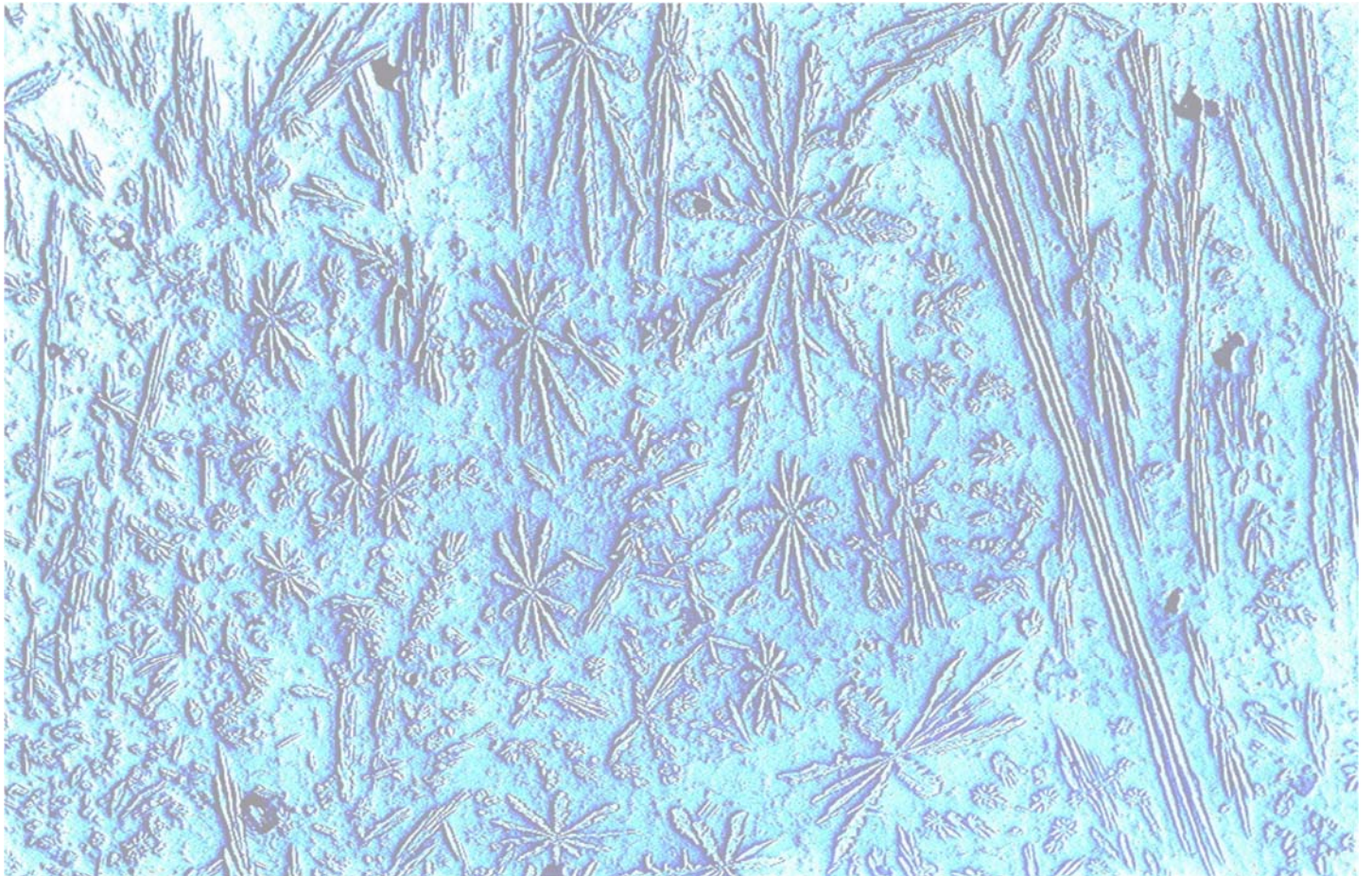# European C-MetAC Days 2020

On-line meeting

December 7 – 10, 2020

PROGRAM

Monday, December 7, 2020
Workshop on "Team skills" guided by Dr. Magdalena Wencka
For enquiries regarding the workshop, please contact magdalena.wencka@ijs.si

Tuesday, December 8, 2020

Chairs: Juri Grin

09:30 – 09:40		Julian Ledieu	*Welcome*
09:40 – 10:00		Vincent Fournée	*Pat Thiel and Quasicrystal surfaces*
10:00 – 10:20	O-1	Laura Agnarelli	$Mg_{29.16}Pt_4$: *a complex intermetallic compound*
10:20 – 10:40	O-2	Yurii Prots	*Structural complexity of* Mn_6Ga_{29}
10:40 – 11:00	O-3	Kristian Bader	*Single crystal growth and characterization of* Ga_3Pd_5
11:00 – 11:30		Break	

Chairs: Peter Gille

09:30 – 09:40 times below:

11:30 – 11:50 O-4 Girma Gebresenbut
Peritectic formation and phase stability of the icosahedral quasicystal i-GdCd and its ternary variants with Zn, Mg, and Y

11:50 – 12:10 O-5 Maike Thal
Quasi-Binary Systems $(Ga_{1-x}Sb_x)Pd_2$ *and* $(Ga_{1-x}Bi_x)Pd_2$

12:10 – 12:30 O-6 Alfred Amon
Crystal structure and bonding in the polar intermetallic compound $Be_{46}Pt_{14}$

12:30 – 13:30　　　　　Lunch

Chairs: Janez Dolinsek

13:30 – 13:50　O-7　Ireneusz Buganski
The distribution moments analysis for the high-temperature X-ray diffraction data of d-AlCuRh

13:50 – 14:10　O-8　Andreja Jelen
Should nanostructure determination in high-entropy alloys be a new standard?

14:10 – 14:30　O-9　Sylwia Gutowska
Electron-phonon mediated superconductivity of LiBi

14:30 – 14:50　O-10　Mitja Krnel
Superconductivity in high-entropy and medium-entropy alloys from the Ti-Zr-Hf-Nb-Ta-Sc system

14:50 – 15:10　O-11　Gabriel Kuderowicz
Soft-mode enhanced type-I superconductivity in LiPd$_2$Ge

15:10 – 15:40　　　　　Break

Chairs: Magdalena Wencka

15:40 – 16:00　O-12　Marko Kuveždić
Universal superconductivity in compositionally complex transition metal alloys

16:00 – 16:20　O-13　Darja Gačnik
The effect of structural inhomogeneity on "dirty" superconductivity in tin-containing alloys

16:20 – 16:40　O-14　Naveen Singh Dhami
Pressure dependent electronic structure of EuTGe$_3$ (T = Co, Rh)

16:40 – 17:10   Poster discussion
                       P1 – Radoslaw Strzałka
                       High-temperature structural studies of d-AlCuRh –
                       new correction for phasons
                       P2 – Oscar Shedwick
                       The study of the surface of a Gallium Nickel binary
                       P3 – Naïma Saadi
                       Utilising 3D-printing to aid visualisation of complex
                       atomic structures

Wednesday, December 9, 2020

Chairs: Silke Bühler-Paschen

09:30 – 09:50   O-15   Gaku Eguchi
Transport study of topological bands: remarkable feature in a thermoelectric material

09:50 – 10:10   O-16   Kamil Ciesielski
Enhanced thermoelectric performance in n-type regime for half-Heusler phase ScNiSb

10:10 – 10:30   O-17   Stanislav Vrtnik
Thermal memory effect in the   -brass type pseudo-binary $Ni_2Mn_{0.3}Zn_{10.7}$ phase

10:30 – 11:00   Break

Chairs: Marc de Boissieu

11:00 – 11:20   O-18   Shelby Turner
Phonon behavior in a random solid solution: A lattice dynamics study on the high-entropy alloy FeCoCrMnNi

11:20 – 11:40   O-19   Geoffroy de Laitre
Dynamical properties of the incommensurately modulated Rb_2ZnCl_4 phase

11:40 – 12:00   O-20   Joanna Smietanska
Molecular dynamics simulation for validation of the phononic ADPs in Hyp-1 protein

12:00 – 12:30   Poster discussion
P4 – Tomasz Toliński
Magnetic and electrical properties of $Gd_5Si_2Ge_2$ thin films
P5 – Karol Synoradzki
Magnetocaloric effect in hexagonal $NdCrGe_3$
P6 – Bruno Gudac
De Haas-van Alphen oscillations in ZrSiS and HfSiS

12:30 – 13:30   Lunch

13:30 – 13:50   O-21   Dominic Burnie
Atomic diffusion on the fivefold surface of the i-Ag-In-Yb quasicrystal

13:50 – 14:10   O-22   Amnah Alofi
Thin film growth of pentacene (Pn) on the two-fold surface of the icosahedral Ag-In-Yb quasicrystal

14:10 – 14:30   O-23   Florian Brix
Tuning adsorption energies and reaction pathways by alloying: PdZn versus Pd for CO_2 reduction to methanol

14:30 – 14:50   O-24   Iryna Antonyshyn
Structural complexity and chemical behaviour of $Hf_2B_2Ir_5$ in oxygen evolution reaction

14:50 – 15:20   Break

15:20 – 15:40   O-25   Sebastian Schenk
Dodecagonal oxide quasicrystal approximant with 72 tiling elements

15:40 – 16:00   O-26   Thiago Trevizam Dorini
Two-dimensional ABO_3/Me oxide quasicrystal approximants: insights from Density Functional Theory

16:00 – 16:20   O-27   Catalina Ruano Merchan
New Quasicrystal Approximants in the SrTiO3/Pt(111)/Al_2O_3(0001) system

16:20 – 16:40   O-28   Fevzi Kafexhiu
Tribological performance of the $AlCoCrFeNi_{2.1}$ eutectic high-entropy alloy in as-cast and aged condition

16:40 – 16:50   Julian Ledieu
Concluding Remarks

Thursday, December 10, 2020

09:30 – 11:00	Science Board Meeting
11:00 – 11:20	Break
11:20 – 12:30	Governing Board Meeting and General Assembly
14:00 – 14:10	Online announcement of the oral and poster prizes

Mg$_{29.16}$Pt$_4$: a complex intermetallic compound

[1,*]L. Agnarelli, [1]Y. Prots, [1]A. Leithe-Jasper, [1]Yu. Grin

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The structural motif of Mg$_{29.16}$Pt$_4$ (space group $F\bar{4}3m$, a = 20.1273 (1) Å) is made up by interpenetrating Mackay clusters. The empty spaces left by the Mackay clusters are filled by tetrahedral units of four PtMg$_9$ tricapped trigonal prisms and Pearce clusters made of tetrahedral units of face-sharing PtMg$_{12}$ icosahedra (Figure 1). This phase reveals an intricate pattern of disorder at the atomic positions of the Mackay icosidodecahedron.
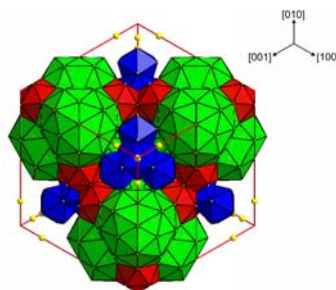

Figure 1. Space filling arrangement of Mackay clusters (green), tetrahedral units of four PtMg$_9$ tricapped trigonal prisms (blue) and the Pearce clusters (red). Unit cell is highlighted in red.

Structural complexity of Mn_6Ga_{29}

Yu. Prots,[1]* I. Antonyshyn,[1] H. Rosner,[1] L. Akselrud,[1,2] I. Margiolaki,[3] Yu. Grin[1]

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The gallium richest phase in the binary Mn−Ga system was synthesized by reaction of elemental Mn with an excess of Ga at different temperatures (430–520 K) and subsequent removal of the flux by high-temperature centrifugation-aided filtration. Combining single crystal and powder X-ray diffraction performed *in-situ* (T = 100−600 K, ESRF, ID22 beamline), four modifications were established: ω_0-**Mn_6Ga_{29}**, monoclinic, *P2/c*, a = 19.7785(1) Å, b = 9.9305(1) Å, c = 12.5612(1) Å, β = 107.62(1) °, low temperatures phase, stable up to ~RT; ω_1-**Mn_6Ga_{29}**, triclinic, $P\bar{1}$, a = 6.3020(5) Å, b = 9.9388(7) Å, c = 18.911(2) Å, α = 90.52(1)°, β = 90.79(1)°, γ = 90.43(1)°, ~290−440 K; ω_2-**Mn_6Ga_{29}**, monoclinic subcell, *P2/m*, a = 6.3209(1) Å, b = 9.9707(1) Å, c = 6.3260(1) Å, β = 90.63(1) °, 440−480 K, development of the superstructure model is in progress; ω_3-**Mn_6Ga_{29}**, monoclinic, *P2/m*, a = 6.3334(1) Å, b = 10.0111(1) Å, c = 6.3373(1) Å, β = 90.037(9) °, from 480 K to peritectic decomposition at 663 K. Due to the low symmetry of ω_0-, ω_1-, and ω_2-modifications and negligible deformation of ω_3-Mn_6Ga_{29} lattice, the unambiguous indexing of the reflections and phase identification is only possible by using high-resolution PXRD patterns. The single-crystal investigations are hampered by presence of multi-twin domains. While Mn_6Ga_{29} undergoes a series of displacive phase transitions, ω_2 and ω_3 modifications cannot be fixed properly by quenching of the samples and $\omega_0 \longleftrightarrow \omega_1$ transition is kinetically slowed down (hysteresis). Due to the negligible thermal effects that associated with structural changes, most of the transitions could not be detected by differential thermal analysis.

All manganese atoms in the crystal structures of Mn_6Ga_{29} are coordinated exclusively by Ga forming distorted tetragonal antiprisms. The monocapped [$MnGa_{8+1}$] antiprisms condense into pairs by sharing their pseudo-quadratic faces and are interconnected via common apexes and edges to form a 3D framework. The structures differ only by small displacements or the deformation of these building blocks.

1 I. Antonyshyn, Yu. Prots, et al. *J. Solid State Chem.* **199** (2013) 141.

Single crystal growth and characterization of Ga$_3$Pd$_5$

[1]K. Bader*, [1]S. Park, [1]J. Schwerin, [2]W. Carrillo-Cabrera, [2]U. Burkhardt, [2]Yu. Grin, [1]P. Gille

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Single crystal growth of Ga$_3$Pd$_5$ from Ga-rich solution using the Czochralski technique is described for the first time.

A single crystal with a mass of more than 3 g could be obtained despite of the narrow temperature window of the solid/liquid equilibrium (1030°C < T < 980°C) in the binary Ga-Pd system [1]. The grown crystal shows a strong anisotropic growth morphology with extended {010} faces which is different from results with structurally related phases such as GaPd$_2$ [2, 3]. Structure analyses using X-ray powder and single crystal diffraction correspond with the known structure model of Ga$_3$Pd$_5$ in the space group *Pbam* [4]. Tiny effects found in thermal analysis led to further investigations of the grown crystal. Ongoing studies by X-ray diffraction, SEM and TEM examinations revealed the presence of coherent precipitates of GaPd ($P2_13$) in annealed samples, indicating a retrograde solubility of Ga in Ga$_3$Pd$_5$ at lower temperatures.

The crystal growth process, structural details and ongoing studies on the thermodynamic stability of Ga$_3$Pd$_5$ are reported.

[1] H. Okamoto, J. Phase Equilib. Diff. 29 (2008) 466–467.
[2] Yu. Grin, Modern Perspectives in Inorganic Crystal Chemistry, E.Parthé (Ed.), Kluwer Academic Publ. 1992, pp. 77-95.
[3] J. Schwerin et al., J. Cryst. Growth 401 (2014) 613–616
[4] K. Schubert et al., Naturwiss. 15 (1958) 360–361.

Peritectic formation and phase stability of the icosahedral quasicystal i-GdCd and its ternary variants with Zn, Mg, and Y

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[2]*Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden.*
[3]*Department of Materials Science and Engineering, Uppsala University, Uppsala, Sweden.*

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Stable binary icosahedral quasicrystals (i-QCs) based on rare earth (RE) and cadmium are typically accessed by solution growth experiments, which operate in very narrow composition and temperature windows. Here we present a procedure, which allows to study peritectic reactions between approximant crystal (AC) phase and liquid yielding i-RECd and exemplify with i-GdCd and ternary variants where Cd is partially replaced by isovalent Zn (i-Gd(Cd,Zn)) or Mg (i-Gd(Cd,Mg)), or the 4f element Gd is replaced by non-magnetic Y (i-(Gd,Y)Cd). The solubility limits for Zn and Mg substitution are about 10 and 20 %, respectively, whereas Gd and Y show a complete solid solution behavior. We find that the peritectic decomposition temperature for i-GdCd is 390 °C, which is decreased when Gd is replaced by Y (i-YCd: 350 °C), and increased when Cd is replaced by Zn (i-Gd($Cd_{90}Zn_{10}$): 440 °C), and especially by Mg (i-Gd($Cd_{80}Mg_{20}$): 520 °C). Whereas substitution decisively alters the decomposition temperature (and hence stability) of the considered i-QCs, the decomposition temperature of the corresponding AC phases remains at around 700 °C. We established the changes in the pseudobinary phase diagrams Gd-($Cd_{95}Zn_5$), Gd-($Cd_{90}Zn_{10}$), and Gd-($Cd_{80}Mg_{20}$) with respect to binary Gd-Cd and find a considerable flattening of the region of exposed liquidus line for solidification of the ternary i-QCs. Accordingly, the ternary i-QCs are more conveniently accessed by solution growth and it was possible to obtain faceted grains with sizes up to 4 x 4 x 4 mm.

Quasi-Binary Systems $(Ga_{1-x}Sb_x)Pd_2$ and $(Ga_{1-x}Bi_x)Pd_2$

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Currently, intermetallic compounds based on the binary system Ga-Pd are of interest in search for new catalyst materials for the semi-hydrogenation of acetylene, e.g. $GaPd_2$ [1] as well as $(Ga_{1-x}Sn_x)Pd_2$ [2]. Therefore, systems based on Ga-Pd which comprise a third metal of the groups 13-15 are promising for above mentioned reaction. In this contribution, focus lies on the ternary phases with bismuth and antimony.

In the isothermal section at 500 °C of the ternary Ga-Sb-Pd system [3,4], two compounds were found on the quasi-binary line $(Ga_{1-x}Sb_x)Pd_2$ which requires further investigation in terms of their thermal stability. In contrast, only one compound with the composition of $Ga_{0.5}Bi_{0.5}Pd_3$ is reported for Ga-Bi-Pd so far [5].

For this study, synthesis of compounds on the quasi-binary lines $(Ga_{1-x}Sb_x)Pd_2$ and $(Ga_{1-x}Bi_x)Pd_2$ is done by varying the content of Sb and Bi. The high frequency furnace was ued for melting the constituent metals, followed by annealing the samples at 773 °C for Sb and 600 °C for Bi, respectively, for two month. Metallographic analysis, as well as electron microscopy, confirm two compounds in the Ga-Sb-Pd system. By powder X-ray diffraction they have been identified as orthorhombic $GaPd_2$ and hexagonal $Ga_{0.47}Sb_{0.53}Pd_2$. This indicates the thermal stability of the latter at 773 °C. The different compounds in the Ga-Bi-Pd system are still under investigation.

References:
[1] M. Armbrüster, K. Kovnir, M. Behrens, D. Teschner, Yu. Grin, R. Schlögl, *J. Am. Chem. Soc.* **2010**, *132*, 14745.
[2] O. Matselko, R. R. Zimmermann, A. Ormeci, U. Burkhardt, R. Gladyshevskii, Yu. Grin, M. Armbrüster, *J. Phys. Chem. C* **2018**, *122*, 21891.
[3] K. W. Richter, H. Ipser, *Ber. Bunsenges. Phys. Chem.* **1998**, *102*, 1245.
[4] O. Matselko, U. Burkhardt, Yu. Grin, R. Gladyshevskii, *Chem. Met. Alloys* **2018**, *11*, 6.
[5] M. El Boragy, K. Schubert, *Z. Metallkd.* **1970**, *61*, 597.

Crystal structure and bonding in the polar intermetallic compound $Be_{46}Pt_{14}$

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L. H. Tjeng, A. Leithe-Jasper, Yu. Grin

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Beryllium-rich intermetallic compounds have aroused interest due to their rich structure chemistry and fascinating properties. Electron deficiency and a high degree of covalency in beryllium-rich compounds yield interesting structural motifs where radii differences can lead to large coordination spheres. Oxidation resistance at high temperatures, high mechanical strength and low density drove the investigations of beryllium alloys with transition metals and recently they attracted attention as possible neutron multiplying blanket materials for the next generation of fusion reactors.

Recently, several new polar intermetallic compounds were reported in the Be-Pt system, such as the narrow-gap semiconductor Be_5Pt and the superconducting complex intermetallic compound $Be_{21}Pt_5$.[1,2]

In this study, we report the new intermetallic compound $Be_{46}Pt_{14}$ which is the first representative of the *anti-*$Gd_{14}Ag_{51-x}$ structure type (Figure 1).

Figure 1. Crystal structure of $Be_{46}Pt_{14}$, projection along [0 0 1].

Here, beryllium atoms form a double-chalice structure around linear chains of Pt atoms. These motifs are connected by stacks of capped triangular prisms.

Electronic structure calculations and hard x-ray photoemission spectra confirmed the suspected charge transfer from Be to the electronegative Pt atoms, exacerbating the valence electron deficiency within the Be-sublattice. The compound $Be_{46}Pt_{14}$ represents an unusual defect variant of the $Gd_{14}Ag_{51-x}$ structure family, as confirmed by detailed crystallographic characterization together with spectroscopic and computational analysis of the electronic structure.

[1] A. Amon, E. Svanidze, et al. *Angew. Chem. Int. Ed.* **2019**, 58, 15928.
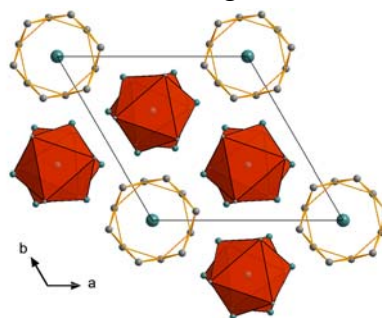[2] A. Amon, A. Ormeci, et al. *Acc. Chem. Res.* **2018**, 51(2), 214.

The distribution moments analysis for the high-temperature X-ray diffraction data of d-AlCuRh

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The atomic structure of the decagonal Al-Cu-Rh quasicrystal with a space group $P10_5/mmc$ is refined based on five X-ray diffraction datasets, collected at 293 K, 1013 K, 1083 K, 1153 K and 1223 K with the use of a synchrotron radiation [1]. The real-space structure solution with the tiling-and-decoration approach is used for every dataset. The Rhombic Penrose Tiling is used as a quasilattice.

The novelty of our work is the application of the moment series expansion of the structure factor that allows to model the phasonic disorder quenched within the atomic structure [2]. The standard generalized Debye-Waller correction is in this approach abandoned.

All the crystallographic R – factors are ranging from 5.9% to 6.4% for the common for all datasets 1460 symmetry-inequivalent peaks. What is the most intriguing is the correlation (Pearson correlation equal to 0.85) between lattice parameters (edge-length of rhombus and the interatomic layer distance) and the residual density that is not correlated with R – factors. Residual density is agglomerated in the origin of the 4D unit cell what has two possible solutions: there is an atom in the center of a decagonal cluster or it is a manifestation of the General Penrose Tiling. Since the residual density is from 2.2% to 3%, what is below the possible density of an atom, we incline to the opinion that the GPT is required for the structure solution.

[1] Kuczera, P., Wolny, J., Steurer, W. (2014). Acta Cryst. B**70**, 306-314
[2] Buganski, I., Strzalka, R., Wolny, J. (2020). J. Appl. Cryst. **53**, 904-913

Should nanostructure determination in high-entropy alloys be a new standard?

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Nanotechnology is one of the hot-topics in science and also materials industry nowadys. Therefore, the electorn micorscopy industry is following this trend by rapid enhancement of the electron microscopes capabilities, like better resolution, higher magnifications, different contrasts visualization, additional manipulations, etc.

For that reason we could observe finer details at nano- and/or atomic level on high-entropy alloys (HEAs) that play a key role in its tangible physical properties and were unexplainable before, due to lack of electorn micorscopes' sensitivity. Example is CoCrFeMnNi HEA (Fig. 1) that is a magnetically concentrated crystalline system with all lattice sites magnetic, containing randomness and frustration that explain some exotic magnetic phenomena.
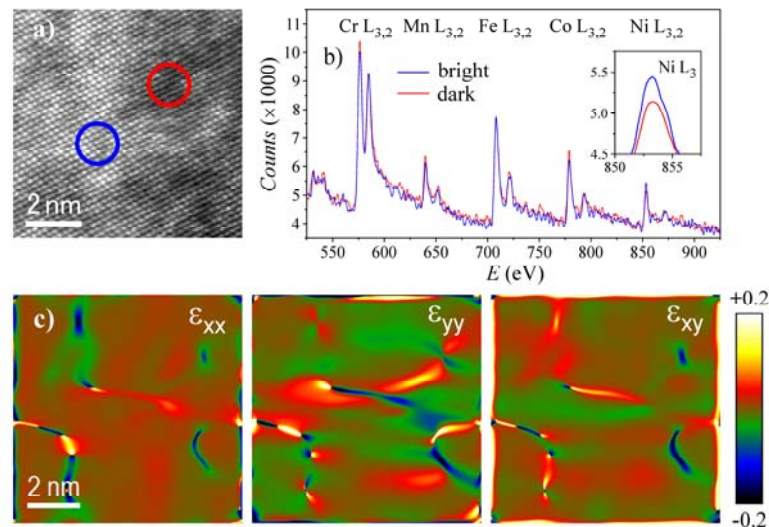

Fig. 1 : **(a)** A HAADF STEM image of the CoCrFeMnNi material. Blue and red circles surround a bright and a dark region, respectively. **(b)** Superimposed EELS spectra of the bright (blue trace) and dark (red trace) regions, normalized to the Fe L_3 intensity. **(c)** Maps of the ε_{xx}, ε_{yy} and ε_{xy} strain tensor components.

Electron-phonon mediated superconductivity of LiBi

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[3]W. Xie, [4]R. J. Cava, [2]T. Klimczuk

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LiBi [1] attracts attention, as it consists of almost the lightest and the heaviest nonradioactive elements of the periodic table: lithium with nearly free-electron Fermi surface and bismuth, which is a basis of topological materials due to its non-trivial Dirac-like electronic states. Moreover LiBi crystallizes in tetragonal crystal structure, which can be seen as distorted *bcc* structure.

Apart from its interesting structural and electronic properties, LiBi is a superconductor with $T_c = 2.45$ K.

Here we will present both the theoretical and experimental studies of LiBi. Firstly, evidence of its superconductivity will be introduced in terms of magnetic susceptibility and heat capacity measurements. Furthermore, the calculated electronic and phonon structure will be shown as well as the electron-phonon interaction function. On this basis two essential features of superconductivity are calculated, the transition temperature and electron-phonon coupling constant.

The band structure of LiBi is determined by an intriguing interplay between dominating p-states of Bi and s-state of Li and is affected by the structural distortion. Besides, its structure becomes almost cubic when external pressure is applied. A significant difference in the masses of atoms is reflected in the phonons. In conclusion its superconductivity is driven by the moderate electron-phonon coupling.

At the end, we will confront properties of isostructural and isoelectronic compounds LiBi and NaBi. The letter one superconducts below T_c=2.15 K and its bandstructure has been reported to show a topological character [2].

[1] K. Górnicka, S. Gutowska, M.J. Winiarski, B. Wiendlocha, W. Xie, R.J. Cava, T. Klimczuk, Chemistry of Materials, *32*(7) (2020) .
[2] R. Li, et al., Scientific Reports 5, 8446 (2015).

Superconductivity in high-entropy and medium-entropy alloys from the Ti-Zr-Hf-Nb-Ta-Sc system

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We investigated superconductivity in six high-entropy and medium-entropy alloys from the system Ti-Zr-Hf-Nb-Ta-Sc, where all samples contain rare earth element Sc. The superconductivity was found to be a robust phenomenon, appearing in all six investigated alloys and is quite insensitive to the degree of structural and chemical disorder in the materials. The superconducting transition temperatures T_c of the samples vary between 6.2 K and 8 K, where samples TiHfTaSc and TiZrTaSc have higher transition temperature than constituting elements. XRD characterization revealed each sample has a bcc and hcp phase. However SEM measurements showed interesting microstructure including dendrites. Specific heat measurements revealed broad peaks indicating that each phase is inhomogeneous. The temperature dependence of the peaks resulting from the formation of Cooper pairs allowed us to estimate the zero-temperature values of upper critical field, ranging from $\mu_0 H_{c2}(0) \approx 10$ T to 16 T. From magnetization measurements we determined that all six samples are type II superconductors and estimated the lower crtical fields $\mu_0 H_{c1}(0)$, ranging from ≈ 100 mT to 700 mT.
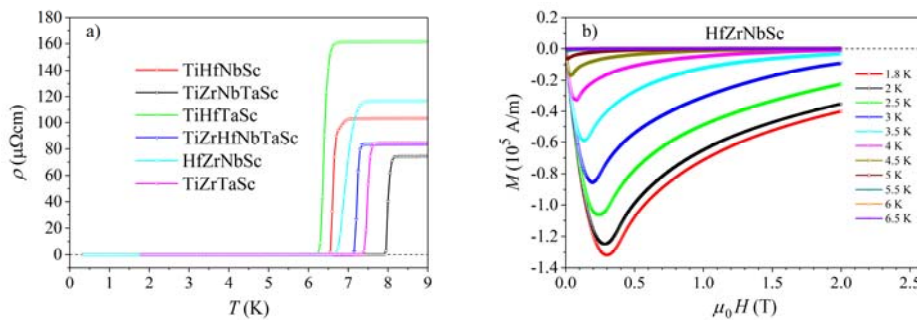

Fig.1: a) Electrical resistivity in zero field for all six samples. b) Isothermal magnetization field dependence for HfZrNbSc sample at various temperatures.

Soft-mode enhanced type-I superconductivity in $LiPd_2Ge$

[1],*G. Kuderowicz, [2]K. Górnicka, [3]E. M. Carnicom, [1]K. Kutorasiński,
[2]T. Klimczuk, [3]R. J. Cava, and [1]B. Wiendlocha

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Electronic structure, phonons and superconductivity of recently synthesized $LiPd_2X$ (X=Si,Ge,Sn) intermetallic compounds is reported. They belong to the Heusler material class which consist of more than 1000 compounds with many kinds of physical properties. Following the discovery of superconductivity in $LiPd_2Ge$ below T_c = 1.96 K, the other two isostructural compounds were synthesized. DFT calculations showed that all $LiPd_2X$ have strong softening of the first acoustic mode. The most pronounced softening occurs in $LiPd_2Ge$ and this compound has highest predict electron-phonon coupling constant λ=(0.53-0.56) and highest T_c, which suggest the correlation between superconductivity and the soft mode.

Universal superconductivity in compositionally complex transition metal alloys

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Using a He^3 cryostat in a superconducting magnet with fields up to 16 T, superconductivity of $(TiZrNbCu)_{1-x}Ni_x$ and $(TiZrNbNi)_{1-x}Cu_x$ metallic glasses was studied over a broad concentration range from the high entropy alloys (HEA) region to the Ni- and Cu-rich alloys, respectively.

We have observed that the upper critical fields of these alloys are Pauli limited and that the superconducting transition temperatures follow the behaviour of the dressed density of states at the Fermi level $N_\gamma(E_F)$, which is common in transition metals and their alloys [1]. In particular, we have shown that the electron-phonon coupling constant λ_{e-p} is proportional to the band density of the state at the Fermi level in our alloys, but also crystalline HEAs [2-4], and in other transition metal alloys. This addresses the problem of unusual superconductivity behaviour [4] which was attributed to the chemical complexity of HEAs but is shown to be inherent to transition metals. Although, minor complications do arise from combining metals of different transition series.

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The effect of structural inhomogeneity on "dirty" superconductivity in tin-containing alloys

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Our study focused on ternary TiZrHf, quaternary TiZrHfSn, and pentary TiZrHfSnX (X = Fe, Cu, Ni, Nb) alloys. Structure characterization revealed that the TiZrHf sample crystallizes in a single-phase hcp crystal structure, while others form multi-phase systems of simple crystal structures, e.g. hcp, bcc, fcc and primitive tetragonal cell, and Mn_5Sn_3, Fe_3Sn, $Fe_{1.67}Sn$ and $HfNi_2Sn$ type intermetallic compounds, respectively. Therefore, the structure inhomogeneity of tin-containing alloys appears in a form of dendritic microstructure as well as within individual phases due to the non-ideal mixing caused by interatomic interactions between different elements.

To investigate electronic inhomogeneity, we performed Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) measurements. Using high resolution low temperature STS, we mapped the local density of states variations of the two-phase TiZrHfSnNb sample and detected the superconducting gaps that varied significantly. The average value was estimated to be around 1 meV, however, some of the grains showed no occurrence of the superconducting gap.

Chemical disorder implies that we are in the "dirty" superconductor limit. For superconducting samples, we measured a rather broad temperature range of the heat capacity peaks and declination in the resistivity, indicating that Cooper pairs do not form instantly and that superconducting phases have nano-regions that vary in critical temperatures.

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Pressure dependent electronic structure of EuTGe$_3$ (T = Co, Rh)

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The 4f electrons are localized inside the atom due to strong Coulomb interaction, yet hybridize with the itinerant conduction electrons. As a result, various anomalous phenomena can emerge, such as valence fluctuations, unconventional superconductivity, and heavy-fermion behavior. The magnetic properties of such systems are directly related to the valence state of rare-earth ions and can be tuned by chemical substitution and external pressure. Most of reported Eu-compounds favor Eu^{2+} (J=7/2) with antiferromagnetic ground state. By applying pressure, the system undergoes a first-order phase transition by changing into a non-magnetic ground state with Eu^{3+} (J=0). While, EuTGe$_3$ (T: transition metal) prefers antiferromagnet ground state with Eu^{2+}, and its magnetic ordering and Eu valence are less sensitive to pressure. I will present pressure dependent electronic structure of EuTGe$_3$ (T=Co, Rh) observed by high-resolution x-ray absorption using partial fluorescence yield. Details of the spectral changes will be discussed in the talk.

Transport study of topological bands: remarkable feature in a thermoelectric material

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Topologically nontrivial material is an emergent venue of new functional material research, and many of highlighted topological insulators and semimetals have originally been known as thermoelectric materials. According to well-known figure of merit concept, large electrical conductivity detached from thermal conductivity is preferred. Topologically nontrivial transport channel can meet the requirement and control of topological bands can boost its thermoelectric performance as recently demonstrated in a metastable thin-film alloy [1].

In this presentation we discuss the role of topological bands in thermoelectric materials, and report recently demonstrated in-situ control of surface transport in a topological insulator $TlBiSe_2$ [2]. Drastic increase of electrical conductivity is observed by stimulating the surface while remain bulk properties unchanged. This surprising discovery raises a number of exciting possibilities, and potential synergies of topological effects and material functionality are discussed.

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Enhanced thermoelectric performance in *n*-type regime for half-Heusler phase ScNiSb

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We studied structural and thermoelectric properties of half-Heusler (HH) phase ScNiSb. X-ray diffraction revealed that the undoped *p*-type material is disordered due to off-centering of Ni atoms from nominal $4c$ (¼, ¼, ¼) Wyckoff site to quarterly occupied position $16e$ (x, x, x) $x = 0.256(2)$ [K. Synoradzki *et al.* Materials 12 (2019) 1723]. Analysis of bipolar thermal conductivity uncovered that electrons in ScNiSb possess 8-times higher mobility than holes. Using this finding as a guide, we prepared *n*-type doped samples $ScNiSb_{1-y}Te_y$. In concert with expectations, the intrinsic mobility rose with doping by an order of magnitude. The effect is supported by change of dominant scattering mechanism from ionized impurity scattering in pristine *p*-type sample to acoustic phonon scattering in doped *n*-type materials. We also observed sizable increase in the effective mass of charge carriers while tuning from holes- to electrons-dominated transport. Maintaining great mobility in *n*-type regime for ScNiSb was possible due to high conduction band anisotropy. Simultaneous increase in effective mass and mobility led to large power factor of 40 $\mu WK^{-2}cm^{-1}$ for $ScNiSb_{0.85}Te_{0.15}$ at 750 K. The project was supported by the National Science Centre (Poland) under research grant no. 2015/18/A/ST3/00057.

Thermal memory effect in the γ-brass type pseudo-binary $Ni_2Mn_{0.3}Zn_{10.7}$ phase

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We present a study of magnetic properties of the γ-brass type pseudo-binary $Ni_2Mn_{0.3}Zn_{10.7}$ phase, recently synthesized while investigating a pseudo-binary Ni-Mn-Zn system. The samples with the composition $Ni_2(Mn_xZn_{11-x})$ and lower Mn content mainly form γ-brass type pseudo-binary phases. The structure can be described by 26-atom γ-clusters centered at the highly symmetric positions of the cubic unit cell $(0,0,0)$ and $(½,½,½)$. The clusters consists of a four polyhedral shells consisting of an inner tetrahedron (IT), outer tetrahedron (OT), octahedron (OH) and distorted cuboctahedron (CO). In the parent γ-Ni_2Zn_{11}, Ni occupies only OT positions with full occupancy and the rest are occupied by Zn. The only difference for the pseudo-binary $Ni_2Mn_{0.3}Zn_{10}$ phase (with low Mn concentration) is that OH sites of the clusters are occupied by Mn/Zn and the rest sites remain intact. Such phase has interesting disordered magnetic sublattice and spins distributed on triangles, resulting in geometrical frustration of spin-spin interactions. Measurements show that the sample is an almost perfect spin glass. The zero-field-cooled (zfc) and field-cooled (fc) dc magnetizations show a spin freezing temperature at about $T_f \approx 15.5$ K with the $M(H)$ hysteresis curves typical for a spin glass. Below T_f we observed zfc-fc magnetization splitting in low magnetic field, frequency-dependent cusp in the ac susceptibility and ultraslow time-decay of the thermoremanent magnetization. All these phenomena show that ergodicity of the spin system is broken on the experimental time scale. The most spectacular manifestation of such an out-of-equilibrium system is the thermal memory effect [1,2] where we could store seven-bit of information (any ASCII character) into the material by pure thermal manipulation.

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

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Interest in high-entropy alloys (HEAs) has grown significantly ever since their debut in 2004 [1-2] due to their exceptional mechanical properties, customizability, and diverse application possibilities [3-5]. HEAs have no principal element, but rather are seen as a random solid solution of four or more elements that have equal concentration, fitting into mostly cubic lattice structures [6]. This perfectly crystalline material with a rather simple structure still hosts a full range of possible short-range chemical disorder. As such, HEAs are especially appealing for studying the effect of disorder on vibrational properties in a system which is between a perfectly ordered crystal and fully disordered amorphous phase.

In this presentation, we provide a detailed lattice dynamics study of the Cantor-Wu HEA FeCoCrMnNi using inelastic X-ray and neutron scattering techniques. We compare phonon dispersions, intrinsic linewidths, and the density of states to those of binary alloy and pure element equivalents, highlighting the effect of the increasing disorder in going from a simple binary alloy to an HEA. Many theoretical studies have shown the importance of mass, atomic size, and elastic constant fluctuations in reducing phonon lifetime, as well as the possible chemical short-range ordering and local strain [7]. Our results are discussed in light of such studies and put into the context of disordered crystalline systems, pinpointing the FCCMN's particular placement on the spectrum between being that of an ordered crystalline system and a metallic glass.

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Dynamical properties of the incommensurately modulated Rb₂ZnCl₄ phase

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Aperiodic crystals are long-range ordered crystals that lack periodicity. Although their structure are in general well understood, their dynamics are more debated. The behaviour and atomic realisation of phason modes arising from the aperiodicity as well as the low thermal conductivity in such systems are to be investigated.

The Rb₂ZnCl₄ phase displays a crystal structure where the orientation of its ZnCl₄ tetrahedrons is incommensurately modulated with an increasing anharmonicity from T_i=303 down to T_C=195K. As theory predicts a different behaviour of phasons depending on the harmonicity regime, it fits well as a probe of the incommensurate phases dynamics. Investigation was conducted through inelastic neutron scattering with the IN6-SHARP, IN5 and IN12 instruments of the ILL, and with the 1T spectrometer of the LLB. Working temperatures ranged from 350K to 140K, covering the incommensurate phase and going beyond the phase transitions.

We measured transverse acoustic phonons and a quasi-elastic scattering signal around the satellite reflections that mark the incommensurability, as well as a localised diffuse inelastic signal at low energies. As expected for an order disorder phase transition no propagative phason mode has been observed. We will present a detailed study of the acoustic phonon width and of the quasielastic signal as a function of the temperature, that might be indirectly coupled to phason fluctuations.

Molecular dynamics simulation for validation of the phononic ADPs in Hyp-1 protein

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Molecular dynamics (MD) simulation was used as a physics-based complementary method to verify the experimental model of Hyp-1 protein from medicinal herb *Hypericum perforatum* with potential application in various pharmaceutical therapies. A nanosecond MD simulation using OPLS-AA reproduced separate distributions of CA and CG atoms within chains A and B. We observed underestimating of experimental ADPs relative to calculated values, which are typically >10 $Å^2$ higher than experimental ones. The average structure factors obtained from simulation confirmed high compliance of experimental and simulated Hyp-1 models. To monitor the conformational variety of the protein analysis of preferred rotamers was performed. Many outliers between experimental and simulated side-chain conformations within the Hyp-1 model were observed, which prompted us to propose more reasonable rotameric forms. Therefore, we confirmed that MD simulation may be applicable for verification of refined, experimental models and explanation of their structural intricacies.

Atomic diffusion on the fivefold surface of the *i*-Ag-In-Yb quasicrystal

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i-Ag-In-Yb is one of the many stable icosahedral quasicrystals observed since their initial discovery by Shechtman in 1982 [1]. Its fivefold high-symmetry surface is considered well-studied. Scanning tunnelling microscopy (STM) investigations have revealed the surface structure [2] and a range of adsorption experiments have been undertaken, often resulting in the formation of quasiperiodic overlayers [3-5].

Here, some of this data will be revisited and some new results will be presented. By analysing successive STM scans taken at room temperature with the same tip conditions, it is apparent that there are moving atoms on the clean fivefold surface of *i*-Ag-In-Yb. To investigate this further, we first map the areas of the surface where diffusion is observed and then calculate the autocorrelation of this map. The autocorrelation indicates a well-ordered map with fivefold symmetry. Migration of diffusing atoms towards the step-edges is not observed. This would be expected if they were remnants of a previous terrace existing prior to the sputter-annealing preparation cycles.

Analysis of a range of metal (Pb, Sb, Bi, In and Ag) adsorption studies on the surface at room temperature indicates that adsorbate species display similar movement. With the areas where diffusion is observed matching previously determined quasiperiodic adsorption sites, order in this distribution is again evident. Intermittent formation of pentagonal motifs between successive STM frames, a structure inherent to this surface, is a common feature throughout each data set. The movement of adsorbates may be related to diffusion in the underlying substrate surface.

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Thin film growth of pentacene (Pn) on the two-fold surface of the icosahedral Ag-In-Yb quasicrystal

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The study of adsorption on quasicrystal surfaces through a wide range of adsorbates both elemental and molecular, has gained a lot of attention recently. The icosahedral (i)– Ag-In–Yb QC is isostructural to i–Cd–Yb [1]and it has readily available high–symmetry surfaces for thin film growth studies. The atomic structure of i–Cd–Yb consists of five atomic shells. The first demonstration of quasicrystalline molecular ordering on fivefold surface of the i–Ag-In–Yb were the Pentacene molecules as reported by Smerdon et al [2]. Pn molecules were adsorbed on Yb sites in that research. Following that study, we have investigated if Pn molecules can grow a quasicrystalline layer on the two-fold surface of the same system, and if Pn molecules are selectively adsorbed on Yb sites.

STM data shows that the molecules are aligned along the 5–fold and 2–fold axes of the substrate. They are ordered in rows along the high–symmetry 5-fold axis of the surface with row separation of either short S $= 0.8 \pm 0.02$ nm or long L $=1.32 \pm 0.02$ nm where the measured separation is perpendicular to the 5–fold symmetry axis. The ratio between them is close to the golden mean $\tau = $ ($\tau=1.618....$) and follows a Fibonacci sequence. The Fast Fourier Transform (FFT) confirms twofold quasicrystalline long-range order.

In conclusion, Pn adsorption on the two-fold surface of i–Ag/In–Yb produced quasicrystalline molecular structure. Additionally, the molecular motif when compared with the model structure of the substrate reveals that Pn molecules adsorb at Yb sites as on the 5-fold surface.

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Tuning adsorption energies and reaction pathways by alloying: PdZn versus Pd for CO$_2$ reduction to methanol

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The decrease of greenhouse gas emission due to fossil fuel combustion is one of the most important challenges to slow down the rate of climate change while replacing fossil sources. Methanol is a safe, easily transportable and fastly biodegradable liquid fuel which could be a carbon neutral alternative to fossil fuels. Catalytic CO$_2$ hydrogenation to methanol (CO$_2$ + H$_2$ → H$_2$O + H$_3$COH), with hydrogen produced from water electrolysis, has proven to be a viable process at the pilot plant scale in several countries. However, efficient catalysts are required to convert the stable CO$_2$ molecule to methanol.

We focus on the PdZn(111) model catalyst, with density functional theory calculations to investigate how the addition of an ancillary metal (Zn) to a metallic catalyst (Pd) influences the mechanism of methanol synthesis through CO$_2$ hydrogenation. We show that the preferred pathway varies with the model catalyst. On pure Pd, the carboxyl route is more likely to be followed and formate routes are favored by the insertion of Zn. The relative donor character of PdZn weakens carbon-bound species and strengthens oxygen-bound species. Alloying Pd with another metal offers then the possibility of tuning the CO$_2$ reduction to methanol by favoring a specific pathway or step on a wisely chosen catalyst. The extension of our study to other ancillary metals combined with Pd may stimulate the discovery of novel alloy catalysts for CO$_2$ hydrogenation to alcohols.
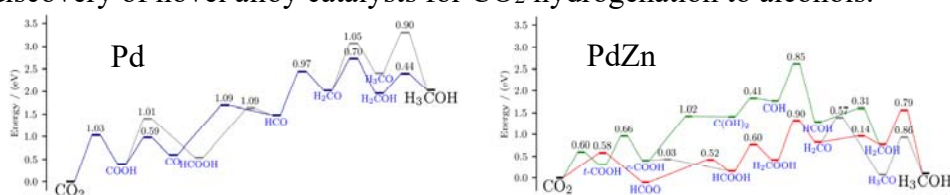

Figure 1: Energy landscape for CO$_2$ hydrogenation to methanol on surfaces

Structural complexity and chemical behaviour of $Hf_2B_2Ir_5$ in oxygen evolution reaction

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Intermetallic compound $Hf_2B_2Ir_5$ crystallizes with own structure type (*Pbam*, a =5.6218(2) Å, b = 11.2456(3) Å, c = 3.8292(1) Å) [1]. Chemical bonding analysis pointed out the cage-like type of crystal structure with B_2Ir_8 groups as main building blocks. These groups form two-dimensional layers parallel to (010) plane, which are interconnected by two- and three-center Ir–Ir interactions into a polyanionic framework. The framework is disordered by random substitution of boron pairs by single iridium atoms. Hafnium cations are incorporated into those „anionic cages".

Possessing a peculiar crystal structure, compound $Hf_2B_2Ir_5$ was investigated as anode material for oxygen evolution reaction (OER) [2]. Harsh oxidation conditions of OER (acidic electrolyte, applied anodic potential, evolving oxygen and presence of various chemically active intermediates) lead to formation of composite material ($Hf_2B_2Ir_5$ matrix + amorphous-like $IrO_x(OH)_y(SO_4)_z$ + crystalline HfO_2), which retain its bulk integrity over 240 h at current densities of 100 mA cm^{-2}. Moreover, the electrochemical activity remains comparable with state-of-the-art Ir-based catalysts over long-term electrochemical experiment. The chemical changes and their influence onto the electrochemical response will be discussed based on electrochemical studies (voltammetry, chrono-potentiometry), material characterization results (PXRD, SEM, XPS) and quantum chemical calculations.

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Dodecagonal oxide quasicrystal approximant with 72 tiling elements

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The discovery of two-dimensional oxide quasicrystals (OQC) has drawn attention to aperiodic structure formation from perovskite materials on Pt(111) [1,2]. On the atomic level, the OQC generates an aperiodic self-similar tiling consisting of triangles, squares and rhombs with Ti atoms at the vertices separated by 6.85 Å.

In this talk, we focus on periodically repeated patches of a quasicrystal known as approximants and discuss low-temperature scanning tunneling microscopy (STM) and surface x-ray diffraction (SXRD) data. Upon annealing of $SrTiO_3$ on Pt(111) we find a periodic structure. Its unit cell contains 48 Ti atoms which occupy the vertices of 48 triangles, 18 squares and 6 rhombs. These tiling elements are furthermore decorated with 48 Sr and 120 O atoms based on a stoichiometry of 1:1:2.5 as determined for a related small unit cell approximant [3].

Based on the intensity of over 500 SXRD diffraction spots recorded at SIXS beamline at SOLEIL, a structure model will be proposed.
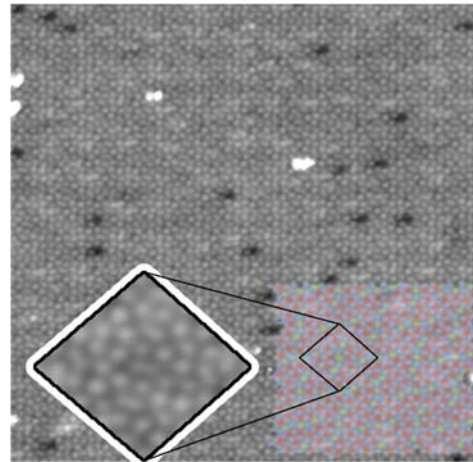

Fig 1: STM image of the large-scale $SrTiO_3$-derived oxide quasicrystal approximant. The bottom right shows the tiling elements as overlay on top. The black box marks the unit cell, where bright protrusions indicate Ti atoms.

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Two-dimensional ABO₃/Me oxide quasicrystal approximants: insights from Density Functional Theory

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Ultrathin metal oxide films play an important role in various technologically important areas, ranging from corrosion protection, microelectronics, to gas sensing, and heterogeneous catalysis. The combination of the low dimension and the quasiperiodic order has been recently reported, with the growth of an oxide quasicrystalline film (OQC), derived from BaTiO₃, on Pt(111) [1]. However, a detailed understanding of the stabilities and properties of OQC films is still lacking. By means of Density Functional Theory (DFT) calculations, using the DFT+U method, we systematically investigate the geometric, electronic, magnetic and thermodynamic properties of aperiodic-like films deposited over a periodic metallic substrate. Starting from the BaTiO₃/Pt(111) oxide approximant structure [2], we consider several ABO3/Me systems, by varying the alkaline metal (A = Ba, Sr, Ca), the transition metal (B = Ti, V, Cr, Mn, Fe, Co, Ni) and the metal substrate (Me = Pt, Pd, Au).

We show that several properties of the oxide layer such as the rumpling, the interfacial electron transfer and the adhesion energies display general trends within the series.
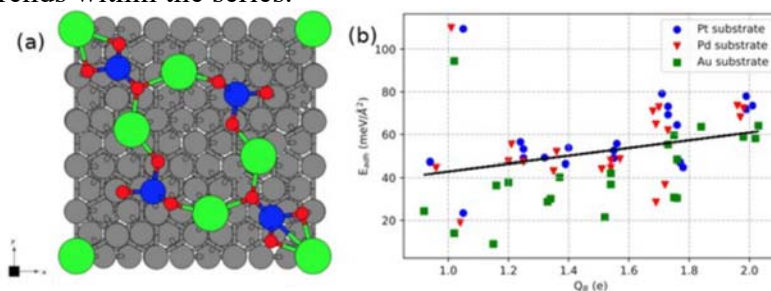

Figure : (a) Structure of the 2D oxide quasicristalline approximant BaBO₃/Pt(111) (top view); (b) Adhesion energy (E_{ads}) of the 2D oxide layer as a function of the Bader charge on the B-type atoms (Q_B).

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[2] S. Förster et al. "Observation and structure determination of an oxide quasicrystal approximant", Phys. Rev. Lett. 2016, 117(9), 095501.

New Quasicrystal Approximants in the SrTiO₃/Pt(111)/Al₂0₃(0001) system.

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Two dimensional oxide quasicrystals (OQCs) were recently discovered by annealing $BaTiO_3$ perovskite thin films epitaxially grown by magnetron sputtering on a single-crystalline Pt(111) substrate [1]. A similar OQC has been obtained by annealing $SrTiO_3$ ultrathin films grown by molecular beam epitaxy (MBE) on Pt(111). In addition, Schenk *et al.* have shown that this OQC coexists with an approximant phase characterized by a monoclinic unit cell [2].

Here, we use a different approach in which the Pt(111) single crystal is replaced by a 10 nm thick Pt(111) buffer layer grown by MBE on Al_2O_3(0001) substrate. Then $SrTiO_3$ thin films of various thicknesses were grown by pulsed-laser deposition and annealed at various temperatures. The growth process was followed *in-situ* by Reflection High Energy Electron Diffraction. The structure and the composition of the interfaces were characterized by X-Ray Diffraction and X-ray Photoelectron Spectroscopy. The formation of a new large square approximant with a lattice parameter equal 44.4 Å is evidenced by scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). High-resolution STM images allowed us to precisely determine the complex tiling consisting in 72 elements arranged as displayed in the figure. Additionally, a hexagonal phase with a lattice parameter of 28 Å has been observed depending on the preparation details as well as other complex 2D oxide phases.
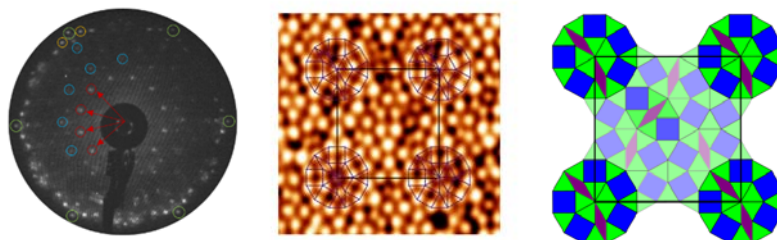

Figure. Left panel: LEED pattern of the approximant phase (50 eV beam energy). First, second, and third order spots of the pseudo-dodecagonal pattern are marked in red, blue, and yellow, respectively. Green circles indicate the reciprocal lattice of the Pt(111) substrate. Central panel: High resolution STM image. Size: 30 nm x 30 nm, tunneling parameters: -1V; 0.1 nA. Right panel: Structural model of the square unit cell approximant.

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Tribological performance of the AlCoCrFeNi$_{2.1}$ eutectic high-entropy alloy in as-cast and aged condition

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Wear behavior of the AlCoCrFeNi$_{2.1}$ eutectic high-entropy alloy (EHEA) in as-cast and aged condition was evaluated for the present study. By aging the material at 800 °C up to 500 h, precipitation of a fine, evenly dispersed micro-phase inside the L1$_2$ takes place. From 500 h to 1000 h of aging, the precipitates coarsen by the Ostwald ripening mechanism. Reciprocating wear tests were characterized by a prevailing abrasive wear mechanism, while adhesive and delamination wear components change with aging conditions. The L1$_2$ phase with lower hardness in the as-cast material preferentially deformed during the wear test, which was not the case after aging the material, i.e., with the presence of precipitates. Aging-induced changes show a similar trend for the coefficient of friction and the L1$_2$ + precipitates phase fraction, whereas changes in specific wear rate are in a good agreement with changes in the B2 phase fraction. In general, aging the AlCoCrFeNi$_{2.1}$ EHEA at 800 °C up to 500 h decreases its coefficient of friction due to reduced adhesive wear component and enhances its wear performance through precipitation strengthening.

High-temperature structural studies of d-AlCuRh – new correction for phasons

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We revisited X-ray diffraction data of decagonal Al-Cu-Rh system collected previously by Kuczera *et al.* [1] at room temperature and at 1013-1223 K. From [1] it is known, that the the best quasiperiodic ordering exists most probably between 1083 and 1153 K. The stability was proven to be most likely not phason-driven entropy lowering.

In our recent studies, we tested an application of the new correction for phasons, based on the statistical approach. It was shown [2,3], that phason flips significantly change the shape of the average unit cell, and therefore influence the structure factor, and thus the diffraction diagram. These changes in the shape of the AUC can be handled analytically. During the structure refinement the new correction for phasons give an extra parameter to fit. The procedure was recently applied to room-temperature d-AlCuRh data [4].

We performed a series of structure refinements including new correction term for phasons alongside the standard perp-space Debye-Waller factor for 5 sets of X-ray diffraction data at 293, 1013, 1083, 1153, and 1223 K. In the case of every dataset, we were able to achieve better *R*-factor values as compared to original results reported in [1].

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The study of the surface of a Gallium Nickel binary

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Gallium nickel binary alloy (Ga_3Ni_2) is used as a heterogeneous catalyst for the reduction of carbon dioxide into methanol [1]. Understanding of its surface atomic structure is important to get insight into catalytical behaviour. However, there is currently no information about the surface atomic structure of this binary alloy.

We have used scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED) to study the structure of three high symmetry surfaces of Ga_3Ni_2. In the first stage, we have figured out the ideal conditions to prepare atomically flat surfaces. This began with getting the surface polished to a mirror shine, either by using a range of different grits diamond pastes to buffer and polish the sample to remove all surface inclusions and damages or in the specific cases where the material has acceptable cleavage planes by applying pressure along those these planes it is possible to remove the top layers revealing an atomically flat plane.

After that initial preparation, the sample is subjected to cycles of sputtering with charged argon particles and then being annealed at a series of temperature for a prolonged period of time to produce a surface that gave high quality LEED and STM images. A range of annealing temperatures was used to observe if this factor had any effect of the results of the LEED and STM data and use the data to get an understanding of what the ideal preparation conditions are for this binary alloy. The results of the STM and LEED images showed that the higher the annealing temperature features such as step terraces seemed to become less well defined when compared to the images taken at lower temperatures. The LEED images show that the face of the sample being probed was exhibiting trigonal symmetries meaning that it was the (001) plane being observed.

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

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Additive manufacturing or 3D-printing has progressed from its initial use in rapid prototyping to creating parts with complex materials, geometries and mechanical properties [1-3]. Quasicrystals are one such complex structure that may benefit from having hand-held models to observe its intricacies in symmetry and geometry, taking visualisation beyond the screen and into the real world.

Presented are two methods to manufacture these structures using a desktop 3D-printing technology. The design approach for both is a multi-step process from initial computer-aided design (CAD) drawing or structural file to printed part. In both cases a stereolithography (SLA) 3D-printer (Formlabs Form 3) is used. In the first method the icosahedral quasicrystal is broken down into 4 'building blocks'. These building blocks are stacked around a landing shape (the rhombic hexecontahedron) [4] using CAD tools. This method is more accessible to the non-expert, requiring only basic knowledge of CAD for use with freeware or industry level software.

The second method involves using crystallography software (such as VESTA). Structural file formats can be used from base (like CIF, PDB, XYZ etc) or structures may be pre-programmed using a desired coding language (in this case Python is used) to produce accurate models. A 3D model file like STL (Standard Tessellation Language) or VRML (Virtual Reality Modelling Language) is exported from the chosen crystallography software. Both methods use the CAD software to finalise details before being sent for printing in 3D.

3D-printing using SLA produced accurate centimetre scale models of icosahedral quasicrystals in differing configurations. Alongside assisting visualisation, 3D-printed models could be used for testing the electromagnetic properties of crystals (scale dependent), the mechanical potential of structural metamaterials and general crystal education. As more crystallography software includes this extension into 3D-printing, it will become easier to conceptualise the true nature of these complex structures.

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Magnetic and electrical properties of Gd$_5$Si$_2$Ge$_2$ thin films

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The search for new magnetic refrigerants gained momentum in 1997 after the discovery of the giant magnetocaloric effect (MCE) at $T_C = 278$ K in the Gd$_5$Si$_2$Ge$_2$ compound by Gschneidner et al. [1]. One of the features characteristic of materials with large MCE is a presence of the first-order type magnetic phase transition often accompanied by the structural transformations. Nowadays, the magnetic refrigeration in a reduced scale attracts growing interest [2-4], however the production of thin films of Gd$_5$(Si$_x$Ge$_{1-x}$)$_4$ remains a challenge. One can think of the dimensions reduction by mechanical milling [5] but in the case of thin films the method of choice is pulsed laser deposition (PLD). In Refs. [3,4] ~800 nm thick thin films of Gd$_5$Si$_{2.7}$Ge$_{1.3}$ and Gd$_5$Si$_{1.3}$Ge$_{2.7}$ have been obtained by PLD and presence of the magneto-structural first order phase transition has been observed at ~194 K followed by magnetic second order phase transition at ~247 K.

In the present study we deposited ultra-thin films of the nominal composition Gd$_5$Si$_2$Ge$_2$ onto naturally oxidized Si substrate using PLD. Commercially available compounds were used to prepare the target. The composition was verified by energy dispersive spectroscopy. Our initial studies were done on films of the thickness 30, 60, 120, and 200 nm. We have observed only a sharp step-like increase of the magnetization at 50 K for the 30nm-thick sample. For thicker films a strong magneto-structural transition is present at about 150 K and a weak transition occurs between 250-300 K, however the latter shows also signatures of first order type phase transition, in contrast to previous studies. We have determined MCE around the characteristic temperatures.

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Magnetocaloric effect in hexagonal NdCrGe$_3$

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As part of our search for new materials that can serve as energy converters, we have investigated the magnetocaloric properties of NdCrGe$_3$ compound. This material, which crystallizes in hexagonal perovskite structure type (space group $P6_3/mmc$), shows ferromagnetic ordering below ~120 K. The magnetic transition was observed in the measurements of magnetization, specific heat and electrical resistivity as a clear anomaly. The change of magnetic entropy, which is a measure of the magnetocaloric effect in a given material, was derived from the measurements of magnetization as a function of the external magnetic field under isothermal conditions and reached up to -2.4(1) J/(K kg) at a magnetic field change from 0 to 5 T. The refrigeration capability (RC) for the same magnetic field change is equal to 91(1) J/kg. In addition, by examining the application potential in the context of the thermoelectric effect, we measured the value of the Seebeck coefficient, which is ~10 µV/K at room temperature.

De Haas-van Alphen oscillations in ZrSiS and HfSiS

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Topological semimetals are group of Dirac materials in which conduction and valence bands cross each other and the crossings are topologically protected. Besides being promising for discovery of novel physical properties, they offer a wide range of possible applications in spintronics, optoelectronics and quantum computing.

Here we show quantum oscillations in magnetization for single crystals of grown ZrSiS and HfSiS, as well as some inbetween compositions as they crystallize in same structure. From shown angular dependence of de Haas-van Alphen oscillations, one can attemp to reconstruct parts of Fermi surface for given material. Analysis of oscillations reveal low effective mass and high mobility for Dirac fermions.