European CMetAC

ECMetAC Newsletter No. 12

January 2024

Dear colleagues of the ECMetAC network,

On behalf of the board of directors, we wish you a Happy New Year 2024! We hope that this new year will bring you great success in your research, fruitful interactions and serenity in your personal life.

Winter had finally arrived and we already had a glimpse of snowfalls during our last ECMetAC Days meeting in Kranjska Gora in Slovenia. Organised by Prof. Janez Dolinšek and his team in a calm and beautiful place, all ingredients were united to generate friendly discussions among the participants and to sit down and plan future collaborations for the coming year. During the event, it was announced that our colleagues, Assoc. Prof. Dr. Mario Novak and Dr. Petar Popčević, will co-host the next ECMetAC Days 2024 which should take place from 25th till 28th November 2024 in Zagreb. It will be 10 years since our last ECMetAC meeting took place in the Croatian capital.
As every year, dedicated workshops will be organised by Research and Activity Domains Leaders, and we encourage you to visit on a regular basis our website to keep up to date with the latest news and meetings. In Autumn, a Euroschool entitled “Advanced Synthesis and Characterisation” will be organised by Dr. M. Heggen at the Ernst Ruska Centre in Jülich, gathering world experts in this topic.
Until then we wish you all a good start for this new year and we are looking forward to welcoming you in 2024 in Jülich and Zagreb.

Best wishes,

Julian Ledieu, Ronan McGrath,
Marc Armbrüster, Jean-Pierre Celis
and Émilie Gaudry

Looking back at ECMetAC Days 2023 in Kranjska Gora

ECMetAC Days 2023 meeting organized by the European Network of European Integrated Centre for the Development of Metallic Alloys & Compounds was held in Kranjska Gora in Slovenia at Hotel Kompas from Nov. 27th to Nov. 30th, 2023. This time the local organizing institutions were the Jožef Stefan Institute from Ljubljana and the University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia. It was already the second time that Slovenia hosted this event after ten years. During the meeting, 67 scientists of 10 European countries represented 17 institutions. Altogether they delivered 33 oral presentations and 23 posters on the following conference topics: 1. Formation, growth and phase stability; 2. Structural and chemical characterization; 3. Physical, chemical and mechanical properties; 4. Surfaces and thin films; 5. Intermetallics for catalysis; 6. Complex metallic alloys, high-entropy alloys, metallic glasses, clathrate compounds, etc.; 7. Thermoelectrics, magnetocalorics; 8. Correlated-electron intermetallic alloys and compounds; 9. Applications and 10. New frontiers in metallic materials. The conference was opened by Dr. Magdalena Wencka (Jožef Stefan Institute, Ljubljana, Slovenia) who represented the Local Organizing Committee and the President of our network Dr. Julian Ledieu (Institut Jean Lamour, Université de Lorraine, France). The scientific part of the conference was opened by Prof. Peter Gille (Ludwig-Maximilians-Universität München, Germany) who presented his new achievements “Single crystal growth of In_7Pd_3: A case study”. During our conference, special attention was paid to our young scientists who

provided altogether 17 oral presentations and 15 posters. During the ECMetAC Days 2023, four laureates of awards dedicated to young researchers were selected. More about this issue will be presented in a separate text. As every year, during the ECMetAC Days 2023 especially important were formal and informal discussions. This time our venue was a snowy alpine town of Kranjska Gora, located only 8 km from the ski jumping hill Planica. We all could enjoy a friendly atmosphere and good Slovenian cuisines and wine. Our annual conference was summarized by Dr. Julian Ledieu and Prof. Janez Dolinšek (Jožef Stefan Institute, Ljubljana, Slovenia), the conference Chair. The Local Organizing Committee (in alphabetic order) consisted of Prof. Janez Dolinšek, Dr. Andreja Jelen, Assist. Prof. Dr. Primož Koželj, Dr. Jože Luzar, Peter Mihor, MSc. Julia Petrović, Dr. Magdalena Wencka and Assist. Prof. Dr. Stanislav Vrtnik.

Conference group photo

Written by:
Dr. Magdalena Wencka
Jožef Stefan Institute, Ljubljana, Slovenia

RAD Equality, Diversity and Inclusion in Material Science

The ECMetAC Days 2023 main event was preceded by a Workshop “Innovative Researcher: End-User Approach for Scientific Project Designing”, dedicated to young and mature members of our network. As always, at the beginning we trained how to give an inclusive and positive feedback. Then we learned about a Design-Thinking approach in general. To understand an end-user approach, we needed to create a person with whom we empathized imagining and defining her/his needs. We created empathy maps that helped

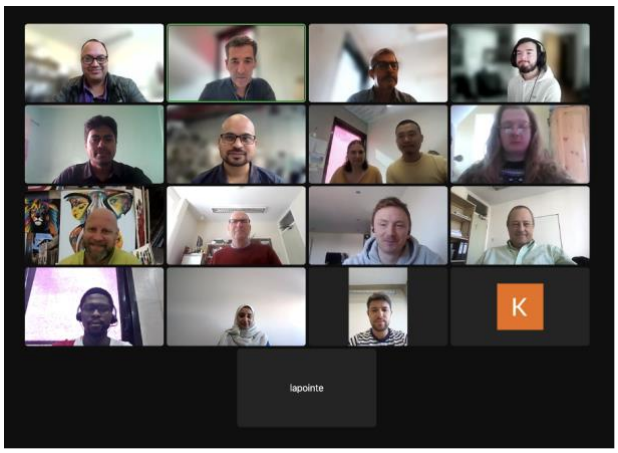
us to make real and personized goals. Then we could bind them with our ideas that we worked with like a personized “food application”. Our effort was supported by MSc. Matjaž Malok from the Jožef Stefan Institute in Ljubljana (Slovenia) who showed us a real end-user approach dedicated to his scientific project designing. Currently he works on the NANOTUL - a miniaturized sensor for counting nanoparticles and droplets in the air. Our guest showed us his presentation about the sensor entitled “Development of miniaturized, portable instrument for detection of respiratory droplets”. Having an interview with Matjaž, we could trace an evolution of the end-user approach as the sensor was originally invented thinking about a single-user who needs to test on the presence of microbes in exhaled air and evolved to a hospital nurse as an operator. Here, especially

valuable was the interview with our young innovator. The Workshop was conceptualized and guided by Dr. Magdalena Wencka.

RAD Atomic Scale Surfaces and Functional Coatings, Thin Films, and Interfaces

The Liverpool Quasicrystal Group organized on 21st September 2023 a one-day workshop on the surface properties of intermetallic compounds. This event was part of the annual activities of the Research and Activity Domain on the Atomic Scale Surfaces and Functional Coatings, Thin Films, and Interfaces (ASCI) of ECMetAC. Dr Hem Raj Sharma and Prof Ronan McGrath from the University of Liverpool serve as the spokesperson for the ECMetAC

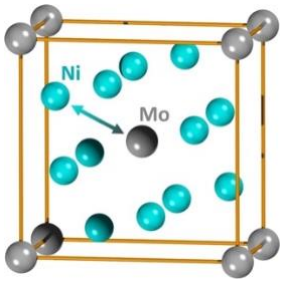
ASCI RAD, and the Secretary-General of ECMetAC, respectively.
The workshop covered the surface properties of a wide range of intermetallic compounds, including quasicrystals, shape memory alloys, high-entropy alloys, and intermetallic catalysts. The workshop was attended by researchers from various European institutes within ECMetAC, as well as from Tribhuvan University and Tel Aviv University



Participants of the online workshop

RAD Materials for Catalysis

Crystal Structure of and Chemical Bonding in MoNi4



Single-phase MoNi4 was prepared by multi-step long-term thermal treatment. The crystal structure was re-evaluated by single-crystal and powder X-ray as well as powder neutron diffraction resulting in space group I4/m and lattice parameters of a=5.7300(6) Å and c=3.5649(6) Å. Despite the formation by complex solid-state reaction, the crystal structure of MoNi4 is fully ordered, whereby the single-crystalline micro-domains feature sizes below 20 µm. The ordering is supported by the strong charge transfer from Mo to Ni hindering the formation of anti-sites. Two types of four-atomic bonds stabilize the crystal structure. The bonding is isotropic, allowing cleavage in different crystallographic directions with mostly nickel atoms on the surface. In combination with the negative effective charge of the nickel species, this enables to shed more light on the behaviour of MoNi4 in catalytic processes.

https://doi.org/10.1002/zaac.202300145

Marc Armbrüster, Leonard Rößner, Yurii Prots, Lev Akselrud, Markus König, Denis Sheptyakov, and Yuri Grin.

Awards

Award Ceremony - ECMetAC Days 2023

Our Laureates (first raw from the right): Priyanka Reddy (University of Zagreb, Zagreb, Croatia), Ahowd Alfahad (University of Liverpool, Liverpool, UK), Federico Mazza |(Vienna University of Technology, Vienna, Austria) and Michael Sannemo (Stockholm University, Stockholm, Sweden) and Dr. Julian Ledieu – President of the ECMetAC and (second raw from the right): Prof. Janez Dolinšek (Jožef Stefan Institute, Ljubljana, Slovenia) – the Conference Chair and the Members of the ECMetAC Young Scientists Oral and Poster Presentation Award Committee: Dr Magdalena Wencka (Jožef Stefan Institute, Ljubljana, Slovenia), Prof. Marc Armbrüster (Chemnitz University of Technology, Chemnitz, Germany) and Prof. Ronan McGrath (University of Liverpool, Liverpool, UK).

ECMetAC Young Scientists Oral Presentation Award: Ahowd Yousef Alfahad

The University of Liverpool (SSRC, UK)

"Surface structure of In_3Ni_2 intermetallic compound"

Ahowd Alfahad is currently a PhD student in her 3rd year at the University of Liverpool within the surface science research group. Her general topic of the talk was dedicated to study surface structure and chemical composition of intermetallic compound In_3Ni_2 under ultra-high vacuum system by X-Ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM).

Study of geometrical structure and chemical properties is important to understanding the catalytic reaction mechanism. My next step will be investigating how exposing pure oxygen to In_3Ni_2 surface will affect the chemical composition of the surface.

I feel interested to study this surface because there is no existing research on the surface structure of In_3Ni_2 under UHV conditions. This work is a collaboration with the Institut Jean Lamour, Université de Lorraine

In my free time, I usually travel with my friends to a new city in the UK because I like to discover a new place and culture.

ECMetAC Young Scientists Oral

Presentation Award: Federico Mazza

Vienna University of Technology (Vienna, Austria)

"Scrutinizing the phonon Kondo effect in intermetallic clathrates"

Federico Mazza is a PhD student in Prof. Silke Bühler-Paschen's group for Solid State Physics and Quantum Materials. His work mainly focuses on experimental techniques conducted in large scale facilities, such as nuclear reactors and particle accelerators where it is possible to investigate physical phenomena non-accessible to conventional measurement techniques usually conducted in university labs. The research topics vary from quantum criticality, quantum phase transitions and entanglement witnesses in Heavy-Fermions metals to phononic studies on type-I clathrates, in order to shed light on those effects that cannot be explained with simple ab-initio theoretical calculations. The best part of the job is essentially the many travels involved and the networking with other researchers. I really enjoy to feel and to be part of a large community where science and discovery are common goals, which eventually lead to several collaborations as well as future endeavors that bring people together.

In my free time I generally like outdoor group activities, even though recently I have taken online classes for programming (in C++ and blueprint) with the long-term goal of making my own video game using Unreal Engine 5. In addition, I frequently go to the gym since it gives me a bit of structure in my daily routine. One of my biggest wishes is to have a pet raccoon one day!

ECMetAC Young Scientists Poster Presentation Award: Priyanka Reddy

Department of Physics, Faculty of Science, University of Zagreb (Croatia)

"Surprising magnetism of murunskite"

Priyanka Reddy, a fourth-year Ph.D. student at the University of Zagreb, Faculty of Science, Department of Physics, is delighted to be recognized by ECMetAC for her outstanding work. This marks her second award from ECMetAC, an achievement that she finds particularly exciting and personally rewarding.

Priyanka's primary research focuses on murunskite ($K_2FeCu_3S_4$) and related compounds, such as $K_2FeCu_3Q_4$ (Q= Se and Te). This work, conceived by Prof. Sunko and her Ph.D. supervisor Prof. Barišić, aims to introduce this new class of materials to bridge the gap between the two well-known high-temperature superconducting families, cuprates, and iron-pnictides. Murunskite is an insulator just like most parent compounds of cuprates, however, it is structurally identical to metallic iron-pnictides. All three classes of compounds exhibit antiferromagnetic-like ordering upon decreasing temperature. The main goal is to explore the substitution of different elements in the pursuit of superconductivity within this family.

At ECMetAC, Priyanka reported novel results on the murunskite parent compound, obtained in collaboration with Dr. Davor Tolj. Namely, at the critical temperature of about 100 K, murunskite transitions from a paramagnetic to an antiferromagnetic-like state with a nearly commensurate quarter-zone wave vector. The only chemically identifiable magnetic atoms are iron, randomly distributed over one-quarter of available crystallographic sites in 2D planes. The remainder are occupied by closed-shell, and thus magnetically inactive, copper. This finding presents a fascinating conundrum – how does robust order emerge from such disorder? Moreover, the irons exhibit a mixed valence

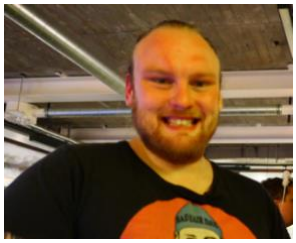
state, with some in the Fe 3+ oxidation state, while the majority are in the 2+ oxidation state, adding to the already present (stoichiometric) randomness of iron.

Priyanka is looking forward to contributing to the organization of ECMetAC 2024, which will be hosted at her home university. Beyond her academic pursuits, Priyanka Reddy is also a proud member of Croatia's first women's international cricket team, and has recently ventured into the world of stand-up comedy.

ECMetAC Young Scientists Poster Presentation Award: Michael Sannemo Targama

Department of Materials & Environmental Chemistry Stockholms Universitet (Stockholm, Sweden)

“Crystal growth and thermal characterization of intermetallic compounds in the Yb-Au-Sn system”



Michael Sannemo Targama is a PhD student at the Stockholm University. He has a love affair with transition metals and my research focuses on mainly exploratory synthesis and characterization of intermetallics with rare-earths, gold and metalloids. Exploring the wonderful intricacies of intermetallics and inorganic materials in general is what drives his curiosity and dedication to contributing to the field.

Outside the lab, Michael partakes in more hobbies than he could ever hope to count. Whether it's crafting, playing guitar, woodworking, 3D-printing, brewing beer, programming or gaming, this unwieldly tangle of interests complements his academic endeavours nicely. He finds that his handiness and continuous crafting bring him peace of mind and more often than not helps him at work when instruments are being rebellious.

European CMetAC

Upcoming Events

ECMetAC Euroschool 2024 in Jülich 3rd till 8th November 2024

We cordially invite you to join us at the *ECMetAC Euroschool 2024: Advances Synthesis and Characterization* which will be held at the Ernst Ruska-Centre, Forschungszentrum Jülich on 3.-8.11.2024. This is an annual event organised by the European Integrated Centre for the Development of New Metallic Alloys and Compounds (ECMetAC). The school will focus on synthesis and characterization of materials in various forms, in particular using microscopy techniques. It will offer lectures by experts in the field revising progress to date and prospect ahead, and tutorials/hands-on trainings. The target audience of the event is Ph.D. students, doctorate fellows, and people new to the field of material science and physics. Young researchers will have an opportunity to establish a network among them.

Related Upcoming Events

APERIODIC 2024

The 11th International Conference on Aperiodic Crystals

24th -28th June 2024, Caen Normandy (France)

Aperiodic is the latest in a series of conferences supported by the Commission on Aperiodic Crystals (CAC) of the International Union of Crystallography (IUCr). These conferences are held essentially every three years, with the most recent meetings in Sapporo (Japan, 2022), Ames Iowa (the USA, 2018), Prague (Czech Republic, 2015), Cairns (Australia, 2012), Liverpool (UK, 2009), Zao (Japan, 2006), Belo Horizonte (Brazil, 2003), Nijmegen (The Netherlands, 2000).

Aperiodic XI provides an excellent opportunity to learn about new results in the field of aperiodic crystals, including incommensurately modulated phases, composite crystals, and quasicrystals. Aperiodic 2024 also offers an opportunity for researchers working in these fields to exchange ideas and encourage collaborations with other research groups, hence promoting material science and engineering.

Aperiodic 2024 (11th International Conference on Aperiodic Crystals) will be held in Michel de Boûard Amphitheatre (right photo) campus 1 at University of Caen Normandy, Caen, France.

ECMetAC Days 2024

The next ECMetAC Days 2024 will be jointly organised by Assoc. Prof. Dr. M. Novak and Dr. P. Popčević respectively from the Faculty of Science and the Institute of Physics from 25th till 28th November 2024 in Zagreb. It has been ten years since the last organisation of this event in Croatia. We are looking forward to welcoming you to ECMetAC Days 2024. More information will be available on our website soon.

ECM34

ECM34 PADOVA 2024 26-30 August

The next ECM conference will take place in Padova from 26th till 31st August 2024. The abstract submission and registration open on 30th January 2024. More information can be found here.

SCTE 2024 - International Conference on Solid Compounds of Transition Elements

The next SCTE conference will be held in Prague from 17th till 21st June 2024. SCTE conferences allow every 2 years to report new discoveries in chemistry and solid-state physics of compounds and materials based on d and f electron elements. Several axes are discussed such as the crystal structure, the chemical bond as well as the various and varied physical properties (magnetic, transport and spectroscopic) of various families of intermetallics (and derivatives such as: hydrides, borides, carbides, silicides, pnictides, chalcogenides, oxides, halides).

For more details, please visit the website.

18th ICC – International Congress on Catalysis

The 18th International Congress on Catalysis, will be held in Lyon on July 14-19, 2024.
More information available on the website.

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