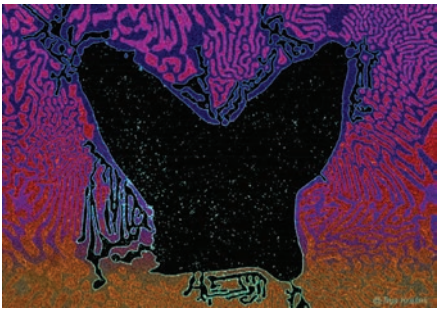
Workshop on

„High-Entropy Alloys: from basic studies to industrial applications”

November 21st
ECMetAC Days 2022, Split, Croatia

Chairperson:
Dr. Magdalena Wencka

SCHEDULE & ABSTRACTS



An art of Slovenian artist's Teja Krašek based on a SEM image of $CrCuFeNiZr_x$ eutectic alloy microstructure taken by Dr. Andreja Jelen (Jožef Stefan Institute, Ljubljana, Slovenia). The alloy was delivered by Prof. Sheng Guo (Chalmers University of Technology, Göteborg, Sweden).

The workshop is dedicated
to honour scientific achievements
of ***Prof. Janez Dolinšek***
the Head of JSI High-Entropy Alloys Group
(Jožef Stefan Institute, Ljubljana, Slovenia)
for his ***65th Birthday Anniversary****.*

The celebrant holds
a single crystal of the i-AgInYb quasicrystal
(Phys. Rev. B, ***84****, 134205 (2011)).*

Schedule:
/presenting authors only/

OPENING:
13:00 – 13:15 *Ante Bilušić, Julian Ledieu, Magdalena Wencka*

Honorary chairing person: Janez Dolinšek

13:15 – 14:00 *Sheng Guo*: Eutectic High-Entropy Alloys & Refractory High-Entropy Alloys: Opportunities and Challenges

Session 1: STRUCTURE and SURFACES
Chairing person: Sheng Guo

14:00 – 14:30 *Anton Meden:* Phase Identification and Quantification in High Entropy Alloys Using X-Ray Powder Diffraction
14:30 – 15:00 *Marc Armbrüster:* HEAs in Catalysis - An Overview
15:00 – 15:20 *Andreja Jelen:* Multi-phase structure of Sn-containing HEAs

15:20 – 16:20 Coffee break (birthday cake & more…)

Session 2: PHYSICAL PROPERTIES
Chairing person: Peter Gille

16:20 – 16:40 *Jože Luzar*: $AlCoFeNiCu_x$ (x = 0.6 – 3.0) zero-magnetostriction magnetically soft high-entropy alloys
16:40 – 17:00 *Primož Koželj*: $Al_{0.5}TiZrPdCuNi$ in HEA vs metallic-glass form: How important is the crystallinity of HEAs for electronic transport?

ROUND-TABLE DISSCUSSION & CLOSING
Chairing person: Magdalena Wencka

17:00 – 17:20 Trends in development of high-entropy alloys
17:20 – 17:30 *Janez Dolinšek, Julian Ledieu*: Closing

Eutectic high-entropy alloys and refractory high-entropy alloys: Opportunities and challenges

S. Guo

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

e-mail: sheng.guo@chalmers.se

The alloying concept of high entropy alloys (HEAs) opens a vast unexplored compositional space potentially leading to numerous new materials and new applications, but also brings new challenges on how to design these alloys properly. In this lecture, I will show opportunities and challenges that are brought by two particular examples of HEAs, refractory HEAs and eutectic HEAs. Refractory HEAs are promising candidates for ultra-high temperature applications, but how to satisfy demanding material requirements to simultaneously obtain decent room-temperature ductility, high-temperature strength and oxidation resistance pose a formidable scientific challenge. Eutectic HEAs, recently becoming prototype dual-phase materials, show a wide spectrum of mechanical properties when they are subject to thermomechanical treatments, while their good castability and decent mechanical properties and corrosion resistance render great application potential where directly cast materials are in need.

Phase Identification and Quantification in High Entropy Alloys Using X-Ray Powder Diffraction

A. Meden

University of Ljubljana, Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia

e-mail: tone.meden@fkkt.uni-lj.si

Ideally, high entropy alloys (HEA) are single phase with randomly mixed atoms of the constituent elements at crystallographic sites of a (simple) crystal structure. In such cases, X-ray powder diffraction (XRPD) is an efficient tool to: 1. prove the phase purity, 2. determine the structure type, 3. determine the exact parameters of the unit cell, 4. estimate the size and strain of the coherently scattering domains.

Often HEAs are (complex) multiphase mixtures, and in such cases the XRPD is an essential tool for phase identification and quantification. For the identified phases, points 2 and 3 above also apply, point 4 is only possible for predominant phases.

The reliability of the results is greatly increased when XRPD methods are used together with scanning electron microscopy techniques (SEM) (BSE imaging and EDS grain analysis).

The above is illustrated with examples (as in Fig. 1).

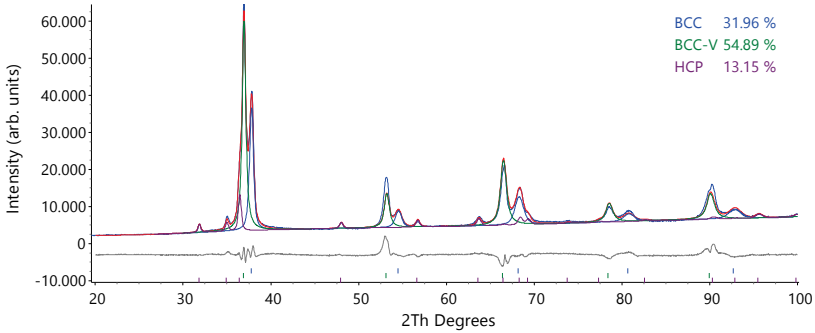


Fig. 1: Rietveld plot of ScHfNbTaZr showing the contributions of the three phases to the measured diffraction pattern and their weight fractions.

HEAs in catalysis – an overview

M. Armbrüster

Institute of Chemistry, Chemnitz University of Technology, Germany

*e-mail: marc.armbruester@chemie.tu-chemnnitz.d*e

High-entropy alloys are an interesting new class of materials and their physical and chemical properties are momentarily explored. For heterogeneous catalysis the randomly occupied crystallographic sites are principally offering a nearly endless variety of potentially active sites. This opens the possibility that there are active sites available for every heterogeneously catalysed reaction resulting in "general" catalysts.

This resulted in tests of HEAs in a number of catalytic reactions. Publications in the field will be presented and critically analysed concerning the phases present and evaluation of the catalytic properties. In addition, a brief outlook on the potential of HEAs in heterogeneous catalysis will be presented.

Multi-phase structure of Sn-containing HEAs

[1,*]A. Jelen, [1]D. Gačnik, [2]A. Meden, [3]Q. Hu, [4]S. Guo, [1]J. Dolinšek

[1]*J. Stefan Institute, Ljubljana, Slovenia*
[2]*Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia*
[3]*Jiangxi Academy of Sciences, Nanchang, PR China*
[4]*Chalmers University, Göteborg, Sweden*

**e-mail: andreja.jelen@ijs.si*

Tailoring of new materials is a playground for many scientists. To combine delicate physical properties in an unusual way, high-entropy alloys (HEAs) serve as an ideal base. We have incorporated Sn into HEAs composed of refractory metals Hf, Nb, Ti and Zr with the addition of 3d transition metals Cu, Fe and Ni. The complex microstructures of those alloys are presented in Fig. 1. All Sn-containing alloys are multi-phase mixtures of intermetallic compounds (in most cases four). A common feature of the alloys is a microstructure of large crystalline grains of a hexagonal $(Hf,Ti,Zr)_5Sn_3$ partially ordered phase embedded in a matrix that also contains many small inclusions.

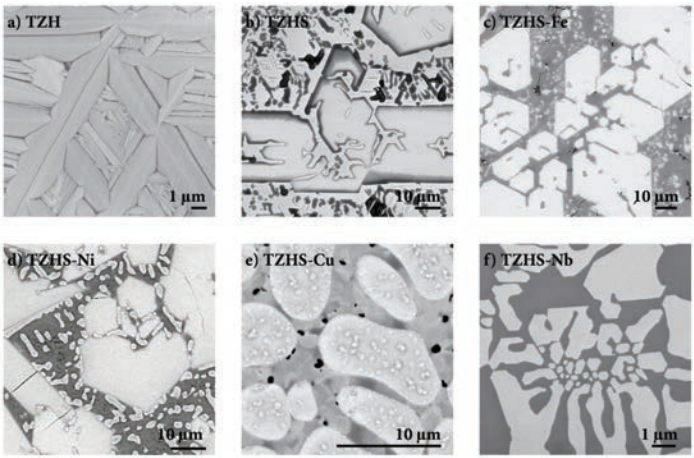


Figure 1: SEM BSE images of (**a**) HfTiZr (HTZ), (**b**) HfTiZrSn (HTZS), (**c**) HfTiZrSnFe (HTZS-Fe), (**d**) HfTiZrSnNi (HTZS-Ni), (**e**) HfTiZrSnCu (HTZS-Cu), (**f**) HfTiZrSnNb (HTZS-Nb).

$AlCoFeNiCu_x$ (x = 0.6 – 3.0) zero-magnetostriction magnetically soft high-entropy alloys

*[1]J. Luzar, [2]P. Priputen, [1]S. Vrtnik, [1,3]P. Koželj, [1]A. Jelen, [1,4]M. Wencka, [1]D. Gačnik, [1]P. Mihor, [1]B. Ambrožič, [5]G. Dražić, [6]A. Meden, [1,3]J. Dolinšek

[1]J. Stefan Institute, Ljubljana, Slovenia
[2]Slovak University of Technology, Faculty of Materials Science and Technology, Bratislava, Slovak Republic
[3]Univ. of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia
[4]Institute of Molecular Physics PAS, Poznań, Poland
[5]National Institute of Chemistry, Ljubljana, Slovenia
[6]Univ. of Ljubljana, Faculty of Chem. and Chem. Tech., Ljubljana, Slovenia

**e-mail: joze.luzar@ijs.si*

This contribution [1] will present our efforts in further advancing soft ferromagnetic high-entropy alloys towards practical magnetic applications via a study of the $AlCoFeNiCu_x$ (x = 0.6 – 3.0) system. $AlCoFeNiCu_{2.0}$ proved to have superior magnetostriction and magnetic softness properties. It shows precisely zero magnetostriction, $\lambda_s = 0$, reasonably low coercivity $H_c \approx 650$ Am^{-1} and substantial saturation magnetic polarization of $J_s \approx 0.55$ T. Near zero magnetostriction was also observed for x = 2.5 and 3.0, so that $AlCoFeNiCu_x$ HEAs for x = 2.0 – 3.0 are all relevant for applications as supersilent (inaudible to a human ear) materials. In the alloys, three phases develop on the microscale and are further nanostructured on the 10-nm scale. It is considered that the ideal zero magnetostriction in the $AlCoFeNiCu_{2.0}$ alloy is a consequence of the three-phase microstructure, in which the magnetostrictions of different signs in the three phases exactly compensate each other. The magnetic softness of the HEAs is attributed to the mechanism of exchange-averaging of magnetic anisotropy.

[1] J. Luzar, P. Priputen, S. Vrtnik, *et al.*, Adv. Mater. Interfaces. *Available online prior to inclusion in an issue:* https://doi.org/10.1002/admi.202201535

$Al_{0.5}TiZrPdCuNi$ in HEA vs metallic-glass form: How important is the crystallinity of HEAs for electronic transport?

[1,2]Magdalena Wencka, [1]M. Krnel, [1]A. Jelen, [1]S. Vrtnik, [1]J. Luzar, *[1,3]P. Koželj, [1]D. Gačnik, [4]A. Meden, [5]Q. Hu, [5]C. Wang, [6]S. Guo and [1,3]J. Dolinšek

[1] *Jožef Stefan Institute, Ljubljana, Slovenia*
[2] *Inst. of Molecular Physics, Polish Academy of Sciences, Poznan, Poland*
[3] *Faculty of Mathematics and Physics, University of Ljubljana, Slovenia*
[4] *Faculty of Chemistry and Chem. Technology, Univ. of Ljubljana, Slovenia*
[5] *Institute of Applied Physics, Jiangxi Academy of Sciences, Nanchang, People's Republic of China*
[6] *Chalmers University of Technology, Göteborg, Sweden*
**e-mail: primoz.kozelj@ijs.si*

High-entropy alloys can be viewed as materials that are half way between ordered crystals and amorphous substances – they exhibit a topologically ordered lattice but on the other hand also an immense amorphous-type chemical disorder. This contribution will present our efforts [1] at determining the importance of the crystal lattice vs the importance of the disorder on the electronic transport in HEAs through a comparative study of a 6-component $Al_{0.5}TiZrPdCuNi$ synthesized in either high-entropy alloy (HEA) or metallic glass (MG) form.
Both forms exhibit a large, negative-temperature-coefficient resistivity, positive thermopower, positive Hall coefficient and small thermal conductivity. A spectral conductivity model within the Kubo-Greenwood formalism allowed us to analyze both modifications on equal footing and reproduce their electronic transport data. The contribution of the phonons to the transport coefficients in both forms is small, so the temperature dependence originates from the electronic properties as described by the spectral conductivity model.
The similarities between the HEA and MG forms of $Al_{0.5}TiZrPdCuNi$ indicate that the immense chemical disorder and not the crystal lattice is the main driving force behind electronic transport in HEAs.

[1] M. Wencka *et al.*, Scientific Reports **12**, 2271 (2022).