylene terephthalate)-alumina composite material

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In this study, the environmentally friendly hybrid composite was developed with the aim to study the influence of composite structure and moisture absorption on the mechanical properties of the hybrid composite. Poly(methyl methacrylate) (PMMA) dissolved in acetone with the addition of modified wood fibers (as a cheap component for producing cartons) was used as a starting composite. Because of the low interfacial adhesion between wood fibers and polymer matrix, wood fibers were modified with 3-mercaptopropyl trimethoxysilan (MTPMS) as a coupling agent. A mixture of pure and recycled poly(ethylene terephthalate) (PET) fibers produced at the vertical molder, as well as modified alumina particles with MTPMS, were added as a reinforcements. Composites were made by the “hot pressing” method. The mechanical properties of the hybrid composite were better when compared to starting composite as evident by an increase in the flexural strength (up to 1.3 times) and the modulus of elasticity (up to 1.2 times). Results of the impact testing showed an increase in the absorbed energy of the hybrid composite than the starting composite. Water absorption was reduced in the hybrid composite, so it can be concluded that modifications of the starting sample led to a reduction in cavities in the composite.

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P.S.III.D.8.

Initial characterization and evaluation of two tailing dumps in Bulgaria for application as precursors for geopolumers

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In Bulgaria, over 33 tailing dumps occur, 21 of which do not operate but are cultivated and 12 tailing dams are actively operating. Turning waste into resource for production of new materials is a step to circular economy. The main effort is the incorporation of mine wastes by utilization and immobilization of toxic metals. The application of this materials is often used in the synthesis of eco- friendly materials, such as geopolymers. In addition, synthesized geopolymers are expected to have properties comparable to those of OPC-based materials. Thus, evaluation of some main characteristics of mine tailing materials is recommended. As a result, the relationship between composition, structure and properties of the analysed materials can be summarized and an appropriate technology of production can be applied, depending on the obtained results.

The potential use of two mine tailings from Bulgaria as precursors for geopolymers was studied. Some structural properties of the raw materials were investigated. The elemental and phase composition were characterized by XRD and XRF. In order to predict the behavior of mine wastes during the polymerization process, leaching tests in strong alkali solutions were conducted. In addition basic measurements of pH, EC, Eh, total heavy metal content, loss of ignition were applied to both samples. Moreover, the samples were subjected to sequential extraction procedure which is fundamental to understanding chemical and physical characteristics of the samples.

The aim of this study is to define the proposed mine tailing materials and to evaluate the possibility of their application as precursors for newly synthesized geopolymers. Nevertheless, additional analysis will be performed depending on the results.

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P.S.III.E.1.

Synthesis, characterization and DFT calculations of Schiff base Co(III) complexes

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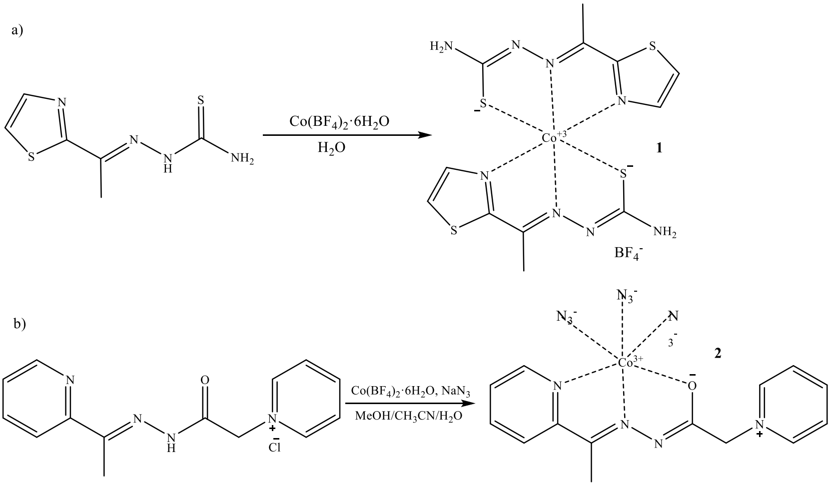
The Co(III) complex (**1**) was synthesized by the reaction of (E)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carbothioamide (**HL^1**) and $Co(BF_4)_2·6H_2O$ in solvent mixture of $MeOH/H_2O$ (Scheme 1a). The Co(III) complex (**2**) was synthesized by the reaction of (E)-1-(2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl)ethyl)pyridin-1-ium chloride (**HL^2**Cl) and $Co(BF_4)_2·6H_2O$ in solution mixture $MeOH/CH_3CN/H_2O$. After complete dissolution of $Co(BF_4)_2·6H_2O$ in the reaction mixture, NaN_3 was added (Scheme 1b). Obtained green crystals were characterized by SCXRD, elemental analysis. IR, NMR and UV/Vis spectroscopy. The Co(III) ions in **1** form mononuclear [Co**L^1**$_2$]BF_4 complex with two **L^1** ligands coordinated through thiazole and imine nitrogen atoms and enolate sulfur atom. The Co(III) ions in **2** form mononuclear [Co**L^2**$(N_3)_3$] complex with **L^2** ligand coordinated through thiazole and imine nitrogen atoms and enolate oxygen atom, while three remaining places are occupied by azide ions.

Density functional theory (DFT) calculations were performed to elucidate the structures of Co(III) complexes in solution.



*Scheme 1. Synthesis of complexes **1** and **2**.*

P.S.III.E.2.

Osteogenic potential of diluted blood and bone marrow in ectopic osteogenesis

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The bone marrow is a rich source of cells for assisted bone reparation which osteoconductive and osteoinductive potential is well documented. Since the amount of bone marrow which can be obtained for clinical application is often limited it is very important to evaluate osteogenic potential of diluted bone marrow. Also, there is more data about the existence of nonadherent cells in the peripheral blood that have characteristics of stem and/or osteoprogenitor cells which recruit blood as potential source of cell which can be used in osteoreparation. The aim of our research was to examine whether and to what extent diluted cells of whole blood and bone marrow in combination with the bone mineral matrix have an impact on the ectopic osteogenic process. The study was conducted on syngenic BALB/c mice, male, 10-12 weeks old. There were three experimental groups BMM (bone mineral matrix), BMM+diluted blood and BMM+ diluted blood+diluted bone marrow. Subcutaneus interscapular implantation was performed and the animals were sacrificed after 1, 2 and 4 weeks after implantation. The implants were analyzed using expression analysis of bone-related genes and histochemical stainings. All types of implants do not induced visible young bone growth but induced creation of necessary preconditions for supporting osteogenic processes. Implants type BMM+diluted blood+diluted bone marrow showed significantly better stimulatory effect on osteogenic processes than BMM+diluted blood and BMM alone. In this study, significant ectopic osteogenic potential of diluted bone marrow and blood in combination with bone mineral matrix was demonstrated.

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P.S.III.E.3.

Novel antimicrobial composites based on calcium- and zinc-alginate hydrogels and activated charcoal

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In this work we have produced novel composite biomaterials based on either Ca- or Zn-alginate hydrogels and activated charcoal (AC) particles impregnated with povidone iodine (PVP-I) for potential applications in wound dressings aimed for treatment of chronic and infected wounds. The obtained composites were analyzed by field-emission scanning electron microscopy and characterized regarding textural parameters, swelling as well as Zn^{2+} and AC release kinetics in the physiological saline solution. PVP-I was easily adsorbed onto AC particles within the composites which was confirmed by UV–visible spectroscopy, energy dispersive X-ray analysis and Fourier transform infrared spectroscopy. Upon contact with physiological fluids, the composite Ca- and Zn-alginate hydrogels swelled and released impregnated AC particles. These released AC particles impregnated with PVP-I exhibited excellent antimicrobial activity especially against multiresistant clinical isolates without the release of iodine into the surrounding environment. This approach enables the development of efficient multifunctional wound dressings using very powerful and at the same time cheap antiseptics such as PVP-I in comparison to new and much more expensive antimicrobial agents (e.g. metal nanoparticles).

P.S.III.E.4.

Characterization and drug release of Zn-Al layered double hydroxyde–nifuroxazide composite

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During last decades, layered double hydroxides ($[M^{II}_{1-x}M^{III}_x(OH)_2]^{x+}(A^-)_{x/n}\cdot yH_2O$, LDHs) have been used in catalysis, ceramics as well as in removal of anionic pollutants. Due to their excellent anion exchange capacity, good biocompatibility and low toxicity, the nanoparticles of LDHs showed an excellent potential as drug carriers. Nifuroxazide ($C_{12}H_9N_3O_5$, NFX) is a broad-spectrum antibacterial drug, poorly soluble in water. Towards to increase the solubility of NFX, Zn-Al-LDH/NFX composite has been prepared by precipitation method at room temperture. Zn-Al-LDH, NFX and the obtained composite were analyzed by Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), simultaneous thermogravimetry-differential thermal analysis (TG-DTA) and Brunauer–Emmett–Teller (BET) method. Characterization of the raw materials and the obtained composite confirmed the intercalation of NFX in Zn-Al-LDH. The in vitro study of drug release in simulated stomach acid and intestinal fluid showed constant release of NFX from Zn-Al-LDH during 24 h, confirming Zn-Al-LDH is a promising drug carrier.

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P.S.III.E.5.

Bio-mimetic bone-like surface structure of Ti-based implants

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To date, the key factor for Ti-based implant success is osseointegration. Previous studies showed modifying surface characteristics, such as topographical configuration and physicochemical properties, can enhance the osteoconductivity of Ti-based implants. A highly developed surface can improve osteogenesis and stronger biomechanical fixation than smooth surfaces. Therefore, implant surface modification is much more demanding, necessitating newer techniques of treatment to be identified. Our investigation aims to combine different methods to obtain surface modification suitable for further in-vitro investigation.

We applied three different methods for increasing the hierarchical surface structure: sandblasting, etching, and alkali treatment. The surface morphology was characterized by scanning electron microscopy (SEM), 2D and 3d tactile profilometry, and atomic force microscopy (AFM), 3D.

Tactile profilometry confirmed that sandblasting treatment leads to formation of micrometric surface features. Subsequent oxalic acid and alkaline treatment did not cause pronounced changes in surface roughness parameters on a micro level. However, AFM measurements, on the areas of 2x2 µm, revealed nanometric changes in surface irregularities on these surfaces. The last alkali treatment caused a porous titanate structure with open pores.

Using the following treatment steps is a bio-mimetic route to forming a bone-like surface structure. The next step of our investigation is to measure the thickness of the obtained layer and its inside structure. The cross-section method would give much more accurate information about the titanate layer and will orient us for suitable biomedical investigation.

P.S.III.E.6.

3D printed scaffold with bisphosphonate for tissue regeneration

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The blend of gelatin and polyvinylpyrrolidone (PVP) was used for the 3D printing of scaffolds with alendronate sodium trihydrate (ALN). This polymer blend is a good choice for tissue engineering applications because of its biocompatibility and optimized mechanical properties. ALN is a bisphosphonate (BP), a drug class used in osteoporosis treatment as an inhibitor of osteoclasts activity. However, orally taken BPs have very low bioavailability (<1%) because of poor absorption and permeability from the gastrointestinal tract (GIT). Also, BPs oral administration can cause mucosal irritation and GIT adverse effects. Because of that, incorporation of ALN in gelatin/PVP scaffold can help overcome these problems and provide local and sustained release of the drug.

Scaffolds with different gelatin/PVP ratios (1:1 and 3:1), with and without a drug, were prepared by the semi-solid 3D printing method. For scaffolds loaded with a drug, the ALN content was 5% on a dry polymer basis. The aim of this work was to examine the influence of polymer blend composition on mechanical properties and in vitro drug release profiles of obtained scaffolds. Chemical interactions during processing were investigated by FTIR spectroscopy. Scaffold morphologies were observed by SEM analysis. In vitro drug release under physiological conditions was performed, and the amount of released ALN from scaffolds was measured. The tensile test revealed that the highest tensile strength and modulus of elasticity were achieved with gelatin/PVP 1:1 ratio loaded with 5% ALN.

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P.S.III.E.7.

Processing and characterization of hybrid chitosan (Ch)/polylactic acid (PLA) composite nanofibrous scaffolds for biomedical application

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Chitosan/PLA blended solution with optimal viscosity is used to obtain electrospun micro/nanofibers with controllable mechanical and biodegradation parameters. The blended solution with polyethylene glycol (PEG) was used to control wettability and increase PCL's biocompatibility. As-spun Ch/PCL membranes were treated with 1M sodium hydroxide (NaOH) to decrease their extreme degradation in aqueous solutions and preserve their nanofibrous structure.

The fabricated nanofibers' diameter (Sample 1 – Ch/PLA and Sample 2 – Ch/PLA/PEG) was sized up to 499 nm for both samples. The test results show that the presence of PEG improves hydrophilicity (from 54,77±20,38° to 21,95±2,17°) and affects the morphology of Ch/PLA nanofibrous membranes. The amount of fibers in 200-299 nm is two times higher for samples with PEG. The addition of PEG to the electrospinning solution leads to uniform distribution of fiber diameters and porosity of chitosan membrane. The pore size of the sample's surface decreased after alkali treatment, although little difference was observed between as-spun and treated samples containing PEG (in the range of 100-199 nm^2). Moreover, the addition of PEG to the spinning solution decreased the weight loss of the electrospun membranes during the degradation experiment. Post-spinning treatment does not significantly change the wettability of both samples. After NaOH post-treatment, hybrid fibrous materials made from Ch/PLA/PEG co-solvent system demonstrate a lower degradation rate (during 1st week of the test) and optimal hydrophilic nature. Optimization of structural and degradation parameters and wettability open the persperspectives biomedical application perspective or tissue engineering constructions.

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P.S.III.E.8.

Nanostructured surface modification and characterization of titanium based materials for medical application

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Nanostructured surface of Ti-13Nb-13Zr alloy (coarse-grained (CG), and ultrafine-grained (UFG), obtained by high pressure torsion - HPT) was formed using electrochemical anodization in the 1M H_3PO_4 + NaF electrolyte, during 30, 60, 90 and 120 minutes. The scanning electron microscopy (SEM) was used to characterise the morphology of the surface, while chemical characterization of the obtained nanostructured surface was performed using energy dispersive spectroscopy (EDS). The surface modulus of elasticity and hardness before and after the surface nanostructure modification, was examined using the nanoindentation test, while the analysis of deformation and damage of the nanostructured surface after nanoindentation was performed using SEM. Cytotoxicity of the tested alloys and cell culture viability were assessed using the tetrazolium salt colorimetric test (MTT test) using mouse fibroblasts (L-929) and human lung fibroblasts (MRC-5) in liquid medium. Morphology and adhesion of cells on the surface were analysed using SEM. The obtained results indicate the strong influence of time, as a parameter of anodization, on the surface morphology. Influence of the HPT processing on the homogeneity of the nanostructured surface obtained by electrochemical anodization has also been shown. The alloys before and after the surface nanostructure modification are adequate in their biocompatibility for use in the implantology. Characterization of the titanium-based materials surface using nanoindentation showed a decrease in the values of modulus of elasticity and hardness for materials with nanostructured surface, which are close to the values of bone tissue in the human body.

P.S.III.E.9.

Electrospun poly(ε-caprolactone) nanofiber mats with cefazolin or yarrow extract powder as urinary catheter-coating materials

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In this study, urinary catheter coating materials were developed as an unexplored alternative to prevent infections caused by urinary catheterization. Nanofiber mats were fabricated from poly(ε-caprolactone) (PCL) solutions containing 20 mas% cefazolin and 10 mas% yarrow extract powder (relative to the weight of the polymer). Blend electrospinning method was applied to produce nanofiber mats. Commercially available silicone and rubber urinary catheters were coated with PCL nanofiber mats by using adhesive n-butyl-2-cyanoacrylate. Adhesion was examined in terms of adhesion strength while the antibacterial activity of the obtained coated catheters against two pathogens was evaluated. Commercial catheters coated with PCL nanofiber mats showed good mechanical stability with adhesion strength in the range 0.015-0.030 N/mm. Coated catheters showed antibacterial activity against S. aureus and E. coli. Inhibition zones indicated that the incorporation of used biologically active agents into polymer nanofibers was successful and that the relevant biological activity was maintained. Based on the obtained results, PCL nanofiber mats with cefazolin could be used as a coating for urinary catheters with pronounced antibacterial activity, while PCL nanofiber mats with yarrow extract powder could be used for the same puropose with aditional activity in terms of antioxidant and would healing properties.

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P.S.III.E.10.

The effect of liposomal pro-healing protein on the rheological properties of mucoadhesive injectable hydrogel

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More significant wounds in the mouth formed after tooth extraction or plastic surgeries are often accompanied by various microorganisms, preventing the wound closure, and prolonging the healing process. To heal these wounds, injectable mucoadhesive material is ideal for promoting wound closure and regeneration[1].

This work aims to prepare an injectable mucoadhesive thermosensitive drug delivery system enriched with pro-healing protein – stable fibroblast growth factor-2 (FGF2-STAB®) and antibacterial enzyme Lysozyme. These active ingredients are further encapsulated into liposomal nanoparticles to prevent protein-matrix interaction and hydrolytic degradation. The mucoadhesive injectable hydrogel is based on poly(lactide-co-glycolide) and poly(ethylene glycol) copolymer (PLGA-PEG-PLGA) functionalized with itaconic acid (ITA), which embodies the mucoadhesive functional groups to the polymer together with the blue-light cross-linkable double bonds[2].

Nanoliposomes with effectively encapsulated pro-healing protein have been successfully incorporated into the PLGA-PEG-PLGA/ITA hydrogel by simple mixing. The liposomes exhibit diameters around 100 nm and low polydispersity.

The focus was on investigating the rheological behaviour, especially the gel-sol transition, of the samples containing protein and encapsulated liposomal nanoparticles together and separately. The temperature ramp tests from 25 to 55 °C were performed using parallel-plate geometry at a heating rate of 0.5 °C/min for more sensitive measurement. The results were compared to those of an unfilled matrix to judge the effect caused by the present nanoparticles. It was determined that the nanoparticles tend to decrease the sol-gel transition by 1 °C, whereas the FGF2-STAB® itself tends to shift the gelation point to higher temperatures.

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1. Kaldybekov D. B. *et al.* European J. of Pharmaceutics and Biopharmaceutics. 143:24-34.
2. Vojtová L. *et al.,* EP 3097134 B1, patent. (2017).

P.S.III.E.11.

Encapsulation of bioactive proteins into thermosensitive biodegradable copolymer nanoparticles based on PLGA-PEG-PLGA

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The use of pro-healing proteins in regenerative medicine has become very widespread recently. One of the problems that can occur with protein release is the incorporation of the protein into the structure of the scaffold, their slow or no release, and their eventual loss of activity. Encapsulation of bioactive substances could prevent all of these problems. The thermosensitive copolymer based on poly(lactic acid), poly(glycolic acid), and poly(ethylene glycol) (PLGA–PEG–PLGA) was used in this work, mainly for the possibility of controlled degradation and gel formation at the human body temperature. The PLGA-PEG-PLGA copolymer consists of two hydrophobic segments (PLGA) and one hydrophilic segment (PEG) placed in the middle. Because of the amphiphilic properties, the copolymer self-assembles and physically cross-links into flower-shaped micelles. A thermostable 9-point mutant of fibroblast growth factor 2 (FGF2-STAB®, Enantis L.t.d.) was chosen as the bioactive component due to its ability to support the growth and the formation of new vessels.

In this work, core-shell spherical nanoparticles of approximately 200 nm having shell from the PLGA-PEG-PLGA copolymer (originally synthesized at CEITEC BUT[1]) and core from the incorporated FGF2-STAB® stabilized protein were prepared via a double-emulsion process. Subsequently, the nanoparticles were characterized in terms of their size, morphology, zeta potential (stability), encapsulation efficiency, and protein release. Although the encapsulation efficiency of FGF2-STAB® in the core-shell particles was pretty high (95.7%) only 25.8% of FGF2-STAB® was released from the core-shell capsules after 21 days. Therefore, further study should be provided to understand the nanoparticle-protein interactions and to enhance the releasing protein amount.

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References:

1. L. Michlovská et al. Macromol. Symp. (2010), 295, 119

P.S.III.E.12.

Composite hydrogels based on gelatin, hydroxypropyl methylcellulose and Mg-doped biphasic calcium phosphate for biomedical applications

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Hydrogels are three-dimensional hydrophilic networks of polymers capable of retaining large amounts of water or biological fluids, which makes them attractive for biomedical and pharmaceutical applications. Although various types of polymers have been investigated as hydrogels for biomedical purposes, those obtained from natural polymers have intrinsic advantages as they are abundant, cheap, biocompatible and biodegradable. Gelatin is a natural polymer that has been applied in biomedicine due to its low price, biocompatibility, and biodegradability. HPMC, a derivative of cellulose, is a hydrophilic, biodegradable, and biocompatible polymer. However, natural polymer-based hydrogels have low mechanical properties and are relatively soluble in physiological conditions, which requires creative cross-linking strategies to improve the functionality of the hydrogels. The citric acid (CA) is an inexpensive and non-toxic compound that has been proven to be an effective crosslinker for natural polymers. In addition, the incorporation of bioactive calcium phosphate particles could further improve mechanical properties and add new functionalities to the hydrogels.

In this work, we present novel composite hydrogels for biomedical applications, based on CA-crosslinked gelatin/HPMC (HPMC-G) matrix and Mg-doped biphasic calcium phosphate filler (BCP). Firstly, the HPMC-G hydrogels crosslinking conditions were optimized. Different CA concentrations, curing temperatures (140-180°C) and times (3-9 min) were applied. During the second step, the optimaly crosslinked HPMC-G hydrogel was incorporated with different amounts of BCP. BCP was obtained by calcination of Mg-doped hydroxyapatite (HA) powder synthesized by the hydrothermal method. XRD analysis confirmed that powder was constituted only of HA and beta-tricalcium phosphate. The obtained composite hydrogels were characterized by mechanical testing, FTIR, SEM, swelling behavior and drug deliverability.

P.S.III.E.13.

Antibiofilm activity of the bioactive ceramic coatings on the 3D printed TC4 scaffold

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Postoperative infections at the site of implantation are one of the main concerns in orthopedic and dental implantology, thus the subject of intensive research is the prevention of bacterial biofilm formation at the surface of the implants. The aim of this study was a coating of 3D printed macroporous TC4 scaffold with bioactive ceramics coupled with metallic ions and an evaluation of their antibiofilm activity.

The macroporous TC4 scaffold was coated with three layers of bioceramics: two silicate bioactive glasses (BAGs) and calcium hydroxyapatite doped with silver and modified with ZnO using sonochemical reaction (Zn_AgHAP). A dip-coating technique followed by annealing at optimized temperature provided uniform coverage of the scaffold.

The obtained and sintered Zn_AgHAP powder was characterized using energy-dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FT-IR), and X-ray diffraction (XRD). The surface morphology and cross-sections of the coated TC4 scaffolds were observed using scanning electron microscopy (SEM). The concentration of released metallic ions in Dulbecco's modified Eagle's medium (DMEM) at 37°C and 5% CO_2 during 2 and 10 days was analyzed using inductively coupled plasma optical emission spectrometry (ICP-OES). The formation of the biofilm at the surface of bare and coated samples after 24 h incubation period was tested using the S. oralis culture.

The EDX, FT-IR, and XRD analyses confirmed the presence of the silver dopant as well as the ZnO phase in the Zn_AgHAP powder. The SEM analysis of the coated scaffold confirmed the successful coating of the ceramic powders. The strong antibiofilm activity against S. oralis suggested the potential of the coated scaffold in further clinical practice.

P.S.III.E.14.

Multicomponent hemostatic dressing may improve bleeding stop and wound regeneration

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The presented research focuses on the preparation and characterization of a new hemostatic wound dressing made from various types of chitosan and cellulose. The dressing has the potential to stop bleeding more effectively while overcoming the limitations that remain of traditional wound dressing, such as a low hemostatic effect, a lack of antimicrobial activity, or possible allergic reactions. The fabrication of hemostatic dressing includes mixing individual blends of different materials in different ratios, followed by a freeze-drying process for two days, which produces highly porous and soft foams.

The synergy of the materials has improved the absorption capacity in comparison to the original materials. The various concentrations of carboxymethylcellulose (CMC) combined with either oxidized cellulose (OC) or chitosan significantly improved the absorption capacity compared to those of the mixtures without the addition of CMC. Moreover, hemostatic properties are also supported by CMC, but mainly when CMC exists at lower concentrations and when chitosan exists at a higher amount. Various combined multicomponent dressings have shown different effects on the clotting time. The combination of various types of cellulose and chitosan led to optimal values, where each component brings a specific feature to the hemostatic dressing. Furthermore, the hemostatic dressings are evaluated with questions that lead to their stability and morphology.

The new dressing will benefit from its multifunctionality of different hemostatic materials, which are easily available and biocompatible. The adhesion of the dressing to the tissue surface and its biodegradation after the required time are believed to greatly accelerate blood stopping and improve wound healing.

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P.S.III.E.15.

Quantum-informational macrophenomena in biomedicine and holistic psychosomatics: quantum-holographic framework

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The Hopfield-like quantum-holographic framework for macroscopic quantum phenomena in biomolecular folding, integrative medicine, transpersonal psychology, and holistic psychosomatics is outlined. This might have significant implications for better understanding of quantum-holographic feedback control mechanisms of morphogenesis, and healing boundary conditions in acupuncture-based and consciousness-based holistic psychosomatics.

P.S.III.E.16.

Chitosan/tripolyphosphate capsule-forming gelation monitored via light scattering curves: Determination of particle forming phases and their effect on physico-chemical and biological parameters

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Chitosan (Chit) is a versatile polymer utilized for various applications in biomedicine. One notable chitosan property is its ability to form nano- to micro-sized capsules via ionic gelation using sodium tripolyphosphate (TPP) as a crosslinker. These capsules have proven their usefulness as drug-delivery systems. The preparation process is facile in theory. However, in practice, the preparation reproducibility in-between laboratories remains challenging, due to the varying nature of chitosan. Two important parameters affecting how the chitosan will act in a chemical setting - degree of deacetylation and molecular weight – are often provided by the supplier in wide ranges and even different batches of the same supplier may have different physico-chemical properties.
In this work, we introduce a novel method using scattering light detected by inexpensive, easily available ultraviolet-visible (UV/VIS) instrumentation to observe Chit/TPP capsule formation. Recorded light scattering curves (SC) depict the relation between turbidity and Chit/TPP ratio. We show, that from these SCs, we can infer the volumes of TPP needed to achieve nanoparticles without aggregation for low molecular weight chitosan. We thus made the Chit/TPP capsule-forming gelation more reproducible in-between laboratories for more controlled encapsulation of antibacterial agents.

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WRTCS
Poster Presentations

W.P.S.F.1.

Biodegradable coatings improved mechanical properties and bioactivity of sintered calcium phosphate scaffolds

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Macro-porous bioactive and biocompatible ceramic materials were intensively developed in last decades in order to enable controlled environment and volume for new bone tissue formation in bioreactors or in vivo. Calcium phosphate nanoparticles doped with different ions, due to the chemical and morphological similarity with human hard tissue minerals, are good basis for scaffold processing. The aim of this study was the optimization of parameters for the processing of bioceramic scaffold based on calcium phosphates simultaneously doped with different cations and anions and further improvement of their mechanical properties and bioactivity by forming of different coatings based on gelatin or chitosan and bioactive nanostructured ceramic fillers. Meso-porous hydroxyapatite nanoparticles doped with magnesium and strontium in combination with different ions with potential antimicrobial activity were synthesized hydrothermally and used as main inorganic phase for scaffold forming by sponge replica method. Different combinations of dopants affected the stabilization of different ratios of bioactive α- and β-tricalcium phosphate phases during the sintering. Soft biodegradable coatings showed great potential for neutralizing the consequences of imperfect sintering and simultaneous improvements of the mechanical properties and bioactivity of biocompatible macro-porous scaffolds with residual antimicrobial potential.

W.P.S.F.2.

Composite scaffolds based on magnesium doped hydroxyapatite and mesoporous nanosized bioactive glass

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Bioceramic materials based on hydroxyapatite (HAP) are widely used as scaffolding material for bone tissue engineering due to their similarity with inorganic part of human bones. Magnesium ion as a dopant in hydroxyapatite was previously shown to improve mechanical properties of HAP based materials, as well as to improve osteoblasts cell proliferation, and induce angiogenesis which stimulate the bone regeneration.

Mesoporous bioactive glass nanoparticles (MBGNPs) present the latest generation of the sol-gel glasses, having high surface area and large pore volume that allow the loading of drugs (anti-inflammatory, anti-osteoporotic, anti-cancer etc.) and growth factors for stimulating cell differentiation and proliferation. MBGNPs are highly soluble and more bioactive compared to the hydroxyapatite. However, their high porosity leads to poor mechanical properties of pure MBGNP-based scaffolds.

Here we propose composite scaffolds based on magnesium doped hydroxyapatite and MBGNPs obtained by a modified microemulsion-assisted sol-gel synthesis for bone tissue engineering application. Hydrothermally obtained hydroxyapatite doped with 5 mol. % of magnesium ions was calcinated at 1000 °C and mixed with 10-20 wt.% MBGNPs to form composite scaffolds by sponge replica method. The addition of MBGNPs has the influence on the sinterability, mechanical properties and bioactivity of the scaffolds

W.P.S.F.3.

Sinterability study of the zeolite-based porous ceramics for water filter application

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Sinterability and structure of zeolite-based porous ceramics were investigated in order to prepare robust ceramics for water filter application. Dry powders of zeolite, kaoline, bentonite and coal/starch were mixed to form powder precursors. Effects of the composition and preparation procedure on the porosity, density, defects and mechanical properties were examined. In order to obtain optimal properties, amounts of kaoline and bentonite were varied together with pore-forming coal and corn strach. Sintered porous ceramics showed promising porous and machanical properties necessary for large scale water filter application.

W.P.S.F.4.

Influence of aluminium anodizing wastes on Flash sintering of alumina

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There is a need for innovative low–carbon technologies to decarbonise Europe and support its transition to climate neutrality. In the ceramic industry, a large part of CO2 emitted is generated in sintering related to the use of high temperatures (800 – 2000 ºC) and prolonged times (h). So, energy reduction is mandatory and one alternative is Flash sintering. Herein, an electric field is applied to the material and, for a specific combination of electric field and heating environment, the material begins to conduct and dissipate heat by Joule effect, densifying in seconds. Alumina, Al2O3, is, nowadays, one of the most important technical ceramics, however, due to its electrical insulator character, Flash does not occur. The present work aims to study the influence of aluminium anodizing wastes on the Flash sintering of alumina. The wastes were pre-treated (900 ºC during 2 h and sieved at 65 μm) and mixed with alumina (planeraty mill - 5 h and 200 rpm) with different proportions: 0, 10, 20 and 40 wt.%. The used aluminium wastes are mainly composed by 64.3 wt.% of Al2O3, 23.4 wt.% of SO3 and 8.7 wt.%, of Na2O. Pressed dried pellets were sintering: a) conventionally – 1550 ºC, for 2 h, with a heating rate of 5 ºC/min; b) by Flash – electric field of 800 V/cm, current limit of 2 mA/mm2 and Flash of 60 s. Our results showed that adition of aluminium wastes allows Flash of alumina to occur. We observed that the Flash temperature decreases with the increase of the waste content, from 1120 ºC to 485 ºC for 10 and 40 wt.% of waste, respectively. Regarding the densification, the increase of the waste content decreases the densification of the material. However, the speciemens sintered by Flash have a higher densification than the ones sintered conventionally, *i.e.* 94 vs 70 % with 20 wt.% of waste. Micrographs of the Flash sintered specimens suggest that diffusion of sodium ions, that come from the residue, may play a role in the conduction behaviour. So, aluminium anodizing wastes allow Flash of alumina to occur with a reduction of up to 800 ºC in the sintering temperature, together with a decrease in the sintering time - from 2 h to 60 s. Hence, our work contributes to the circular economy due to the use of an industrial waste and is aligned with need of low–carbon technologies to decarbonise Europe due to the energy reduction achieved by Flash sintering

Virtual Presentations

VIRTUAL OFFLINE ORAL PRESENTATIONS

V.O.S.1.

Enhanced superconductivity in nanoscale amorphous films

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Due to robust superconducting (S) properties, ease of growth, high critical temperatures (T_c), extraordinary phase homogeneity, and little requirements on the substrate layer, amorphous superconductors have become attractive candidate materials for superconducting micro- and nanoscale devices, in particular, nanowire single photon detectors, offering low noise, highest count rates, and improved spectral sensitivity. While applications of crystalline S films have been studied extensively, the search for useful amorphous counterparts is relatively rare.

This study focuses on the properties of germanium- and silicon-based amorphous α-MoGe and α-MoSi nm-thick layers grown by magnetron sputtering. We have examined how composition and growth conditions affect nanofilm properties. For thicknesses of several tens nm, we report maximum T_c‘s about 6 K when the films were deposited on commercial silicon substrates at room temperature and without extra substrate heating. The transition temperature and amorphous character could be improved by cooling of the substrate during growth, which inhibits formation of a crystalline phase. In this case, α-MoGe and α-MoSi layers exhibited T_c‘s slightly above 7 K. X-ray diffraction and transmission electron microscopy studies confirm the absence of long range order. The area, in which these films have not yet received proper applications, is S-I-S Josephson junctions based on amorphous S materials and ~1 nm thick insulating (I) interlayer. It was shown [1] that such junctions demonstrate high homogeneity of their tunneling properties due to the uniformity of the surface morphology in Mo-based amorphous S films.

We argue that superconductivity in highly disordered nm-thick films is strongly coupled, with the ratio of the superconducting gap Δ to the critical temperature T_c much larger than the conventional BCS prediction, $2\Delta/k_BT_c >> 3.528$. In this case, we should follow Eliashberg theory of phonon-mediated superconductivity. Within its framework, one can understand the effect of structural disorder by taking into account the presence of a so-called boson peak naturally arisen from the competition between propagation of elastic phononic waves and their viscous damping.

1. I. P. Nevirkovets *et al. Supercond. Sci. Technol.* **35** 035008 (2022)

V.O.S.2.

Phase structure, microstructure and mechanical properties of high-entropy alloys $Ta_{29-x}Ti_{40}V_xZr_{26}Al_5$ (x = 0, 5, 10, 15, 20, 29)

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Refractory multicomponent concentrated alloys (RMCA) have high strength characteristics in a wide temperature range, which makes them perspective for various applications. Unfortunately, most of these alloys have low plasticity during tensile tests at room temperature, which creates additional technological difficulties in product manufacturing. High plasticity was recently observed for alloy $Ta_{29-x}Ti_{40}V_xZr_{26}Al_5$, which is also of interest due to its unusual mechanical behavior. The purpose of this work was to study the patterns of changes in the structure and properties of alloys of this system with a change in the relative concentration of tantalum and vanadium - elements with the same concentration of valence electrons, but significantly different atomic radii and melting temperatures.

The ingots of $Ta_{29-x}Ti_{40}V_xZr_{26}Al_5$ alloys with x = 0, 5, 10, 15, 20, 29 (at.%) were produced by arc melting. The microstructure of as-cast samples was studied using a metallographic Olympus GX51 and scanning JSM 7001F (equipped with a system for (EDS) INCA ENERGY 350) microscopes. XRD patterns of the as-cast specimens were recorded using «DRON-4-07» diffractometer.

Investigation of alloys' phase composition shown that in the absence of vanadium (x = 0), the alloy has single-phase bcc structure with lattice parameter a = 3,309Å. With maximum vanadium concentration (x = 29) there are two identified bcc phases. The lattice parameter of bcc1 phase is a = 3,296Å, and lattice parameter of bcc2 phase is a = 3,384Å. Metallographic investigations have shown that all the alloys have a similar microstructure, characterized by the presence of grains, within which a dendritic liquation is observed. Local analysis has shown that the content of elements in dendrites and interdendritic areas differs noticeably: Ti and V are distributed uniformly, whereas Ta significantly enriches dendrites and Zr and Al are located in the interdendritic areas. So, two bcc "phases" in some alloys are connected with dendritic and interdendritic areas.

Criteria, based on the thermodynamic parameters of the binary alloys, melting temperatures of the components, geometric and electronic characteristics of individual atoms were used to calculate the possible phase-structural state of the alloys; results were compared with experimental data.

V.O.S.3.

Antitumor effect of complexes based on redox-active inorganic nanoparticles with menadione

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Complexes of redox-active NPs /menadione were used in combination with vitamin C to assess antitumor efficacy and generation of reactive oxygen species in the L929 mouse fibrosarcoma model within a week and thereafter.

Complexes of extra-small (1-2 nm) inorganic orthovanadate (GdYVO4/Eu3+) NPs or cerium oxide (CeO2) NPs with menadione (M) were obtained and characterized. L929 mouse fibrosarcoma cells (~ 2 x 10^4 cells/ml) were incubated in DMEM/F12 with 3% FBS in humidified atmosphere with 5% CO2 within a week in the presence of the complexes (NPs/M - 10 µg/ml/20 µmol) and with or without vitamin C (2-4 mM). Cells were sampled for MTT-test each 72 h after introduction of the complexes into the medium. In addition, after treatment cells incubated without complexes for the next 72 h to analyze cell recovering. Cells vitality was also evaluated by microfluorimetry with propidium iodide (PI); the superoxide generation inside the cells was visualized with dihydroethidium (DHE) fluorescence using an inverted epifluorescence microscope (IX-71; Olympus, Tokyo, Japan).

CeO2 NPs had no toxic effect for any of used concentration unlike orthovanadate NPs that decreased the cell viability at concentrations starting from 25µg/ml. However, when NPs-based complexes were used, a significant suppressive effect was observed. The best result was observed for CeO2 NPs /M complexes in the presence of vitamin C (0.507 ±0.042RU to control values in 24h after the first application, 0.099±0.013 RU in 72h after the first application, 0.071±0.022 RU in 72h after the second application, and 0.173±0.001 RU – thereafter effect). Under these conditions, within 24 h exposition with the both complexes (with about 25% higher effectiveness of CeO2 NPs/M) increased a generation of superoxide radicals according to the microfluorimetry of the DHE probe in cells. This is consistent with the literature data indicating the mitochondrial generation of the superoxide radicals as a result of the interaction of the components used in the system. In conclusion, redox-active NPs/M complexes and vitamin C can be used as malignant cell destructors due to synergism of redox-active components.

V.O.S.4.

RE-doped nanoceria with pre-determined luminescent and redox properties

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Cerium oxide nanocrystals are widely discussed now due to their unique physical and biological properties. Variable valence of cerium ions (Ce^{3+}/Ce^{4+}) opens the way for ROS scavenging by ceria nanocrystals, while high anionic conductivity in cerium oxide bulk materials and nanocrystals makes these materials perspective for development of solid oxide fuel cells. In our study we have used the methods of luminescent spectroscopy we have revealed the features of formation and redox action of RE-doped colloidal nanoceria. RE-doped nanocrystals were obtained using the method of co-precipitiation of RE chlorides and novel method of cation exchange leading to formation of RE^{3+}-doped nanoceria in the presence of RE^{3+} ions in undoped nanoceria colloids. The dynamics of increase of RE^{3+} luminescence intensity during cation exchange at different conditions (UV irradiation, H_2O_2 addition) reveals a key role of Ce^{3+}-Vo-Ce^{3+} complexes in the processes of incorporation of RE^{3+} ions into ceria nanoparticles.

Preferential occurrence of Ce^{3+} ions in the form of Ce^{3+}-V_o-Ce^{3+} complexes prevents formation of hydroxyl radicals during HP decomposition by colloidal nanoceria, which is one of the key factors of enzyme-like action of nanoceria. At the same time, for CeO_2: Re^{3+} (Re = Y, Eu) nanoparticles HP interaction with Ce^{3+}-V_o-Re^{3+} complexes occurs preferentially via Fenton reaction involving formation of hydroxyl radicals and hampering HP decomposition. So, the variation of the type of doped ions opens the possibility to change both the luminescence properties and efficiency of redox activity of nanoceria.

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V.O.S.5.

A new highly developed titanate surface layer on titanium can support attachment and proliferation of human cells

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Titanium (Ti) implants are widely used in dentistry and in orthopedic practice. Still, Ti surface often requires additional modifications for better osseointegration and tissue connectivity. Both morphology and chemical composition of the surface play important roles in ensuring the long term stability of the implants. We have developed a combined protocol to obtain highly developed, porous and hydrophilic surfaces on the commercially pure Ti. We then aimed at investigating biomedical properties of the new Ti surfaces.

The surface layers were obtained on Ti longitudinally truncated cylinder specimens with 3.1x8 mm upper/bottom faces via consecutive treatments by polishing, sandblasting, acid etching and NaOH curation. Then, the specimens were immersed in simulated body fluid (SBF) to prime deposition of calcium phosphates. Human umbilical cord mesenchymal stem cells were plated and cell attachment and proliferation were evaluated by resazurin reduction assay (RR), fluorescence microscopy (FM) and scanning electron microscopy (SEM).

We observed that all the surfaces were able to support attachment and proliferation of the cells. We did not detect significant differences in the RR assay, although the surface after SBF immersion showed a trend to better support the attachment and proliferation of the cells.

The FM revealed that the cells attached and grew on both protruding and sunken niches of the surfaces. The cells looked less flat and uniform on the developed surfaces than on the even polished surfaces, which suggests that the cells were able to attach to the sides of the microgrooves and microridges. This was confirmed by the fact that the cells on the developed surfaces were in various focal planes. The SEM imaging corroborated that on the developed surfaces the cells grew in various planes and retained various shapes; and that the cells looked more flattered on the even polished surface. We concluded that the designed combined treatment protocol for Ti surfaces could be employed in the development of Ti implants with increased osteoconductive capacity. These results call for continuation of the studies with specimens with larger surface area and with specialized osteogenic cell types.

OFFLINE POSTER PRESENTATION

V.P.S.1.

Vortex-matter manipulation in nm-thin type-II superconducting layers

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Tuning the critical current in type-II superconducting layers plays a substantial role in the performance of related superconducting devices. The traditional way to avoid deterioration of transport characteristics is to immobilize magnetic flux lines by natural or artificially introduced pinning sites *inside* the nanolayer. An alternative approach can be realized in planar superconductor/ferromagnet bi- or tri-layers where the nm-thin films are placed in close proximity. An interaction between Abrikosov vortices and the magnetization texture in a ferromagnetic layer provides a pinning potential for them. The effect, called *magnetic pinning*, wa studied in coupled metallic multilayers based on different combinations of a weak diluted ferromagnetic (NiCu) and superconducting (NbN) films. The latter include those with an ultra-thin insulating interlayer (AlN) between the two strips, thus cutting off short-range proximity effect. Measurements of the temperature effect on current-voltage curves for samples with different stacking order of the films have been performed. In some configurations, we found a strong growth of the critical current followed by moderate changes in the critical temperature or their complete absence. Related analysis shows that the underlying mechanism of the supercurrent growth in the NbN film is indeed *magnetic vortex pinning* that can be enhanced further through magnetization engineering enabling optimization of the pinning strength in desired field ranges.

The second part of the work was devoted to the passage of a charge current through a heavy non-magnetic metal (Pt) that causes a ransverse spin current because of the asymmetric spin scattering mediated by spin-orbit coupling, the well-known spin-Hall effect. At the interface between NbN and Pt nm-thin layers which breaks the translational symmetry of the heterostructure, spin accumulates on a length scale of the spin-flip diffusion length. Changes in the critical temperature and the supercurrent parallel to the NbN/Pt interface are found to be well reproduced by a concerned phenomenological model.

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