

European CMetAC

ECMetAC Newsletter No. 3

January 2021

Dear colleagues of the ECMetAC network,

Best wishes for 2021 from the Executive Board!

Last year, we had to reinvent the way we work as a consortium. This led to the successful organisation of the ECMetAC Days 2020. This year will offer new perspectives for our research activities and interactions.

Soon, we will meet again on site somewhere in Europe. We will collect our conference badges and move to the Welcome party to find friendly and familiar faces and to meet new members. On-site events are vital for our research works and are essential to continue developing new collaborations among our members, which *in fine* transform into better Science. It also leads to fantastic opportunities on many levels from career perspectives to the discovery of new cultures and history. These scientific meetings are crucial for those young scientists waiting to discover the atmosphere of conferences and this unforgettable moment of delivering your first oral presentation in front of a large audience.

Until the situation improves, scientific exchanges will continue remotely. This year, several events are already planned by ECMetAC including workshops organised by the Research and Activity Domain (RAD) speakers, an online Euroschool organised by the Liverpool group and the ECMetAC Days 2021 that we hope will take place in Split next December. More details about these events are given later in the newsletter. Don't forget that news will be regularly posted on our website <https://ecmetac.eu/> and we encourage you to send us your latest results, positions

open or others relevant information for our members.

We are looking forward to seeing you soon!

Stay healthy and best wishes.

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

A new Speaker for the Research and Activity Domain in Catalysis

“Chemistry journey” of Iryna started at the *Ivan Franko National University of Lviv* (Ukraine) in 2001 as an enthusiastic and active student of the Department of Chemistry. Inspired by chemistry study and further eager by engaging research during PhD time, her scientific interest on intermetallic compounds was growing every day. Insight into the “world” of crystal structures and phase equilibria in ternary systems of Ga and Sb with transition- and rare-earth metals during PhD was accompanied with an excellent opportunity of DAAD scholarship at *Max-Planck-Institut für Chemische Physik fester Stoffe* in 2008-2009. This explores a vision on methods, techniques and approaches for study of intermetallic compounds and adds even more taste and passion to deal with



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scientific challenges, puzzling scientific questions and search for optimal solutions. The year 2011 starts from the successful defense of PhD thesis in Lviv and ends with the movement from native town to Dresden. The postdoc period in the group of Prof. Juri Grin offers another view on intermetallic compounds and their possible applications, particularly in the field of thermoelectric materials. This experience clearly underlined the importance of chemical nature and chemical properties of intermetallic compounds. Starting from 2015, the research becomes to be focused on the chemical properties of intermetallic compounds and the catalysis field offers a perfect “playground” for such studies. The experimental work was smoothly complemented by planning and responsibility for laboratory and endures with the responsible role of a group leader at MPI CPfS in 2019. The core of her actual research interests are **chemical properties of intermetallic compounds** under dynamic reaction conditions and their understanding based on the crystal structure and chemical bonding, building a “bridge” for interpretation of catalytic performance and search of new catalytic materials.

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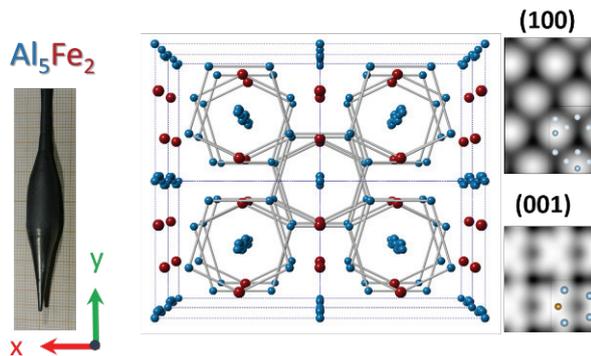
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News from the Research and Activity Domains (RADs)

RAD Atomic scale surfaces and functional coatings, thin films and interfaces

Unraveling the surface structure of the Al_5Fe_2 intermetallic compound

<https://doi.org/10.1016/j.apsusc.2020.148540>



The Al_5Fe_2 is an intermetallic that has been known for a long time. It is a technologically important compound used to protect steel against corrosion and oxidation. It easily forms through Al diffusion into steel during aluminum pack cementation or hot dipping of steel parts into molten Al bath, resulting in a thick protective coating of the intermetallic phase. Its structure consists in an ordered framework of pentagonal antiprims with composition Al_2Fe inside which nearly continuous chains of fractionally occupied Al sites exist. It was only recently discovered that some ordering of these Al channel atoms can occur at low temperature leading to various superstructures.

The article reports the first detailed surface investigation at the atomic scale of this compound [1]. The growth of a large single crystal of the Al_5Fe_2 compound is described. X-ray diffraction and transmission electron microscopy investigations indicate that the bulk structure corresponds to the low temperature polymorph η phase described as an incommensurately modulated

ed crystal. Extensive density functional theory calculations were performed to determine its formation enthalpy and its electronic structure. Two samples were extracted presenting either the (100) or (001) orientation, which were further investigated by different surface techniques (XPS, LEED and STM). Both surfaces exhibited superstructures, whose origin can be explained in the light of density functional calculations performed on model surfaces.

[1] L. Boulley, D. Kandaskalov, M.C. de Weerd, S. Migot, J. Ghanbaja, S. Sturm, P. Boulet, J. Ledieu, E. Gaudry, V. Fournée. *App. Surf. Sci.*, 542 (2021) 148540.

RAD Equality and Diversity in Materials Science - Action 2020: on-line

by Dr. Magdalena Wencka

For ECMetAC Days 2020, a set of activities developing soft skills dedicated especially to young researches of our network was proposed. First of all, ten licences for Gallup tests granted by our Network were distributed among the first ten young scientists who showed interest to get them. Gallup tests, called also Clifton-34-Strengths, were designed by Don Clifton, the father of strengths psychology. Following Clifton's thought "There is no more effective way to empower people than to see each person in terms of his or her strengths", our young researchers could find particular knowledge about their five principle talents belonging to four groups of executing, influencing, relationship building and strategic thinking. Our young scientists joined to almost 24,4 million people around the world who run such tests and who know that STRENGTH (ability to provide near-perfect performance) =

TALENT (natural way of thinking, feeling or behaving) * INVESTMENT (time spent practicing, developing skills and building knowledge base) [1]. Following science taken from CliftonStrengths statistics, it is clearly visible that people who processed these tests are six times more engaged in their jobs and agree that they have chance to do what they do best every day, so that their quality of life increased significantly. Strengths science supports then developing scientific carriers as every scientist is the leader of his/her own career and the same holds for the collaboration in scientific teams. Then, “Personal skills for team work” workshop was held on Dec. 2nd 2020 and was dedicated to personal skills development basing on CliftonStrengths. The workshop was guided by a coach, a manager and psychotherapist specialized in social skills Adam Bekier from SWPS University Clinic (Poznań, Poland). The basic task here was to process the knowledge coming from the CliftonStrengths tests and finding ways how to develop them. Especially the task “Name it, claim it, aim it” was a great tool to manage with freshly described skills. The third event of the Equality and Diversity in Material Sciences Action 2020 was the workshop on “Team skills” held on Dec. 7th 2020 and guided by dr. Magdalena Wencka – a physicist, scientific project leader and innovation manager at the J. Stefan Institute (Ljubljana, Slovenia). Here, participants working in small groups on imagined project could embed personal skills into their own teams. According to the team skills, special attention was put on inclusiveness [2] and its authentic commitment to diversity and challenge to status quo, humanity in a shape of creating space for others to contribute, awareness of bias to avoid personal blind spots and flaws in systems, curiosity about others like listening without judgement and seeking with empathy to understand people around and finally cultural intelligence that means to be attentive to other’s cultures. According to the effec-

tive collaboration within the scientific teams, the participants of the workshop practiced empowering others, paying attention to diversity of thinking and psychological safety and focusing on team consolidation.

Summarizing all Equality and Diversity in Material Sciences Action 2020 activities, let’s hear the voice of the participants who summed up:

“I had a great time when we worked in groups, when we shared our hobbies, talents and discussion. It was challenging as I am not used to talk about myself with people that I am not close to... I gained the wider knowledge about myself and possibility to look on every individual person as the unique talent.” M.

“Congratulations on the very interesting and fruitful workshop.” F.

“I was really surprised by the participants’ readiness and openness. It was a real game-changer... And thus, we get to the main point: the innovative and opening idea to organize such a workshop. Kudos to the organizers, there is a far greater potential within this group yet to be discovered”. A.

Next workshop on “Working within team of extreme individualists” will be held during EUROSCHOOL 2021. See you then!

[1] <https://www.gallup.com/cliftonstrengths/en/253790/science-of-cliftonstrengths.aspx>

[2] <https://hbr.org/2020/03/the-key-to-inclusive-leadership>

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Reports

ECMetAC Days 2020

Contrary to many events that have been cancelled, the ECMetAC Days 2020 went ahead from 7th to 10th December. Originally planned in Split, it was organised online thanks to the support of the Board of Directors who are greatly acknowledged here. The event followed the workshop on "Team skills" and brought together (albeit virtually) 78 participants over two days. It included 28 oral contributions and 6 posters with a priority given to young scientists. A special contribution given by V. Fournée was dedicated in memoria of Prof. P.A. Thiel, an outstanding scientist and friend for many of us, who we deeply miss.

While online, the high quality of the presentations generated exciting interactions among the participants. More details about the ECMetAC Days 2020 program can be found [here](#).

ECMetAC Young Scientists Oral Presentation Award: Shelby Turner

Institute: University Grenoble Alpes, CNRS, Grenoble-INP, Labs: Institut Laue-Langevin, SIMaP Grenoble, and ILM Lyon.

Title of talk: Phonon behavior in a random solid solution: A lattice dynamics study on the high-entropy alloy FeCoCrMnNi

Shelby Turner is currently a PhD student in her 3rd year at the Institut Laue-

Langevin in Grenoble, France. She uses x-ray and neutron techniques at large scale



facilities and nuclear reactors to study fundamental thermal and transport properties of materials in order to engineer better thermoelectric materials. She says "I am working towards

bridging the gap between ordered, crystalline systems and disordered, glass systems, in the context of heat transport, through the understanding of phonon scattering mechanisms."

She is interested in several types of materials, such as type-I clathrates, high-entropy alloys, yttria-stabilized zirconia, barium fluoride, and iron antimonide. She received the award for her presentation entitled "Phonon behavior in a random solid solution: A lattice dynamics study on the high-entropy alloy FeCoCrMnNi." On this topic, she says "there is a lot of momentum right now behind the study of high-entropy alloys, and it is very motivating to feel like I am playing a small part. I think we still have a lot to learn about these materials, and in the future I hope to be able to study a series of high-entropy alloys in order to better decouple the different disorder effects we are seeing in the phonon behavior."

Favorite hobby: Shelby is trying to take full advantage of these three years living in the French Alps: skiing, hiking, mushroom picking...she is learning that the French have mountain-related activities for every season!

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ECMetAC Young Scientists Oral Presentation Award: Sebastian Schenk

Institute: Martin-Luther-University Halle-Wittenberg (Halle, Germany)

Title of Talk: Dodecagonal oxide quasicrystal approximant with 72 tiling elements



Sebastian Schenk is currently a PhD student at the Martin-Luther-University Halle-Wittenberg within a French-German research project focusing on aperiodic crystals. He uses several experimental tools, such as surface X-ray diffraction and scanning

tunneling microscopy, to investigate the surface structure of the two-dimensional quasicrystalline phases discovered recently in the group. He received the award for his presentation entitled "Dodecagonal oxide quasicrystal approximant with 72 tiling elements". He says "During my time as PhD student we investigated the growth of our quasicrystalline systems and wanted to deeply understand the aperiodic structure on the atomic scale. Therefore we took our samples and went to beamtimes at two different synchrotrons. I am still impressed about the scale and complexity of these research facilities. On the other side I developed several custom routines to analyze aperiodic structures in physical and internal space."

In his free time he likes to play games. Video games and also board games, where he is not afraid of complex rules. Another big part in his life are his two cats.

ECMetAC Young Scientists Oral Presentation Award: Sylwia Gutowska

Institute: AGH University of Science and Technology, Krakow, Poland.

Title of Talk: Electron-phonon mediated superconductivity of LiBi

Sylwia Gutowska is currently a PhD student in her 4th year at the AGH University of Science and Technology. She describes the superconductivity of materials using ab initio methods. Her objective is to understand the influence of various properties of



electronic and phonon structure on superconductivity. She received the award for her presentation entitled "Electron-phonon mediated superconductivity of LiBi". She says "LiBi has caught our attention because it consists of almost the lightest and heaviest stable elements and crystallizes in a tetragonal crystal structure with square sublattices of Bi, very unusual for Bi-based compounds. Such a simple structure was an excellent opportunity to study in details the properties of electron-phonon interactions and superconductivity. Our next research focuses on more complex materials such as the Ir based Laves phase. We are trying to answer the question of how accompanied by the Kohn anomaly conversion from the Ir fcc structure to the fcc Laves phase causes a rela-

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tively high critical temperature of the Laves phase compared to Ir."

Favourite hobby: sci-fi literature.

ECMetAC Young Scientists Poster Award: Naïma Saadi

Institute: University of Liverpool (Liverpool, UK), Faculty: School of Engineering.

Title of poster: Utilising 3D-printing to aid visualisation of complex atomic structures



Naïma Saadi is currently a PhD student in her 2nd year on a multi-disciplinary project encompassing Engineering, Physics and Materials. She uses several 3D-printing technologies including resin and extrusion-based meth-

ods to manufacture complex geometries. A mixture of computer-aided design skills and crystallography have made visualising icosahedral quasicrystals more accessible. She received the award for her poster entitled "Utilising 3D-printing to aid visualisation of complex atomic structures". She says "An incredible amount of research has gone into optimising 3D-printing over the years, and likewise with understanding quasicrystals. It's about time these two areas merged. We were all excited when our first aperiodic structures were printed, now it's time to take things a step further". She wonders how these structures perform mechanically – under load bearing conditions for example. "Could quasicrys-

tals be beneficial beyond having electromagnetic band gap properties? It's a very new area within metamaterials and we would like to find out".

Favourite hobbies: She admits there are too many to name although, after receiving a telescope that was about to be thrown in the bin, stargazing has taken up a lot of Naïma's time – weather permitting of course. Her aim is to revisit Norway (when possible) to continue her dark sky exploration in the middle of nowhere. "I'm absolutely taking advantage of my sister living there, the solitude is humbling and the viewing conditions are immense".

Welcome to our new Member!

On 10th December, the Department of Physics, University of Zagreb represented by Dr. Mario Novak was accepted as new active member of ECMetAC by the Governing Board of the consortium and the General Assembly of ECMetAC NSU.



Please visit our new member website for further information:

<https://www.pmf.unizg.hr/en>

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Upcoming Events

ECMetAC Days

The ECMetAC Days 2021 will be organised by the University of Split from 7th -10th December. At this stage, we are planning for a onsite meeting. The main purpose of ECMetAC Days is to provide comprehensive information on recent results achieved within the current year of the ECMetAC network and to discuss directions for future research. Contributions will cover the field of metallic alloys and compounds ranging from basic to application oriented research: Development of new metallic alloys and compounds Structure determination, stability Physical, chemical and mechanical properties Surfaces of complex metallic alloys Materials for thermoelectricity and magneto-caloric application Materials for catalysis Coating technologies Complexity in periodic and aperiodic metallic alloys and compounds (theory and experiment) High-entropy alloys.

ECMetAC EuroSchool 2021

The next Euroschool 2021 entitled “**Complex Intermetallic Compounds for Applications**” will be held online by the Liverpool group from 24th-28th May 2021. Started in 2006, this is an annual event organised by ECMetAC. The school will focus on potential applications of complex intermetallic in various areas. The school 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 present their research activities in the poster session and establish a network among them. The list of previous EuroSchools is accessible on our website.

High Entropy Alloys Workshops

The next workshop organized within the ECMetAC will be dedicated to “High Entropy Alloys: from basics to Industrial Applications”. The event will take place online on 18th March 2021. We encourage you to visit our website as more details and the full program will soon be available.

Related Upcoming Events

IRN Aperiodic Seminar

by Marc de Boissieu

Friday 9th April from 9:00-10:30 Paris time

SCTE 2021 online

11th-16th of April 2021, Wrocław

<http://scte2020.intibs.pl/>

Kick-off meeting IRN Aperiodic

Postponed in October 2021, Carry le Rouet <http://irn-aperiodic.grenoble.cnrs.fr/>

25th Congress of the IUCr

14th-22nd August 2021-01-22, Prague, Czech Republic <https://iucr2020.org/>

Missing Content?

If you have any news items for circulation, either on our website <https://ecmetac.eu/> or in this newsletter, please send them to Julian Ledieu (julian.ledieu@univ-lorraine.fr).

Newsletter Subscription

If you are interested in receiving the ECMetAC newsletter on a regular basis, please go to <https://ecmetac.eu/> and subscribe for the newsletter at the bottom of the webpage

Imprint

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