ECMetAC Euroschool 2021: Complex Intermetallic Compounds for Applications

24-28 May 2021
(Online Through Zoom)

Program and Abstracts

Organised by: European Integrated Centre for the Development of New Metallic Alloys and Compounds (ECMetAC)

Host: The University of Liverpool

Dear participants,

Welcome to **ECMetAC Euroschool 2021: Complex Intermetallic Compounds for Applications** being held online on 24-28 May 2021.

Since more than 10 years, the Euroschools, organised by the European Integrated Center for the Development of New Metallic Alloys and Compounds (ECmetAC), trains young researchers in the field of Materials Science. Initially hosted by the Josef Stefan Institute in Ljubljana (Slovenia, 2009 and 2010), the Euroschool then travelled all over Europe (Germany, France, Croatia, UK, Poland, Belgium, Slovakia) on an annual basis. Each Euroschool proposes a different program, focusing on a either a theoretical, experimental or applicative topic. This event focuses on applications of complex intermetallic compounds.

Due to the Covid crisis, the Euroschool planed in 2020 at TU Chemnitz has been cancelled. In 2021, because the health situation is still worrying in several European countries, the Euroschool is held online, hosted by the University of Liverpool.

Based on lectures given by experts of the field, the Euroschool aim to enhance the scientific performance, creativity, and ethical standards of young researchers, in order to allow them to evolve throughout their career as agile players in universities, companies and organisations. The international environment - each Euroschool brings together researchers from several European countries - is useful to the development of collaborations between participants. We hope that the Euroschool 2021 will provide you with useful knowledge to build a future consistent with your projects!

We thank all speakers and participants for their valuable time amidst the unprecedented time.

Stay Safe!

Dr Hem Raj Sharma
Chair, Euroschool 2021
The University of Liverpool, UK

Prof Emilie Gaudry
Coordinator, RAD Euroschool
Université de Lorraine/CNRS, Nancy, France

24 May 2021

Introduction:

'ECMetAC Euroschool 2021: Complex Intermetallic Compounds for Applications' will be held online on 24-28 May 2021. This is an annual event (15th in series) organised by the European Integrated Centre for the Development of New Metallic Alloys and Compounds (ECMetAC). The school will focus on potential applications of complex intermetallics in various areas. It will offer lectures by experts in the field revising progress to date and prospects 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 the opportunity to establish a network among them.

Topics:

- Basic introduction to complex metallic alloys (structure, physical properties, growth)
- Surface structure and properties
- Magnetic properties
- Materials for energy (catalysts, thermoelectricity, magneto-calorimetry)
- Thin films and coatings
- Mechanical properties
- Additive manufacturing materials

Speakers:

- Prof Bostjan Markoli, University of Ljubljana, Slovenia; *Metallurgy and properties of Al-based alloys*
- Dr Constantin Vahlas, French National Centre for Scientific Research (CNRS), Paris, France; *Chemical vapor deposition and atomic layer deposition: principles and challenges towards the processing of complex intermetallic films*
- Prof Emilie Gaudry, Université de Lorraine/CNRS, Nancy, France; *An introduction to the atomic and electronic structures of complex metallic alloys*
- Dr Hari Dahal, American Physical Society, USA; *Scientific publication and peer-review process*
- Dr Hem Raj Sharma and Prof Ronan McGarth, The University of Liverpool, UK; *Surface properties of complex metallic alloys*
- Dr Iryna Antonyshyn, Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany; *Intermetallic compounds in (electro)catalysis and important features of solid catalyst*
- Dr Jon Alaria, The University of Liverpool, UK; *Magnetocaloric properties of metallic alloys*
- Prof Julia Dshemuchadse, Cornell University, New York, USA; Dr Kirsty Young, Nu Instruments, UK; and Dr Sebastián Alarcón Villaseca, Osram Opto Semiconductors, Regensburg, Germany; *Career Opportunities*
- Dr Magdalena Wencka, Polish Academy of Sciences, Poznań, Poland; *Communication and negotiation skills for researchers*
- Dr Marc Heggen, Forschungszentrum Jülich, Germany; *Plastic deformation mechanisms in CMAs: Dislocations and metadislocations*
- Prof Paul Canfield, Iowa State University, USA; *Cooking, fishing and jogging through phase space: a practical guide to giscovering and understanding new materials*

- Prof Silke Bühler-Paschen, Vienna University of Technology, Austria; *Complex intermetallic compounds for thermoelectric applications*
- Dr Vincent Fournee, Université de Lorraine/CNRS, Nancy, France; *Complex metallic alloys as new materials for additive manufacturing: current and future applications*

Program (Central European Time):

	24/05/2021 Monday	25/05/2021 Tuesday	26/05/2021 Wednesday	27/05/2021 Thursday	28/05/2021 Friday
09:50-10:00	Opening remarks (Sharma)				
10:00-11:00	**Lecture:** General introduction to CMA (Gaudry)	**Lecture:** Magnetocaloric materials (Alaria)	**Lecture:** Intermetallic compounds in (electro)catalysis (Antonyshyn)	**Lecture:** CMA for Thermoelectric applications (Bühler-Paschen)	**Lecture:** Thin films and coatings (Vahlas)
11:00-11:15	Break				
11:15-12:30	**Activity:** Draw crystallographic structures (Gaudry)	**Activity:** Magnetocaloric materials (TBC)	**Activity:** Important features of solid catalyst Catalysis (Antonyshyn)	**Activity:** CMA for Thermoelectric applications (Bühler-Paschen)	**Activity:** Thin films and coatings (Vahlas)
12:30-13:00	Break				
13:00-14:00	**Lecture:** Surface properties of CMAs (McGrath & Sharma)	**Lecture:** Discovering and understanding new materials (Canfield)	**Workshop:** Communication and negotiation skills for researchers (Wencka)	**Lecture:** Additive manufacturing (Fournee)	**Lecture:** Metallurgy and properties of Al-based alloys (Markoli)
14:00-14:15	Break				
14:15-15:30	**Activity**: Analysis of surface atomic structure data of CMA (McGrath & Sharma)	**Lecture:** Scientific publication and peer-review process (Dahal)	**Workshop:** Communication and negotiation skills for researchers (Wencka)	**Lecture:** Career opportunities (Dshemuchadsem, Young & Villaseca)	**Lecture:** Mechanical properties (Heggen)
15:30-16:30			**Workshop:** Communication and negotiation		Closing remarks (McGrath)

			skills for researchers (Wencka)		

Deadlines:

Date	Action	Remarks
15 January 2021	Internal circulation	√
30 January 2021	First circulation	√
30 January 2021	Identify lecturers	√
28 February 2021	Finalise program	√
8 March 2021	Second circulation/Launch website	√
31 March	Abstract submission deadline	√
10 May 2021	Registration deadline	√
15 May 2021	Final circulation	√
24-28 May 2021	Euro school	

Registration:
Registration is free for anyone from an ECMetAC member institution. Non-ECMetAC members may join upon payment of a registration fee of €100. The registration deadline is 30 April 2021. The link to registration is https://forms.gle/FUtxcNuSgcfPghq1A.

Satellite Meeting
"Materials for energy" meeting will be held as "virtual satellite" to the Euroschool, on May 31. The plan is to have a few short presentations on topics related to energy materials, followed by discussions on ongoing and possible new joint work. We will interpret the topic "Materials for energy" in a broad sense. In particular, also materials with (putative) topological properties can be included (as there is frequent overlap with good thermoelectric properties).

Zoom link (the same zoom link for Euroschool and satellite meeting):
https://liverpool-ac-uk.zoom.us/j/97285524993?pwd=enFGbzlXYThGNDBRVWo4c1l4aEJHQT09

Meeting ID: 972 8552 4993
Passcode: VnLs1+S8

Please contact h.r.sharma@liverpool.ac.uk or Dominic.Burnie@liverpool.ac.uk for any technical difficulties.

Organising Committee:

- Hem Raj Sharma, The University of Liverpool
- Ronan McGrath, The University of Liverpool
- Dominic Burnie, The University of Liverpool
- Emilie Gaudry, Université de Lorraine/CNRS, Nancy, France
- Julian Ledieu, Université de Lorraine/CNRS, Nancy, France

Contact:
Dr. Hem Raj Sharma
Department of Physics and Surface Science Research Centre
The University of Liverpool
Liverpool L69 3BX, UK
Email: H.R.Sharma@liverpool.ac.uk

An Introduction to the Atomic and Electronic Structures of Complex Metallic Alloys

*Émilie Gaudry

Univ. Lorraine, CNRS, Institut Jean Lamour, Nancy, France

**e-mail: emilie.gaudry@univ-lorraine.fr*

Structurally complex alloy phases are atypical metallic systems based on crystal structures with giant unit cells, containing from several tens to several thousands of atoms, arranged into high-symmetry clusters connected together. They represent interesting new materials, since until recently hardly any studies have been carried out on their physical properties.

In this talk, I will introduce the atomic and electronic structures of complex metallic alloys. The emphasis will be on the specific bonding network occuring in these compounds, on the existence of two different physical length scales, one representing the cluster substructure, the other the long-range periodicity, as well as on the mechanisms, contributing to the electronic stabilization of these systems (Fig. 1). During the tutorial, several complex structures will be investigated using the VESTA sofware [1].

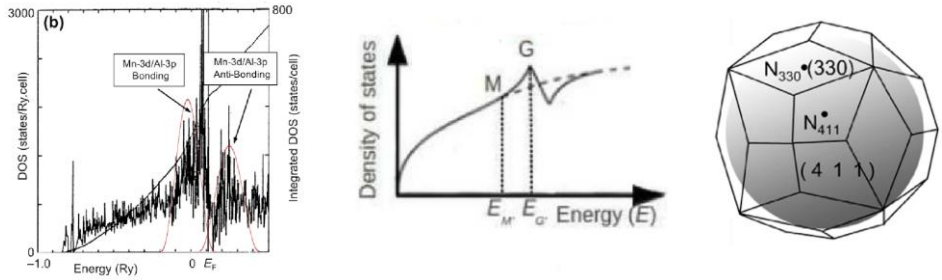

Figure 1 – (a) Electronic structure of the α-$Al_{114}Mn_{24}$ complex alloy. (b) Schematic density of states showing a pseudo-gap that originates from a Hume-Rothery stabilization mechanism. (c) Fermi sphere - Brillouin zone interaction in a γ-brass structure. From Ref. [2].

[1] K. Momma and F. Izumi, J. Appl. Crystallogr. 44 (2011) 1272
[2] Mizutani et al., Electron Theory of Complex Metallic Alloys, in Physical Metallurgy: Fifth Edition (2014), pages 103-202; in Physical Metallurgy: Fifth Edition Eds D. Laughlin and K. Hono, Elsevier Oxford

Surface Properties of Complex Metallic Alloys

*Ronan McGrath and Hem Raj Sharma

The University of Liverpool, UK

**e-mail: r.mcgrath@liverpool.ac.uk*

The lecture will cover some basics of surface science and experimental techniques (LEED: Low energy electron diffraction; AFM: Atomic force microscopy; STM: Scanning tunnelling microscopy; XPS: X-ray photoelectron spectroscopy; AES: Auger electron spectroscopy; UPS: Ultraviolet photoemission spectroscopy. We will then move on to surface structure of quasicrystals and approximants and finally epitaxy on quasicrystals.

Magnetocaloric Materials

Jonathan Alaria

The University of Liverpool, UK

email: alariaj@liverpool.ac.uk

Cooking, Fishing and Jogging through Phase Space: A Practical Guide to Discovering and Understanding New Materials

Paul C. Canfield

Iowa State University, Iowa, USA

e-mail: canfield@ameslab.gov

The design, discovery, characterization and control of novel materials is perhaps the most important research area for humanity as it moves into the 21st century. A myriad of societal problems concerning energy, clean water and air, and medicine all need to be solved by the discovery of new compounds with dramatically improved, or even new, properties. The search for such materials requires a blending of skills and mindsets that, traditionally, have been segregated into different academic disciplines: physics, chemistry, metallurgy, materials science. In this colloquium I will outline the basic philosophy and techniques that we use to search for novel materials. These include a combination of intuition, experience, compulsive optimism and a desire to share discovery [1].

In the second half of the lecture, the specific case of superconductivity will be used as an example of one such search. Over the past couple of decades, a growing sense of where and even how to search for new superconductors has been developing, with the recent discoveries of MgB2 and the FeAs based materials providing, at least for me, clear guidance.

[1] Paul C. Canfield, *Rep. Prog. Phys.* **83** [2020] 016501

Scientific Publication and Peer Review Process

Hari Prasad Dahal

Associate Editor, Physical Review Materials, American Physical Society

email: *hari@aps.org*

The global scientific publication landscape is evolving and expanding rapidly. The area of research, size of the scientific community and number of published scientific literature are growing tremendously. The publication process follows different publishing models but the foundation of all models remains almost the same, the peer review process managed by the editorial system. The interaction between the authors and anonymous reviewers mediated by the editors is at the heart of the peer review process. The Authors, Reviewers and Editors play important roles, as well as face unique difficulties at times. The presentation will cover these aspects of scientific publication. The presenter will share the Editors' side of the story, and would like to hear from the Authors and Reviewers.

Intermetallic Compounds in (Electro)Catalysis and Important Features of Solid Catalysts

Iryna Antonyshyn

Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

e-mail: Iryna.Antonyshyn@cpfs.mpg.de

Intermetallic compounds (IMCs) represent a fascinating class of compounds with variety of different crystal structures, plenty of possible chemical bonding scenarios and, therefore, a busket of intriguing physical and chemical properties. Considering catalyst as a substance that provides an alternative pathway of the chemical reaction, lowering the activation barrier and enhancing the reaction rate, IMCs are the promising catalyst candidates. On one hand, their well-defined crystal structure and different nature of the chemical bonding (e.g. combination of ionic and covalent interactions) allow to tailor the catalyst activity, selectivity and/or stability. On another hand, the IMCs can be used as model systems for investigation of reaction mechanisms and the nature of the active sites. Depending on the type of reaction, IMCs can be considered as catalysts themselves or as precursor substances for formation of catalytically active material. Different examples of IMC application in heterogeneous catalysis and electrocatalysis will be presented and role of intermetallic compound will be illustrated.

To enhance the potential power of intermetallic compounds for their application in (electro)catalysis field, the important features of solid catalysts will be outlined during the „Learning activities“.

Communication and Negotiation Skills for Researchers

[1,2*]M. Wencka, [3]M. Frątczak

[1]*J. Stefan Institute, Ljubljana, Slovenia*

[2]*Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*

[3]*Collegium Da Vinci, Poznań, Poland*

**e-mail: magdalena.wencka@ijs.si*

We shall propose workshop improving communication and negotiation skills towards better understanding of inclusiveness that is the quality of including many different types of people and treating them all fairly and equally [1]. The main values behind inclusiveness are as follows:

- humanity to create space for others to contribute at equal way;
- awareness of bias that shows awareness of personal blind spots and flaws in the systems, value talents, effort and achievements than wealth and social position;
- curiosity about others to demonstrate open mindset and deep curiosity about others, listening without judgment and seeking with empathy to understand others;
- cultural intelligence toward being attentive to other's cultures and adapt as required;
- effective collaboration that empower others, paying attention to diversity of thinking and psychological safety toward focusing on team cohesion.

Our training program contains block of communication with elements of interculturalism, roles in groups according to Meredith Belbin, stress management and savoir vivre. The second part of our workshop will be dedicated to negotiation skills including negotiations styles, self-presentations for negotiations, issue of difficult co-worker and assertiveness in difficult conversations. We shall propose practical exercises on team roles, assertiveness in difficult conversations including conversation with a supervisor. Our workshop will be guided by Mariusz Frątczak, who is Board Member and Sales and Marketing Director of Collegium Da Vinci in Poznań, Poland. He is experienced sales trainer and business coach specialized in communication, public speaking, customer service and trade negotiation. He conducted more than 200 research and consulting projects in banking, financial support, education service and renewable energy (wind farms).

[1] https://dictionary.cambridge.org/dictionary/english/inclusiveness

Complex Intermetallic Compounds for Thermoelectric Applications

Silke Bühler-Paschen

Vienna University of Technology, Austria

email: paschen@ifp.tuwien.ac.at

Thermoelectric materials can convert temperature gradients into electric field gradients and vice versa. As such they are of interest for thermoelectric generators and heat pumps. For this conversion to be efficient, the physical quantities entering the thermoelectric figure of merit have to be optimized. After a general introduction I will discuss various materials design strategies to do so. Special emphasis will be put on cage compounds where rattling guest atoms can be used to boost two key quantities, the thermopower and the phonon thermal conductivity in intriguing ways.

Complex Metallic Alloys as New Materials for Additive Manufacturing: Current and Future Applications

S. Kenzari, B. Boy, D. Bonina, J.M. Dubois, *V. Fournée.

Institut Jean Lamour, Université de Lorraine/CNRS, Nancy, France

**e-mail: vincent.fournee@univ-lorraine.fr*

Additive manufacturing processes allow freeform fabrication of the physical representation of a three-dimensional computer-aided design (CAD) data model. This area has been expanding rapidly over the last 25 years. It includes several techniques such as selective laser sintering, selective laser melting and stereolithography. The range of materials used today is restricted while there is a real demand for manufacturing lighter functional parts or parts with improved functional properties. In this presentation, we summarize recent work performed in this field, introducing new composite materials containing complex metallic alloys. These are mainly Al-based quasicrystalline alloys whose properties differ from those of conventional alloys. The use of these materials allows us to produce light-weight parts consisting of either metal–matrix composites or of polymer–matrix composites with improved properties. Functional parts using these alloys are now commercialized. We will review current applications of these new materials as well as potential ones, from automotive industry to medical implants and anti-counterfeiting objects.

Career Opportunities

[1,*]Julia Dshemuchadse, [2]Kirsty Young, and [3]Sebastián Alarcón Villaseca

[1]Cornell University, New York, USA
[2]Nu Instruments, UK
[3]Osram Opto Semiconductors, Regensburg, Germany

[*]email: mwencka@ifmpan.poznan.pl

You are working on your PhD or postdoc in the field of complex and new intermetallic alloys and compounds. What do you want to do next? What job options do you have and how do they align with the skills you have developed and the networks that you have built? We will discuss these and other questions that you might have about career opportunities in industry and in academia.

All three panelists have earned their PhDs in the community that is now ECMetAC, after which they have followed different paths. After his PhD work conducted at CNRS in Nancy, France, Sebastián Alarcón Villaseca worked at two research institutes in Germany before entering industry as a research and development engineer. Kirsty Young earned her PhD at the University of Liverpool in the UK before joining Nu Instruments UK. After finishing her PhD at ETH Zurich, Switzerland, Julia Dshemuchadse moved to the USA as a postdoc before starting at Cornell University as an assistant professor.

Chemical Vapor Deposition and Atomic Layer Deposition: Principles and Challenges towards the Processing of Complex Intermetallic Films

Constantin Vahlas

CIRIMAT – CNRS, Toulouse

email:constantin.vahlas@ensiacet.fr

Functional properties of complex metallic alloys, oxide systems and compounds are often enhanced by the processing of these materials in the form of thin films and coatings. This is due to the high surface to volume ratio of films, which illuminates their particular surface properties. It also compensates their often-brittle character in the bulk form and contributes in savings of highly valuable, complex in producing, materials. However, the screening of such films and coatings and the implementation to the market of appropriate compositions and microstructures, depends on the capacity to process them on predefined substrates. Gas phase deposition techniques under various atmospheres, is a privileged means to achieve this objective. Among them, chemical vapor deposition (CVD) and atomic layer deposition (ALD) allow processing films with the desirable elemental composition and tunable microstructure on complex-in-shape substrates and at low to moderate temperatures, thus preserving the structural integrity of thermally sensitive parts.

The present lecture will focus on the fundamentals of CVD and ALD techniques, with the aim to reveal their potential and the hard points to overcome in view of the processing of functional films and coatings that can be implemented in all Key Enabling Technologies [1]. The classic structure – properties correlation in materials science will be complemented with the process – structure one, which is a prerequisite for crossing all technology readiness levels to the market. The utility of multiscale and multiphysics process modeling to meet this objective will be highlighted [2,3]. These concepts will be illustrated with case studies including CVD of approximant phases [4-6] and ALD of aluminum oxide [7].

[1] N. Alford, J. Amouroux, D. Barbier, G. Bauer, A. Borg, J. P. Condé, A. González-Elipe, H. G. Grimmeiss, A. Jaeger-Waldau, D. J. Jarvis, T. Lippert, S. Maier, H. J. Muessig, E. Olsson, J. Perriere, L. Pfitzner, F. Priolo, H. Richter, A.-C. Ritschkoff, P. Siffert, A. Slaoui and C. Vahlas, Materials for Key Enabling Technologies, Strasbourg, 2011.
[2] G. P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, B. Caussat and A. G. Boudouvis, Chem. Eng. Res. Des., **132**, 795-811 (2018).
[3] I. G. Aviziotis, N. Cheimarios, T. Duguet, C. Vahlas and A. G. Boudouvis, Chem. Eng. Sci., **155**, 449-458 (2016).
[4] L. Aloui, T. Duguet, F. Haidara, M.-C. Record, D. Samélor, F. Senocq, D. Mangelinck and C. Vahlas, Appl. Surf. Sci., **258**, 6425-6430 (2012).
[5] N. Prud'homme, T. Duguet, D. Samélor, F. Senocq and C. Vahlas, Appl. Surf. Sci., **283**, 788-793 (2013).
[6] I. G. Aviziotis, T. Duguet, K. Soussi, M. Heggen, M. C. Lafont, F. Morfin, S. Mishra, S. Daniele, A. G. Boudouvis and C. Vahlas, Phys. Status Solidi A, 215 (2018).
[7] G. P. Gakis, H. Vergnes, E. Scheid, C. Vahlas, A. G. Boudouvis and B. Caussat, Chem. Eng. Sci., **195**, 399-412 (2019).

Plastic Deformation Mechanisms in CMAs: Dislocations and Metadislocations

*M. Heggen, and M. Feuerbacher

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

**e-mail: m.heggen@fz-juelich.de*

Complex Metallic Alloys (CMAs) show remarkable mechanical and plastic properties and novel mechanisms of plastic deformation. This talk will focus on the plastic deformation properties and characterisation of defects in CMAs using electron microscopy. After an introduction of the basic ex- and in-situ transmission electron microscopy techniques, several examples for new mechanisms and defects in various CMA-phases are given, including ε-type AlPdMn, T-AlMnPd, μ-AlMn, and $Al_{13}Co_4$ [1]. In the phase T-AlMnPd for instance, a novel and highly complex deformation mechanism was found, which is based on the movement of so-called metadislocations mediating strain and separate phason defects [2]. Upon deformation, the phason defects move ahead and locally transform the T-phase structure for accommodation of the dislocation core. Dislocation core and phason defects leave a slab of a modified complex phase, which can be interpreted as a stack of stacking faults. In general, deformation of CMAs implies orchestrated movements of tens or hundreds of atoms per elementary glide step along various crystallographic directions [3]. Although these mechanisms are fairly complex, they can be described by simple tiling descriptions.

[1] M Feuerbacher, M Heggen, "Dislocations in Solids: Metadislocations" Vol 16. ed. J.P. Hirth and L. Kubin, (Elsevier, Amsterdam) p. 110.
[2] M Heggen, L Houben, M Feuerbacher, Nature Materials **9**, 332 (2010).
[3] M Heidelmann, Mc Heggen, C Dwyer, M Feuerbacher, Scripta Materialia **98**, 24 (2015).