Workshop / Veranstaltung:

Functional High Entropy Alloys / Hochentropiefunktionswerkstoffe

29th March 2022 10:00 am - 05:00 pm CET

- Organizers:
  Prof. Dr. Alfred Ludwig, Materials Discovery, Ruhr-Universität Bochum
  Prof. Dr. Oliver Gutfleisch, Functional Materials, TU Darmstadt

- Venue: Ruhr-Universität Bochum, ZGH - http://zgh.rub.de
- Format: in presence/ hybrid, all talks invited
- Language: English

High entropy alloys, as a fundamentally new material design concept, are a rapidly growing field of research in recent years with a wide range of possibilities for tailoring new materials with interesting combinations of properties. These almost unlimited design options are based on the alloy structure of five or more elements, which can often be present in simple crystal structures. After the original focus on mechanical properties, the functional properties of this exciting class of materials are now coming to the fore.
Current examples are high entropy alloys for electrocatalysis, hydrogen storage and magnetic applications as well as high entropy oxides for batteries.
The workshop will briefly introduce the basics of high entropy materials and then discuss the most exciting developments in the field of functional materials.

Hochentropielegierungen als ein grundlegend neues Materialdesignkonzept sind ein in den letzten Jahren stark wachsendes Forschungsfeld mit vielfältigen Möglichkeiten, neue Werkstoffe mit interessanten Eigenschaftskombinationen maßzuschneidern. Diese nahezu unbeschränkten Designoptionen beruhen auf dem Legierungsaufbau aus fünf oder mehr Elementen, die oft in einfachen Kristallstrukturen vorliegen können. Nach dem ursprünglichen Fokus auf mechanische Eigenschaften, rücken nun die Funktionseigenschaften dieser spannenden Materialklasse in den Vordergrund.
Aktuelle Beispiele sind Hochentropielegierungen für die Elektrokatalyse, für die Wasserstoffspeicherung und für magnetische Anwendungen sowie Hochentropieoxide für Batterien.
Der Workshop wird die Grundlagen der Hochentropiematerialien kurz vorstellen und dann die spannendsten Entwicklungen im Bereich der Funktionswerkstoffe diskutieren.

Programme:

	Speakers	Affiliation	Title
10:10	Prof. Sheng Guo	Chalmers University of Technology, Sweden	Physical Metallurgy of High-Entropy Alloys
10:40	Dr. Abhishek Sarkar	Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology	High Entropy Oxides: Opportunities and Challenges
11:10	Prof. Jan Frenzel	Ruhr-Universität Bochum	Microstructures, martensitic trans-formations and atomic mobilities in high-entropy shape memory alloys
11:40	Prof. Oliver Gutfleisch	TU Darmstadt	Potential of high-entropy alloys for hard and soft magnets
12:10	Prof. Victorino Franco	University of Seville, Spain	Pushing the limits of magnetocaloric high-entropy alloys
13:30	Dr. Natalia Shkodich	Universität Duisburg-Essen	Tailoring magnetism of nanocrystal-line of CoCrFeNiGax (x = 0.5, 1.0) high entropy alloys by high energy ball milling
14:00	Dr. Ziyuan Rao	Max-Planck-Institut für Eisenforschung Düsseldorf	Machine learning enabled fast high-entropy alloy discovery – a case study on novel INVAR alloys
14:30	Prof. Wolfgang Schuhmann	Ruhr-Universität Bochum	High-entropy materials catalysts - from high-throughput discovery to novel catalysts for energy conversion reactions
15:20	Prof. Martin Sahlberg	Uppsala University, Sweden	High entropy alloys for hydrogen compression and storage
15:50	Prof. Babak Anasori	Mechanical and Energy Engineering, Indiana University-Purdue University, USA	High-entropy 2D Transition Metal Carbide MXenes
16:20	Prof. Alfred Ludwig	Ruhr-Universität Bochum	Exploration of the multidimensional HEA search space using high-throughput experimentation

Supported by:

- Materials Discovery & Interfaces, Ruhr-Universität Bochum
- ZGH Center for Interface-Dominated High Performance Materials
- Functional Materials, TU Darmstadt
- Cooperate Research Center CRC/TRR 270 HoMMage
- DGM

DGM Expert Committee Functional Materials:
https://dgm.de/de/netzwerk/fach-gemeinschaftsausschuesse/funktionswerkstoffe
https://dgm.de/en/network/expert-joint-committees/functional-materials

Prof. Sheng Guo (Chalmers University of Technology, Sweden)

A Brief Introduction to

Physical Metallurgy of High-Entropy Alloys

Sheng Guo

Industrial and Materials Science, Chalmers University of Technology, 41296 Göteborg, Sweden

Since about 18 years ago, there has been a new trend in designing alloys in the physical metallurgy community, which differs significantly to previous practices. In the new category of alloys, high-entropy alloys (HEAs), there is no longer a clear distinction of dominant alloying element and other elements, and basically all alloying elements are mixed equiatomically or close to equiatomically. This novel alloy design strategy opens up a vast unexplored compositional space, and potentially new opportunities to numerous new materials and new applications, but also brings new challenges on how to design these alloys properly. In this lecture, I will give an overview of HEAs from the physical metallurgy perspective, starting from the definition, moving to the alloy design strategies that are currently adopted to HEAs, and then some typical properties of this relatively new class of metallic materials. The focus will be on mechanical properties, but some functional properties will also be covered.

Dr. Sheng Guo is currently a Professor at the Department of Industrial and Materials Science, Chalmers University of Technology in Sweden. Sheng joined Chalmers as an Assistant Professor in 2013, and was promoted to Associate Professor in 2016, and to Professor in 2020. Before joining Chalmers, Sheng spent four years working as a postdoctoral researcher in two universities in Hong Kong, City University of Hong Kong, and Polytechnic University of Hong Kong, respectively. Sheng's research activities nowadays are focused on alloy design and mechanical properties of high-entropy alloys (HEAs), but he is also actively looking for opportunities to expand his research areas to functional properties of novel metallic materials including HEAs.

Dr. Abhishek Sarkar (Karlsruhe Institute of Technology, Institute of Nanotechnology)

High Entropy Oxides: Opportunities and Challenges

Horst Hahn, Abhishek Sarkar, Leonardo Velasco, Ben Breitung, Miriam Botros, Yanjiao Ma,

High entropy oxides (HEOs) are an emerging class of single-phase solid solutions consisting of multiple cations in near-equiatomic proportion. The field of HEOs has rapidly grown in the last half a decade to include numerous compositions along with several crystallographic structures, e.g., rocksalt, fluorite, perovskites, spinels, pyrochlores, etc. Consequently, the extensive compositional flexibility of HEOs offers the possibility to tailor a plethora of functional properties. Examples of some of their improved functionalities compared to conventional oxides are the enhanced electrochemical cyclic stability, superior ionic conductivity, higher catalytic activity, greater thermal insulation and exotic magneto-electronic properties. This being the opportunities that can be harvested for future applications, researchers working on HEOs face multiple challenges in terms of precise understanding of their atomistic features, such as local elemental distribution, distortion and bonding characteristics. Information-based approaches can help to identify optimized compositions and structures. Hence, the talk will provide an overview of the current state of research on HEOs along with the possible approaches to tackle the aforementioned challenges benefitting future research endeavors.

Abhishek Sarkar is a postodoctoral researcher in the group of Prof. Horst Hahn at the Joint Laboratory Nanomaterials - Technische Universität Darmstadt and Karlsruhe Institute of Technology. He received his M. Tech. degree from Indian Institute of Technology, Madras in 2016 and PhD in material science from TU Darmstadt in 2020. His research interests include synthesis and structure-property correlations in high entropy materials with emphasis on their magnetic, electronic, optical and electrochemical properties. He has published more than 20 articles in the field of high entropy ceramic materials.

Prof. Jan Frenzel (Ruhr-Universität Bochum)

Microstructures, martensitic transformations and atomic mobilities in high entropy shape memory alloys

J. Frenzel, O. Oluwabi, D. Piorunek, G. Eggeler

Institut für Werkstoffe, Ruhr-Universität Bochum, Universitätsstr. 150, 44801 Bochum
jan.a.frenzel@rub.de

High entropy shape memory alloys (HE-SMAs) represent a young class of materials which show reversible martensitic phase transformations. HE-SMAs were derived from binary NiTi, to which the elements Cu, Pd, Zr and Hf are added. HE-SMAs represent ordered complex solid solutions. Their high temperature phase is of B2 type, where the different elements occupy specific sites in the former Ni- and Ti-sub-lattices. In the present work, we study how an increasing chemical complexity as well as deviations from the ideal stoichiometry affect microstructures and phase transformation behavior. The results show that microstructural features in HE-SMAs were inherited from nine different binary HE-SMA sub-systems (e.g. Ti-Pd, Ni-Zr, Ni-Ti, etc.). As a striking observation, the dependence of martensite start temperatures on the degree of off-stoichiometry differs in HE-SMAs from what is known for the binary reference system NiTi. Our findings are discussed in the light of previous studies on the concentration dependence of transformation temperatures in shape memory alloys. We also present recent results on the effects of chemical complexity on atomic mobilities in HE-SMAs. Using diffusion couples, it has been observed that adding Pd to binary NiTi speeds up interdiffusion, whereas the opposite was found for Zr and Hf additions.

Apl. Prof. Dr.-Ing. habil. Jan André Frenzel

Chair for Materials Science and Engineering
Institute for Materials, Faculty Mechanical Engineering
Ruhr University Bochum, ICFO 04/323
44801 Bochum, Germany
e-mail: jan.a.frenzel@rub.de

Education and degrees

12/2018 Habilitation at the Ruhr University Bochum (RUB), Germany
11/2005 Dr.-Ing. degree in Materials Science / Mechanical Engineering obtained at the RUB
03/2003 Dipl.-Ing. degree, Ruhr University Bochum

Positions held

1) 11/2019: Appointment as adjunct professor at the Institute for Materials, RUB, Germany
2) Since 01/2008: Head of the Advanced Study Group „Input Data and Validation“ in the Interdisciplinary Center for Advanced Materials Simulation (ICAMS)
3) Since 11/2005: Head of the „Processing“ group, Institute for Materials, RUB
4) Post-Doc, research visits at Oak Ridge National Laboratory (Prof. Easo George, 2006) and Northwestern University (Prof. David Dunand, 2007)

Prof. Oliver Gutfleisch (TU Darmstadt)

Potential of high-entropy alloys for hard and soft magnets

Oliver Gutfleisch[1,2], Fernando Maccari [1]
Liuliu Han[3], Zhiming Li[3], Ziyuan Rao[3], Dierk Raabe[3]

[1] TU Darmstadt, Material Science
[2] MPG Group "De Magnete", MPIE Düsseldorf
[3] Max-Planck-Institut für Eisenforschung, Düsseldorf

First, we describe shortly the material attributes for high performance hard magnets, soft magnets and magnetocaloric materials. We need to consider these intrinsic and extrinsic magnetic properties when extending the parameter range to “new” magnets with secondary functionalities such as complex geometry by additive manufacturing, local vs. effective anisotropy and exchange, mechanical, (directional) thermal and electrical properties. Here, the vast compositional space with multiple principal elements and tuning possibilities of defects with specific structural and chemical configurations in high entropy alloys (HEA) or compositionally complex alloys (CCA) becomes interesting. The extension of the demonstrated attractive mechanical properties combinations in HEAs to functional materials like magnetic compounds is fascinating and challenging. However, they might help to answer the more and more demanding property sets in electrical machines. We give some examples of how coherent and incoherent precipitates in HEAs can be used to tune the critical magnetisation reversal processes while improving greatly secondary functionalities like strength and ductility.

O. Gutfleisch, M. A. Willard, E. Brück, C. H. Chen, S. G. Sankar, J. P. Liu, Magnetic materials and devices for the 21st century: stronger, lighter, and more energy efficient, Adv. Mater. 23 (2011) 821-842.

T. Gottschall, K.P. Skokov, M. Fries, A. Taubel, I. Radulov, F. Scheibel, D. Benke, S. Riegg, O. Gutfleisch, Making a cool choice: the materials library of magnetic refrigeration, Progress Rep. in Adv. Energy Mat. 9 (2019) 1901322.

G. Herzer, Modern soft magnets: Amorphous and nanocrystalline materials, Acta Mat 61 (2013) 718–734.

L. Han, Z. Rao, I.R. Souza Filho, F. Maccari, Y. Wei, G. Wu, A. Ahmadian, X. Zhou, O. Gutfleisch, D. Ponge, D. Raabe, Z. Li, Ultrastrong and ductile soft magnetic high-entropy alloys via coherent ordered nanoprecipitates, Advanced Materials 2102139 (2021) 9p.

Z. Rao, B. Dutta, F. Körmann, D. Ponge, L. Li, J. He, L. Stephenson, B. Gault, L. Schäfer, K.P. Skokov, O. Gutfleisch, D. Raabe, Z. Li, Unveiling the mechanism of abnormal magnetic behavior of FeNiCoMnCu high-entropy alloys through a joint experimental - theoretical study, Phys. Rev. Materials 4 (2020) 014402.

Z. Rao, B. Dutta, F. Körmann, W. Lu, X. Zhou, C. Liu, A. K. Silva, U. Wiedwald, M. Spasova, M. Farle, D. Ponge, B. Gault, J. Neugebauer, D. Raabe, Z. Li, Beyond Solid Solution High-Entropy Alloys: Tailoring Magnetic Properties via Spinodal Decomposition, Adv. Funct. Mater. 31 (2020) 2007668.

Liuliu Han, Fernando Maccari, Isnaldi R. Souza Filho, Nicolas J. Peter, Ye Wei, Baptiste Gault,, Oliver Gutfleisch,, Zhiming Li, Dierk Raabe, A mechanically strong and ductile soft magnet with extremely low coercivity, submitted.

Oliver Gutfleisch is a Professor for Functional Materials at TU Darmstadt, a scientific consultant at Fraunhofer IWKS Hanau and is running the external Max-Planck Research Group De Magnete at MPI for Iron Research Düsseldorf. His scientific interests span from permanent magnets for power applications to solid state energy efficient caloric cooling, ferromagnetic shape memory alloys, magnetic nanoparticles for biomedicine, with emphasis on tailoring structural and chemical properties on the nanoscale. He has published more than 460 papers, was awarded an EU ERC Advanced Grant (Cool Innov), is an IEEE Fellow and is the speaker of the DFG Cooperate Research Center 270 Hysteresis Design of Magnetic Materials for Efficient Energy Conversion.

Prof. Victorino Franco (University of Seville, Spain)

Pushing the limits of magnetocaloric high entropy alloys

V. Franco, J.Y. Law
University of Seville, Spain.

Until recently, magnetocaloric high entropy alloys were either limited to low-temperature applications or had sub-par performance, making them less attractive than conventional materials [1]. In the low temperature range, rare-earth HEAs have a relevant magnetocaloric performance [2]. At higher temperatures, implementing a magnetostructural phase transition in rare-earth free HEAs boosts MCE response, increasing it by one order of magnitude, bridging the gap with respect to the more conventional magnetocaloric materials [3,4]. We will show that, to obtain the desired properties, the search inside the huge compositional space of HEAs has to be performed with a directed search strategy that takes the material from a low or medium-entropy alloy with the desired functionality toward the HEA space.

[1] J.Y. Law, V. Franco, APL Mater. **9**, 080702 (2021).
[2] H. Yin, J. Law, Y. Huang, V. Franco, H. Shen, S. Jiang, Y. Bao, and J. Sun, Mater. Des. **206**, 109824 (2021)
[3] J. Y. Law, L. M. Moreno-Ramírez, Á. Díaz-García, A. Martín-Cid, S. Kobayashi, S. Kawaguchi, T. Nakamura, and V. Franco, J. Alloys Compd. **855**, 157424 (2021)
[4] J. Y. Law, Á. Díaz-García, L. M. Moreno-Ramírez, and V. Franco, Acta Mater. **212**, 116931 (2021)

Victorino Franco is a Professor at the Condensed Matter Physics Department of University of Seville. His research focuses on magnetic materials for energy applications, including soft magnetic and magnetocaloric materials. He has published more than 200 papers and has an h-index of 42. He received young scientist awards from the Royal Order of Chivalry of Seville and from the Spanish Royal Physics Society and was named 2019 IEEE Magnetics Society Distinguished Lecturer. He served as chair of the Spain Chapter of the IEEE Magnetics Society, chair of the Magnetic Materials Committee of the Minerals, Metals & Materials Society (TMS), and was General Chair for the 2022 Joint MMM-INTERMAG Conference.

Dr. Natalia Shkodich (Universität Duisburg-Essen)

Tailoring magnetism of nanocrystalline of CoCrFeNiGax (x = 0.5, 1.0) high entropy alloys by high energy ball milling.

N. F. Shkodich, M. Spasova, U. Wiedwald, M. Farle.

Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany

The high energy ball milling (HEBM) in planetary ball mills can yield stable microstructures and nanocrystalline high entropy alloys (HEAs) with better homogeneity compared to other non-equilibrium processes.

We report the successful fabrication of nanocrystalline singe *fcc* phase CoCrFeNiGa *x* (*x* = 0.5, 1.0) powder particles with good structural and compositional homogeneity by HEBM. The XRD, SEM/EDX, and TEM/EDX results showed that *fcc* phase with refined microstructure of nanosized grains (~10 nm) could be obtained after 190 min of HEBM at 900 rpm.

Based on DSC results the produced HEA powders demonstrated a thermal stability of up to 1273K which is remarkable in regard to the low melting temperature T_{melt} =302.9 K of Ga.

We used HEBM - produced CoCrFeNiGa *x* (*x* = 0.5, 1.0) powders to fabricate *homogeneous* nanocrystalline bulk HEAs by spark plasma sintering (SPS). SPS at 1073 K of the $CoCrFeNiGa_{0.5}$ powder increased the crystallinity of the *fcc* phase, while for the equiatomic CoCrFeNiGa powder a partial transformation of *fcc* structure into a *bcc* one was observed. Direct SPS of an elemental powder blend of Co, Cr, Fe, Ni and Ga ingots on the other hand resulted in a less homogeneous compositions.

The obtained nanocrystalline HEA CoCrFeNiGa *x* (*x* = 0.5, 1.0) powders showed a paramagnetic behavior at room temperature and a Curie temperature (T_c) is of 130K-150K. After SPS consolidation the equiatomic CoCrFeNiGa bulk material show a ferromagnetic behavior up to T_c=735-750K. Its saturation magnetization M_s^{FM} (300K) increased by a factor of 10 compared to the one of HEA powder connected to the partial phase transition from a fcc to a *bcc* phase. The SPS consolidation at 1073K of $CoCrFeNiGa_{0.5}$ HEA powder, however, did not change its paramagnetic nature at room temperature.

In collaboration with M. Spasova, M. Farle, U. Wiedwald. Financial support through DFG– Project-ID 405553726 – TRR 270 is acknowledged.

Dr. Natalia Shkodich
Junior Research Project Leader
(CRC/TRR 270 HoMMage)

University Duisburg -Essen
Faculty of Physics
Experimental Physics – AG Farle
Lotharstr. 1, 47057 Duisburg,
Germany

Phone: +49 (0)203 379-4284

e-mail:
natalia.shkodich@uni-due.de

Education
Diploma (Chemical Engineering & Technology, 2006), KNRTU, Russia PhD (Physics and Mathematics), ISMAN of Russian Academy of Science, Russia

Research interests
✓ Synthesis of nanostructured materials (high-entropy alloys, metallic glasses, pseudo alloys) by combined use of high energy ball milling and by Spark plasma synthesis for magnetic applications
✓ Characterization of structure–composition–magnetic–mechanical properties relationships

Awards
• Prize-2018 from Moscow Region Governor for achievements in scientific research and innovations (endowed of 10000 €)
• Gold medal for the development of "Nanocomposite electrocontact material and the method of its production" of the XX Moscow International Salon of Inventions and Innovative Technologies "Archimedes-2017".

Dr. Ziyuan Rao (Max-Planck-Institut für Eisenforschung Düsseldorf)

Machine learning-enabled fast high-entropy alloy discovery - a case study on novel Invar alloys

High-entropy alloys are solid solutions of multiple principal elements, capable of reaching composition and feature regimes inaccessible for dilute materials. Discovering novel materials with valuable properties, however, relies on serendipity, as thermodynamic alloy design rules alone often fail in high-dimensional composition spaces. Here, we propose an active-learning strategy to accelerate the design of novel Invar alloys in a practically infinite compositional space of high-entropy alloys, based on very sparse data. Our approach works as a closed-loop integrating machine learning with density-functional theory, thermodynamic calculations, and experiments. After processing and characterizing 17 new alloys, we identified 7 novel high-entropy Invar alloys with extremely low thermal expansion coefficients below 5×10-6 K-1. We demonstrated that our approach has more than 50 times higher efficiency than trial and error. Our study thus opens a new pathway for the fast and automated discovery of novel functional high-entropy alloys with optimal magnetic, thermal and electrical properties.

Name: Ziyuan Rao

E-mail: z.rao@mpie.de

Education:

May 2021– present: Postdoc at Max-Planck institute for iron research, Düsseldorf

Sep. 2017 – Nov. 2021: PhD at Max-Planck institute for iron research, Düsseldorf

Sep. 2014 – Jan. 2017: Master at University of Science and Technology Beijing, Beijing

Sep.2010 - Jul. 2014: Bachelor at University of Science and Technology Beijing, Beijing

Brief research statement:

I am interested in studying high-entropy magnetic and Invar alloys with various approaches including machine learning and atom probe tomography.

Prof. Wolfgang Schuhmann (Ruhr-Universität Bochum)

High-entropy materials catalysts - from high-throughput discovery to novel catalysts for energy conversion reactions

Ieva Cechanavičiūtė[1], Olga Krysiak[1], Tim Bobrowski[1], Tobias Löffler[1], Chanikarn Tomon[1], Lars Banko[2], Corina Andronescu[3], Alfred Ludwig [2], Wolfgang Schuhmann[1]

[1] Analytical Chemistry - Center for Electrochemical Sciences (CES); Faculty of Chemistry and Biochemistry; Ruhr University Bochum; Universitätsstraße 150, D-44780 Bochum, Germany
[2] Materials Discovery and Interfaces; Institute for Materials; Ruhr University Bochum; Universitätsstraße 150, D-44801 Bochum, Germany
[3] Chemical Technology III, Faculty of Chemistry and CENIDE; Center for Nanointegration University Duisburg Essen; Carl-Benz-Straße 199, 47057 Duisburg, Germany

High entropy alloys (HEA) comprising four or more constituent elements, are an interesting new class of materials with tunable chemical composition. The often surprisingly high electrocatalytic activity of HEA is related to an abundance and variation of active sites, resulting from the statistical distribution of the elements on the surface. The challenge involved with the experimental exploration of HEA materials, lies in the enormous number of possible combinations of chemical elements and their mixing ratios, leading to a huge option space for the development of new catalysts. With millions of possible element combinations and roughly 10^4 possible mixing ratios for each material system, fundamentally new research strategies are required.

A high-throughput experimentation strategy is reported, enabling rapid synthesis and screening of possible HEA catalysts materials for important reaction in the field of energy conversion and storage. Combinatorial co-deposition using magnetron sputtering is applied to cover substantial parts of the total composition space of quinary HEA material systems in materials libraries. Electrochemical high-throughput screening is applied to map the electrocatalytic activity over the chemical compositions. Moreover, if a hit composition is discovered, different synthesis approaches were implemented which allow for the development of powder-type electrocatalysts and hence a successful initial scale-up of the discovered material.

Examples concerning the discovery and electrochemical evaluation of novel high-entropy materials for energy conversion reactions will be provided.

Acknowledgements: I am grateful to all coworkers and cooperation partners for their input in the research I am allowed to present as well as to a variety of funding agencies including the DFG, the BMBF, and the ERC.

Wolfgang Schuhmann studied chemistry at the University of Karlsruhe, and completed his PhD in 1986 at the Technical University of Munich. After finishing his habilitation at Technical University of Munich in 1993, he was appointed professor for Analytical Chemistry at the Ruhr University Bochum in 1996. His research interests cover a broad spectrum of different fields of electrochemistry, including biosensors, biofuel cells, batteries, photoelectrochemistry, electrocatalysts for energy conversion including high-entropy materials, scanning electrochemical microscopy, scanning electrochemical cell microscopy, in-situ electrochemistry-spectroscopy techniques, micro- and nanoelectrochemistry, among others.

Prof. Martin Sahlberg (Uppsala University, Sweden)

High entropy alloys for the hydrogen society

When switching the energy system to renewable sources, metal hydrides have many uses including rechargeable batteries, hydrogen storage, hydrogen compression and thermal storage. State of the art materials for these applications such as LaNi5 and TiFe, however, suffer certain limitations such as degradation during repeated hydrogen cycling and harsh activation conditions for initial hydrogen uptake, promoting the need for novel materials. One class of materials that are interesting options are High Entropy Alloys. Due to the random distribution of the elements, there is a large variety of local environments for hydrogen, potentially unlocking sites that are unavailable in conventional transition metal hydrides. It is therefore imperative to establish design rules to enable tuning of the hydrogen sorption properties. The effect of having many differently sized metals on the crystal structure is also not fully understood, and is believed to have a high impact on the bulk properties such as hydrogen sorption in these materials.
This talk will cover synthesis and evaluation of a wide range of HEAs, focusing on structural and hydrogen sorption properties. Several new design rules have been established, and verified using a combination of experiments and statistical/machine learning methods.

Martin Sahlberg is a professor in materials chemistry at the Ångström Laboratory, Uppsala University, Sweden. Since his PhD in 2009, his research has focused on materials design for sustainable development, with emphasis on metal hydrides and magnetic materials. He is also heavily involved in neutron scattering activities in Sweden, with focus on ESS. He is currently Director for SwedNess, a Swedish research school in neutron scattering employing 40 PhD-students in functional materials, life science, basic chemistry and physics, and engineering.

Prof. Babak Anasori (Mechanical and Energy Engineering, Indiana University-Purdue University, USA)

High-entropy 2D Transition Metal Carbide MXenes

Babak Anasori

Department of Mechanical and Energy Engineering, Purdue School of Engineering and Technology, Indiana University-Purdue University Indianapolis (IUPUI), Indianapolis, Indiana, 46202, United States

The family of two-dimensional (2D) transition metal carbides and nitrides MXenes is one of the largest families of 2D materials in terms of the number of possible compositions, with more than forty synthesized compositions (e.g., Ti2C, Ti3C2, Nb2C, Mo2C) and many more that are predicted to exist. Ordered double-transition metals carbides have been synthesized by using two transition metals, such as in Mo1.3Y0.6C, Cr2TiC2, and Mo2Ti2C3, with either in-plane or out-of-plane atomic ordering. In the ordered double transition metal carbides (MXenes), physical, electrochemical, and mechanical properties, such as electrical conductivity and optical properties, can be tuned by controlling the transition metals ordered chemistry.
In 2021, by combining the two fields of double-metal MXenes and high-entropy alloys, a new area in the MXenes field has emerged, as high-entropy MXenes. In these MXenes, four transition metals are combined in the form of solid solutions in the 2D atomic planes of MXenes. We have successfully synthesized two high-entropy MXenes of TiVNbMoC3Tx and TiVCrMoC3Tx. In this talk, the rationale behind high-entropy MXenes, their synthesis conditions, and some of their properties will be discussed.

Reference:
High-Entropy 2D Carbide MXenes: TiVNbMoC3 and TiVCrMoC3, **ACS Nano**, 15, 12815-12825 (2021)

Dr. Babak Anasori received his PhD at Drexel University in 2014 in the Materials Science and Engineering Department, the birthplace of MXenes. Before joining Purdue School of Engineering & Technology, IUPUI, he was a Research Assistant Professor at the A.J. Drexel Nanomaterials Institute and Materials Science and Engineering at Drexel University from 2016 to 2019. Dr. Anasori is the second most published author in MXenes, with more than 140 refereed publications on MXenes and their precursors. Dr. Anasori is among the Web of Science Highly Cited Researchers in 2019, 2020, and 2021. He has received several international awards, including the 2016 Materials Research Society (MRS) Postdoctoral Award, 2021 Drexel University 40-under-40, and the 2021 WIN Rising Star Award in Nanoscience and Nanotechnology.

banasori@iupui.edu

https://www.babakanasori.com

Prof. Alfred Ludwig (Ruhr-Universität Bochum)

Exploration of the multidimensional high entropy alloy search space using high-throughput experimentation

Prof. Dr.-Ing. Alfred Ludwig
Institute for Materials and ZGH, Ruhr University Bochum, Bochum, Germany
https://www.mdi.ruhr-uni-bochum.de/index.html.en

Discovery of new materials is a key challenge in materials science: e.g. new materials for sustainable production/storage/conversion of energy carriers are necessary to improve existing and to enable future energy systems. Compositionally complex materials ("high entropy alloys") promise new discoveries in a however extremely large search space. For the exploration and exploitation of this multidimensional search space, efficient methods for discovery and optimization are necessary: Thin-film combinatorial materials science (1) is an effective means to produce large datasets on new materials. This approach is useful for validation of theoretical predictions (e.g. from high-throughput computations), and production of large, consistent and complete experimental datasets which can be used for materials informatics. The approach comprises fabrication and processing of thin-film materials libraries by combinatorial sputter deposition processes and optional post-deposition treatments, followed by the high-throughput characterization of the different thin-film samples contained in these libraries, and finally the organization of the acquired multi-dimensional data in adequate databases as well as their effective computational analysis and visualization. High-throughput material characterization methods are automated, fast, and mostly non-destructive: examples are EDX for composition, XRD for crystal structure, high-throughput test stands for temperature-dependent resistance (phase transformation), magnetic, optical and mechanical properties as well as scanning droplet cells for (photo)electrochemical properties screening. Results for up to quinary systems are visualized in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will cover and discuss examples of combinatorial discoveries and development of new compositionally complex materials in different materials classes and forms (films, nanoparticles) (e.g. (2)). Furthermore, a new approach (3) to accelerate atomic-scale measurements for complex alloys is presented as well as applications of materials informatics to accelerate and improve the materials discovery process (4, 5).

(1) A. Ludwig (2019) *Discovery of new materials using combinatorial synthesis and high-throughput characterization of thin-film materials libraries combined with computational methods*, npj computational materials 5, 70
(2) T. Löffler, H. Meyer, A. Savan, P. Wilde, A. Garzón Manjón, Y. T. Chen, E. Ventosa, C. Scheu, A. Ludwig, W. Schuhmann (2018) *Discovery of a multinary noble metal free oxygen reduction catalyst*, Adv. Energy Mater. 8, 1802269
(3) Y. J. Li, A. Savan, A. Kostka, H. S. Stein, A. Ludwig (2018) *Accelerated atomic-scale exploration of phase evolution in compositionally complex materials*, Materials Horizons 5, 86 - 92
(4) P. M. Maffettone, L. Banko, P. Cui, Y. Lysogorskiy, M. Little, D. Olds, A. Ludwig, A. I. Cooper (2021) *Crystallography companion agent for high-throughput materials discovery*, Nature Computational Science 1, 290 – 297.
(5) L. Banko, O. A. Krysiak, J. K. Pedersen, B. Xiao, A. Savan, T. Löffler, S. Baha, J. Rossmeisl, W. Schuhmann, A. Ludwig (2022) *Unravelling composition-activity-stability trends in high entropy alloy electrocatalysts by using a data-guided combinatorial synthesis strategy and computational modelling*, Adv. Energy Mater., 2103312

Alfred Ludwig is Professor for Materials Discovery and Interfaces at the Institute for Materials of Ruhr University Bochum (RUB). In 1999 he received his Ph.D. in mechanical engineering from University of Karlsruhe. He then worked at the caesar research center in Bonn and became head of the research group "Combinatorial Materials Science" in 2002. At the same time, he started at RUB as junior professor and became full professor in 2012. He initiated and organised the research center ZGH (Center for Interface-Dominated High Performance Materials) of which he is the scientific director. In 2021 he became as well one of the founding directors of the Research Alliance Ruhr research center "Future Energy Materials and Systems". His research interests include combinatorial materials science, high-throughput experimentation, material informatics, autonomous experimentation, materials for nano/microsystems, thin films and multinary nanoparticles, with a focus on multifunctional materials for future energy systems, e.g. novel electrocatalysts.