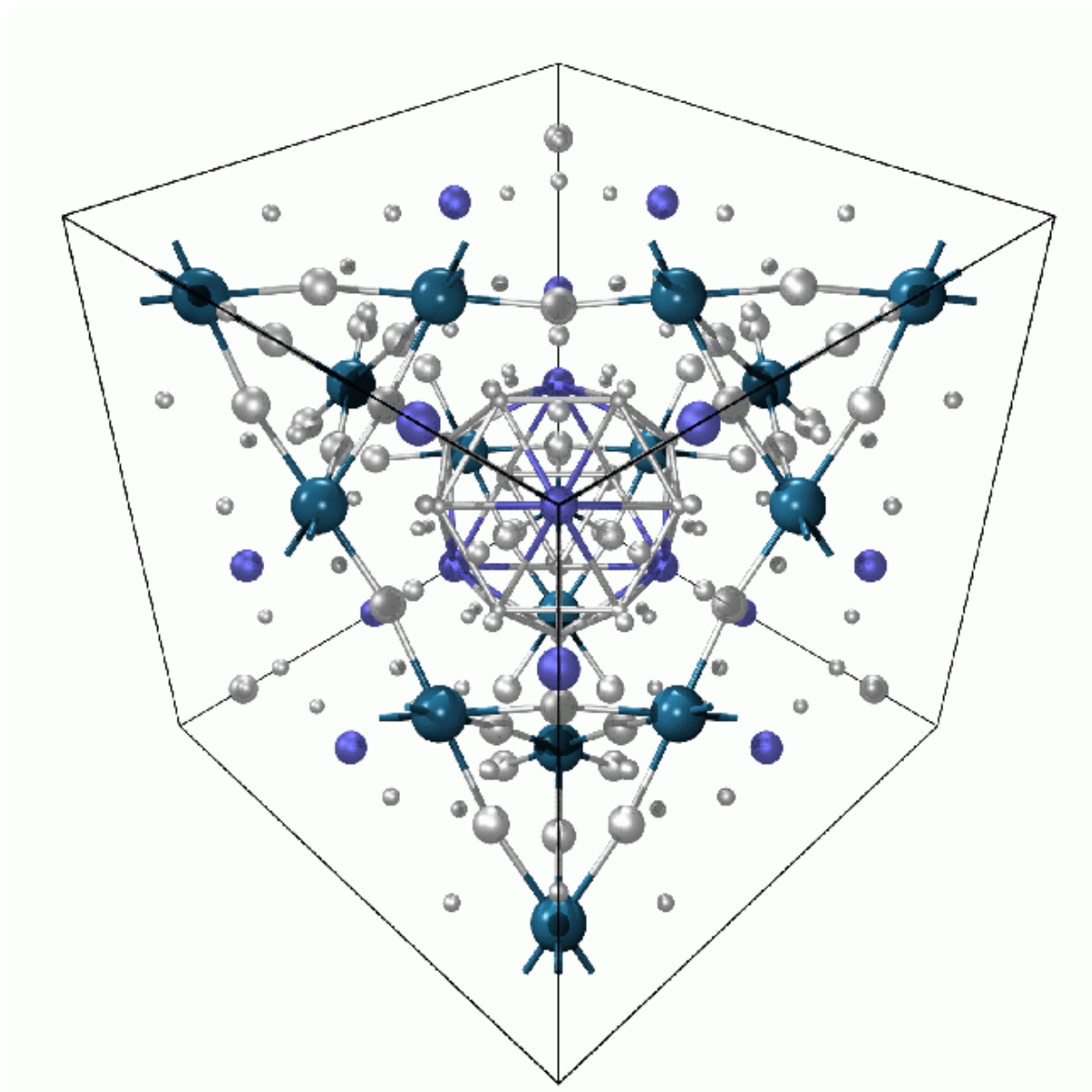


C-MAC Euroschool 2015

**Material Synthesis and Characterization
Applied to Complex Metallic Alloys**



Program and Abstracts

Bratislava, Slovakia, June 1 -5, 2015

C-MAC EUROSCHOOL 2015

Material Synthesis and Characterization Applied to Complex Metallic Alloys

Program and Abstracts

Editors:

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Slovak Academy of Sciences
and European Integrated Centre for the Development of Metallic Alloys and Compounds

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Conference logo – Al₁₀V crystal structure, courtesy of M. Jahňatek

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Material Synthesis and Characterization
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and Compounds

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C-MAC EUROSCHOOL 2015

Material Synthesis and Characterization Applied to Complex Metallic Alloys Bratislava, Slovakia, June 1 – 5, 2015

Program

Sunday, May 31, 2015

16:00 - 19:00 Registration

19:00 - 20:30 Welcome and refreshments

Monday, June 1, 2015

08:00 - 09:00 Registration (continued)

Chairperson: Marc de Boissieu

09:00 - 09:10 **Marc de Boissieu, Marek Mihalkovic:** Welcome to the participants

09:10 - 10:30 **Catherine Tassin:** Thermodynamics

10:30 - 11:00 **Coffee Break**

Chairperson: M. de Boissieu

11:00 - 12:30 **Catherine Tassin:** Thermodynamics (plus tutorial)

12:30 - 14:00 **Lunch Break**

Chairperson: Catherine Tassin

14:00 - 15:30 Peter Gille: Bulk materials preparation

15:30 - 16:00 Coffee Break

Chairperson: Catherine Tassin

16:00 - 17:30 Peter Gille: Bulk materials preparation

Tuesday, June 2, 2015

Chairperson: Constantin Vahlas

09:00 - 10:30 Marek Mihalkovic: Introduction on the structure of CMA

10:30 - 11:00 Coffee Break

Chairperson: Constantin Vahlas

11:00 - 12:30 Marc de Boissieu: X-ray and neutron characterization

12:30 - 14:00 Lunch Break

Chairperson: Peter Gille

14:00 - 15:30 Marc de Boissieu: X-ray and neutron characterization

15:30 - 16:00 Coffee Break

Chairperson: Peter Gille

16:00 - 17:30 Catherine Tassin: Thermodynamics (tutorial)

17:30 - 20:30 Poster Session

Wednesday, June 3, 2015

Chairperson: Marek Mihalkovic

09:00 - 10:30 **Constantin Vahlas:** Coatings

10:30 - 11:00 **Coffee Break**

Chairperson: Marek Mihalkovic

11:00 - 12:30 **Constantin Vahlas:** Coatings

12:30 - 14:00 **Lunch Break**

Chairperson: Peter Svec

14:00 - 15:30 **Richard Portier:** Transmission electron microscopy (tutorial)

15:30 - 16:00 **Coffee Break**

Chairperson: Peter Gille

16:00 - 17:30 **Marek Mihalkovic:** Crystal structure prediction

17:30 - 20:30 **Poster Session**

Thursday, June 4, 2015

Chairperson: Marek Mihalkovic

09:00 - 10:30 **Richard Portier:** Transmission electron microscopy and SEM

10:30 - 11:00 **Coffee Break**

Chairperson: Marek Mihalkovic

11:00 - 12:30 **Richard Portier:** Transmission electron microscopy and SEM

12:30 - 14:00 **Lunch Break**

Chairperson: Peter Svec

14:00 - 15:30 **Marc de Boissieu, Richard Portier, Marek Mihalkovic:** Tutorial
Crystallography and X-ray diffraction

15:30 - 16:00 **Coffee Break**

16:00 - 17:30 **Lab visit**

19:00 - 20:30 **Gala Dinner**

Friday, June 5, 2015

Chairperson: Richard Portier

09:00 - 10:30 Peter Svec: Nanostructures

10:30 - 11:00 Coffee Break

Chairperson: Richard Portier

11:00 - 12:30 Peter Svec: Nanostructures

12:30 - 14:00 Lunch Break

14:00 - 17:30 Excursion to Volkswagen Plant, Bratislava – Devinska Nova Ves

17:30 - 17:45 Marc de Boissieu, Marek Mihalkovic: Closing remarks

End of the Conference

List of Poster Contributions

P01: L. Prochaska, A. M. Andrews, H. Detz, D. MacFarland, W. Schrenk, G. Strasser, T. Zederbauer, and S. Paschen,

Developing heavy fermion film growth by molecular beam epitaxy

P02: Andreja Jelen, Mitja Krnel, Primož Koželj, Stanislav Vrtnik, Gregor Kapun, Janez Dolinšek,

Investigation of GaPd₂ intermetallic catalyst

P03: Baran Sarac, Daniel Sopy, Steffen Oswald, Mihai Stoica, Jürgen Eckert,

Tailoring Property-Structure Relationship in Bulk Metallic Glasses

P04: Manisha Pathak, Alexander Ovchinnikov, Matej Bobnar, Walter Schnelle, Peter Höhn, Yuri Grin,

Synthesis and Crystal Structure Novel Nitridogermanate Ca₆[Ge₂N₆]

P05: Mirtha Pillaca, Viviane Cocivera, Tamara Maletin, Peter Gille,

Crystal growth of Sb-based binary alloys prepared by modified Bridgman technique

P06: Janez Lužnik, Jože Luzar, Jin Bae Lee, Hae Jin Kim, Andreja Jelen, Damir Pajić, Magdalena Wencka, Zvonko Jagličić, Anton Meden, Janez Dolinšek,

Synthesis and magnetic properties of hematite particles in a "nanomedusa" morphology

P07: M. Solecka, M. Rozmus-Górnikowska, A. Radziszewska, J. Kusiński,

Investigations of Inconel 625 and Inconel 686 after high-temperature corrosion at the waste incineration ash

P08: S. Thorn, S. Hars, M. Lowe, R. McGrath, H. R. Sharma,

Growth of Pb on the Three-Fold Surface of a Ag-In-Yb Quasicrystal

P09: P. Koželj, S. Vrtnik, A. Jelen, S. Jazbec, Z. Jagličić, S. Maiti, M. Feuerbacher, W. Steurer, J. Dolinšek,

An analysis of the physical properties of Ta₃₄Nb₃₃Hf₈Zr₁₄Ti₁₁ – the first high-entropy alloy superconductor

P10: Irena Janotová, J. Zigo, P. Švec, I. Mat'ko, D. Janičkovič, P. Švec Sr.,

Crystallization in rapidly quenched Fe-B-Si system with additions of C and Cu

P11: Girma Hailu Gebresenbut, Cesar Pay Gomez

Syntheses and crystal structure determination of quasicrystal approximants in the RE-Au-Si systems (RE = Gd, Tb, Dy, Ho and Yb)

P12: B. Podmiljšak, J.-H. Kim, P.J. McGuinness, S. Kobe,

Influence of Ni on the magnetocaloric effect in Fe_{84-x}Ni_xZr₆B₁₀ soft-magnetic amorphous alloys

P13: Marija Sorić, Ivo Batistić, Petar Popčević, Jovica Ivkov, Peter Gille, Ana Smontara,

DFT modeling and transport properties of palladium based intermetallic compounds

P14: Peter Svec, Juraj Zigo, Irena Janotova, Dusan Janickovic, Jozef Marcin, Ivan Skorvanek, Peter Svec Sr.,

Structure and Properties of Equiatomic Fe-M-Nb-B (M=Co, Ni) and M-rich Metallic Glasses

P15: J. Kadok, Y. Prots, J. Grin, J. Ledieu, V. Fournee, M.-C. de Weerd, P. Boulet,

The Aluminum-Iridium binary system and Al-Ir based ternary compounds

P16: Abdullah Sirindil, Loïc Perriere, Phillippe Vermaut, Marianne Quiquandon, Richard Portier, Denis Gratias,

Elaboration and study of the $\text{Sc}_{57}\text{Ru}_{13}$ 1/1 cubic approximant of icosahedral structures in the (Sc,Ru) system

Abstracts

Poster Contributions

Developing heavy fermion film growth by molecular beam epitaxy

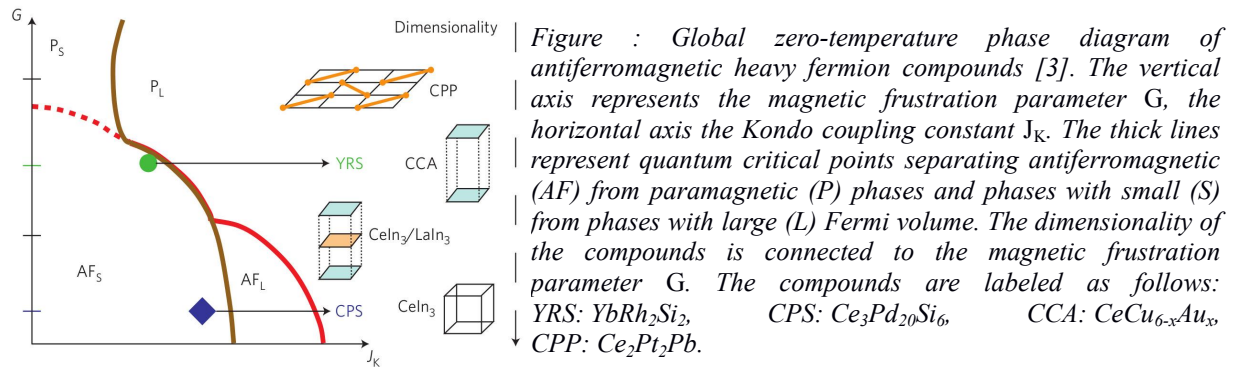
¹L. Prochaska, ²A. M. Andrews, ³H. Detz, ²D. MacFarland, ³W. Schrenk, ^{2,3}G. Strasser, ³T. Zederbauer, and ¹S. Paschen

¹*Institute of Solid State Physics, Vienna University of Technology, Austria*

²*Institute of Solid State Electronics, Vienna University of Technology, Austria*

³*Center for Micro- and Nanostructures, Vienna University of Technology, Austria*

YbRh₂Si₂ is a prototypical heavy fermion compound. It exhibits a Kondo destruction quantum critical point as its antiferromagnetic phase is fully suppressed by the application of a small magnetic field [1]. From studies of the cubic compound Ce₃Pd₂₀Si₆ it is concluded that dimensionality is an efficient way to tune through the theoretically suggested [2] global phase diagram for antiferromagnetic heavy fermion compounds [3]. The technique of molecular beam epitaxy (MBE) provides the ability to grow single crystalline thin films of YbRh₂Si₂ and tune this material to the extreme 2-dimensional limit. There have been very encouraging results recently for CeIn₃/LaIn₃ [4] and CeCoIn₅/YbCoIn₅ [5] superlattices. We have set up an MBE system equipped with a standard evaporation cell for Yb and two electron beam evaporators for Rh and Si.



We acknowledge financial support by the European Research Council (ERC Advanced Grant No. 227378) and the Austrian Science Fund (FWF Doctoral School Solids4Fun W1243).

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[4] H. Shishido, T. Shibauchi, K. Yasu, T. Kato, H. Kontani, T. Terashima and Y. Matsuda, Science 327, 980 (2010).

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INVESTIGATION OF GaPd₂ INTERMETALLIC CATALYST

Andreja Jelen¹, Mitja Krnel¹, Primož Koželj¹, Stanislav Vrtnik¹, Gregor Kapun²,
Janez Dolinšek¹.

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Intermetallic compounds from the Ga-Pd system (GaPd, GaPd₂ and Ga₇Pd₃) are highly selective catalyst materials for the reaction of semi-hydrogenation of acetylene [1]. The catalytical selectivity of these compounds is considered to follow the active-site isolation concept[1]. This concept is valid for GaPd and Ga₇Pd₃, whereas its validity is not obvious for GaPd₂. In order to test this concept, we conducted a comparative study of physical properties of the GaPd₂ phase to the GaPd phase (with the emphasis on the electronic properties), where the physical properties of GaPd were reported recently [2]. We investigated properties of bulk monocrystalline GaPd₂ samples and GaPd₂ nanoparticles on SiO₂ support.

With present contribution, we would like to focus mainly on material crystal structure characterization by means of X-ray diffraction and final materials characterization by means of different physical properties and scanning electron microscopy (SEM). An example of SEM backscattered electron (BSE) images is shown in Figure 1.

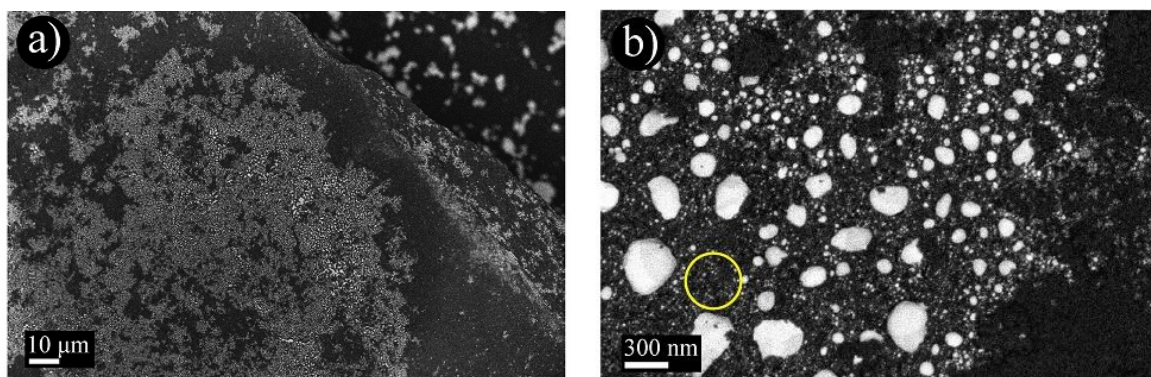


Figure 1. (a) BSE image of the GaPd₂/SiO₂ supported nanoparticles at low magnification. The nanoparticles' region is shown magnified in panel (b). The larger ("white") nanoparticles are metallic Pd, whereas the slightly darker small nanoparticles in the regions between the white nanoparticles are the GaPd₂ nanoparticles (like those encircled) [3].

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[3] M. Wencka et al.: GaPd₂ Intermetallic Catalyst in the Bulk and Nanoparticle Morphology and the Relevance of Active-Site-Isolation Concept for its Catalytic Selectivity (sent for publication).

Tailoring Property-Structure Relationship in Bulk Metallic Glasses

^{1*} Baran Sarac, ¹ Daniel Sopu, ¹ Steffen Oswald, ^{1,2} Mihai Stoica, ^{1,3} Jürgen Eckert

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Bulk metallic glasses (BMGs) exhibit ultra-high strength (up to 6 GPa) and elasticity (about 2%) in sequence with plastic-like processing capability when heated above its glass transition temperature. Albeit these favorable properties, the Achilles' heel of monolithic BMGs is the limited ductility particularly under tension. On the micron-scale, this challenge can be overcome by the incorporation of a rather soft second phase within the matrix, which can arrest and/or nucleate the shear bands. This approach reports a unique method which describes a tangible and quantitative route to investigate the significance of second phase parameters (e.g. size, spacing, distribution) on the toughening phenomena. Fabrication of the periodic pores (acting as the second phase) requires a joint process of photolithography and Bosch etch of Silicon templates followed by thermoplastic forming of BMGs to replicate the imprinted pattern. High feature precision and batch-processing are the key advantages of this multi-step fabrication. BMGs with a variety of embedded pore patterns were subjected to quasi-static uniaxial tensile test, where the results highlighted the importance of selecting the spacing of the pores perpendicular to loading smaller than the intrinsic crack length of the monolithic BMG. In addition, we identified the ratio of pore size to spacing, as well as pore architecture other criteria for tensile ductility optimization. Subsequent fracture analysis revealed three different deformation regions, where molten spots were observed on the fracture surface which are the indications of local melting due to excessive heat release during rupture. Compositional fluctuations (maximum of 5 at%) between deformed and undeformed regions were confirmed by EDX and Auger spectra. Finally, we conducted molecular dynamic simulations in order to assess the behaviour of porous metallic glasses on the nanometer scale.

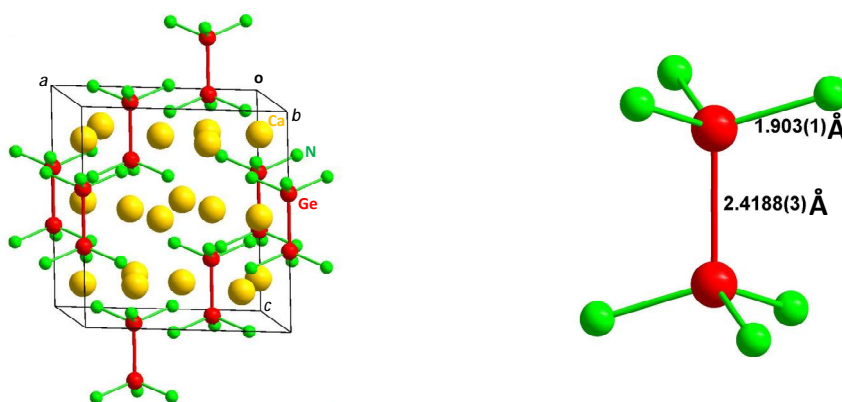
Synthesis and Crystal Structure Novel Nitridogermanate $\text{Ca}_6[\text{Ge}_2\text{N}_6]$

Manisha Pathak, Alexander Ovchinnikov, Matej Bobnar, Walter Schnelle,
Peter Höhn, Yuri Grin

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Characteristic structural features of most of the ternary alkaline earth (*AE*) germanium nitrogen compounds are isolated or condensed nitridogermanate anions $[\text{Ge}_x\text{N}_y]^{z-}$ surrounded by electropositive *AE* cations; previously known nitridogermanates with Ca include $\text{Ca}[\text{GeN}_2]^{[1]}$, $\text{Ca}_2[\text{GeN}_2]^{[2]}$, $\text{Ca}_5[\text{Ge}_2\text{N}_6]^{[2]}$, $\text{Ca}_4[\text{GeN}_4]^{[2]}$, and $\text{Ca}_7[\text{GeN}_4]\text{N}_2^{[3]}$, in contrast to anti-perovskite calcium germanide nitride $\text{Ca}_3\text{GeN}^{[4]}$.

In the present contribution, we report the novel calcium nitridogermanate $\text{Ca}_6\text{Ge}_2\text{N}_6$. The new phase crystallizes trigonal (*R*3 (No.148), $a = 9.2124(2) \text{ \AA}$, $c = 9.2675(3) \text{ \AA}$, $Z = 3$). $\text{Ca}_6[\text{Ge}^{\text{III}}_2\text{N}_6]$ is the first example of a nitridogermanate containing $[\text{Ge}_2\text{N}_6]^{12-}$ dimers with Ge-Ge bonds. Ge in 3+ oxidation state is tetrahedrally coordinated by Ge and 3 N with Ge-Ge bond length of $2.4188(3) \text{ \AA}$ and Ge-N distances of $1.903(1) \text{ \AA}$, (3x). Previously reported phases $\text{Ca}_2[\text{Ge}^{\text{II}}\text{N}_2]$, $\text{Ca}_4[\text{Ge}^{\text{IV}}\text{N}_4]$ & $\text{Ca}_7[\text{Ge}^{\text{IV}}\text{N}_4]\text{N}_2$, $\text{Ca}_5[\text{Ge}^{\text{IV}}\text{N}_3]_2$, and $\text{CaGe}^{\text{IV}}\text{N}_2$, contain nitridogermanates in the form of bent anions of $[\text{GeN}_2]^{4-}$, isolated tetrahedra $[\text{GeN}_4]^{8-}$, infinite chains of $^{1-}_\infty[\text{GeN}_2\text{N}_{2/2}^{5-}]$, and 3D network of $[\text{GeN}_{4/2}^{2-}]$, respectively. The isolated N^{3-} in $\text{Ca}_7[\text{Ge}^{\text{IV}}\text{N}_4]\text{N}_2$ is coordinated by six Ca^{2+} .



Synthesis of $\text{Ca}_6[\text{Ge}_2\text{N}_6]$ was performed from Ca_3N_2 and Ge in molar ratio of 3 : 1 in sealed tantalum ampoules at 750°C using molten Na as flux and NaN_3 as a source of N_2 . After the reaction, excess Na was removed under dynamic vacuum at 300°C . The heavy atom positions of isotypic $\text{Ca}_6[\text{Cr}_2\text{N}_6]\text{H}^{[5]}$ phase were used as a starting model in Rietveld refinement, however no indications for any occupation of the H-site were observed.

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Crystal growth of Sb-based binary alloys prepared by modified Bridgman technique

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Currently, antimony-based alloys are receiving detailed examination owing to their potentially efficient thermoelectric behavior. Binary compounds (FeSb_2 and CoSb_3) and third-component modifications based on them were found to be particularly promising. These peritectically melting compounds cannot be crystallized from congruent melts but have to be grown below their specific peritectic temperature from Sb-rich solutions containing more than 90 at. % Sb. Moreover, due to the relatively high Sb vapor pressure crystal growth has to be carried out in closed ampoules, e.g. using the Bridgman method from a high-temperature solution. Unfortunately, liquid-phase mixing in closed Bridgman-type ampoules is not easy to be achieved, but is necessary to remove the rejected Sb excess from the phase boundary of the growing crystal to avoid second-phase inclusion formation of pure Sb.

Our previous results in vertical Bridgman growth of FeSb_2 and CoSb_3 show a high density of Sb inclusions, even with extremely low growth rates of less than 1 mm/d. Also in experiments using a Bridgman configuration being inclined with respect to the vector of gravity, buoyancy-driven convection could not be remarkably increased to avoid second-phase inclusions. That is, why we added a continuous rotation of the growth ampoule to the inclination of the Bridgman furnace. With a Bridgman-type set-up being tilted by 15° against the horizontal, the growing crystal rotates together with the ampoule while the Sb-rich liquid tries to keep its horizontal surface level. This results in a strongly forced convection within the solution, especially next to the growth interface where materials transport is needed most to avoid constitutional supercooling. First experiments using this rotary Bridgman growth resulted in single-phase ingots of FeSb_2 and CoSb_3 .

It is worth mentioning that the advantage of this modified growth technique is not at all restricted to the Sb-based thermoelectric materials. Therefore, it may be a powerful approach in unidirectional solidification from off-stoichiometric melts, in general.

Synthesis and magnetic properties of hematite particles in a "nanomedusa" morphology

^{2*}Janez Lužnik, ²Jože Luzar, ¹Jin Bae Lee, ¹Hae Jin Kim, ¹Andreja Jelen, ³Damir Pajić, ⁴Magdalena Wencka, ⁵Zvonko Jagličić, ⁶Anton Meden, and ¹Janez Dolinšek

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We present the synthesis, characterization, and magnetic properties of hematite particles in a peculiar "nanomedusa" morphology. The particles were prepared from an iron-silica complex by a hydrothermal process in a solution consisting of ethyl acetate and ethanol. The particles' morphology, structure, and chemical composition were investigated by transmission electron microscopy, powder X-ray diffraction, and scanning electron microscope equipped with an energy-dispersive X-ray spectrometer. The "hairy" particles consist of a spherical-like core of about 100 nm diameter and fibrous exterior composed of thin "legs" of 5 nm diameter grown along one preferential direction. The particles' cores are crystalline and undergo a magnetic phase transition to a weakly ferromagnetic state at a temperature of 930 K that matches reasonably the Néel temperature of bulk hematite. However, unlike bulk hematite that undergoes Morin transition to an antiferromagnetic state around room temperature and small hematite nanoparticles that are superparamagnetic, the "nanomedusa" particles remain weakly ferromagnetic down to the lowest investigated temperature of 2 K. Each particle thus represents a nanodimensional "hairy" ferromagnet in a very broad temperature interval, extending much above the room temperature. Such high-temperature ferromagnetic nanoparticles are not frequently found among the nanomaterials.

Investigations of Inconel 625 and Inconel 686 after high-temperature corrosion at the waste incineration ash

^{1*}M. Solecka, ¹M. Rozmus-Górnikowska, ¹A. Radziszewska, ¹J. Kusiński

¹*Department of Surface Engineering and Materials Characterisation, Faculty of Metals Engineering and Industrial Computer Science, AGH University of Science and Technology in Krakow, Poland*

Inconel alloys 625 and 686 is a Ni-Cr-Mo alloys used for its high strength, outstanding corrosion resistance, and excellent fabricability. For this reason, these alloys are typically used as a one of the most important coating material and can be applied in a different environments and elements of devices, having various applications. To perform the Ni-base weld overlays, without introducing too much Fe, a new weld technique called Cold Metal Transfer (CMT) was used [1,3]. The cold metal transfer process as called CMT which was invented by Fronius company is a modified Metal Inert Gas (MIG) welding process.

This paper presents the causes and mechanisms of high-temperature corrosion of boiler elements during the incineration of waste. Tests results of the Inconel 625 and Inconel 686 coated boiler tubes exposed into the waste incineration ashes were performed using scanning electron microscopy supported by energy dispersive X-ray spectroscopy.

Microstructure examinations of the Inconel 625 and Inconel 686 corroded surface were carried out by using scanning electron microscopy (SEM) namely a Nano SEM 450 manufactured by the FEI Company (Fig. 1). The metallographic microsections were subjected to qualitative and quantitative analyses of chemical composition by means of X-ray spectroscopy with energy dispersion (EDS) using detector manufactured by the EDAX company.

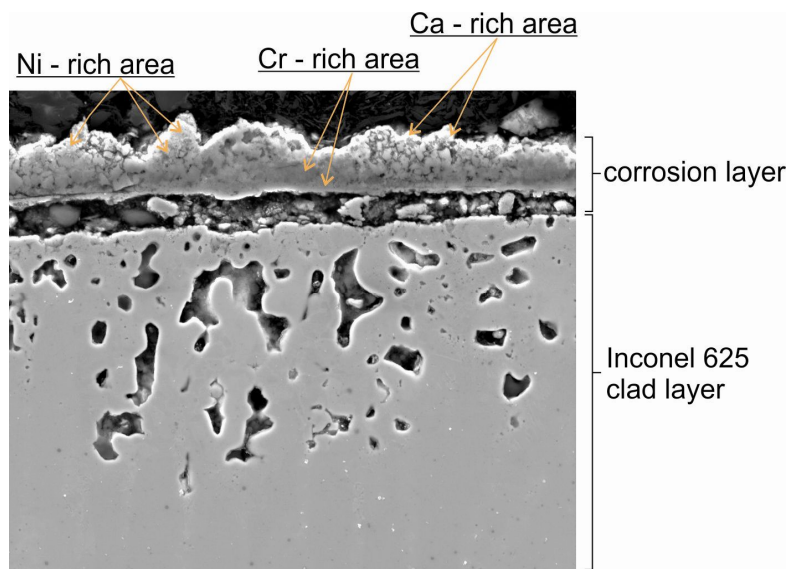


Fig. 1. Inconel 625 after corrosion test at the waste incineration ash (650°C for 500h)

Growth of Pb on the Three-Fold Surface of a Ag-In-Yb Quasicrystal

¹S.Thorn, ¹S.Hars, ¹M.Lowe, ¹R.McGrath, ¹H.R.Sharma

¹Surface Science Research Centre, Department of Physics, University of Liverpool, UK

Since the availability of single grain quasicrystals (QCs), much research has been done on deposition of elements/molecules onto these surfaces [1]. This research has predominantly been related to how the adsorbates will arrange themselves according to the structure onto which they are being adsorbed. The icosahedral (i-) Ag-In-Yb QC is one such sample in which recent work of this manner has been carried out [2-5], whereas previous work has been with Al-based QCs. It is considered that i-Ag-In-Yb is comprised of Tsai-type clusters [6]. These clusters are interlocking shells of the constituent elements, ending in a rhombic triacontahedral (RTH) cluster. Due to the minimisation of surface energies the Ag-In-Yb QC is preferentially cut through the cluster centre, which has a high atomic density (indicative of relative stability) rich in Yb. This provides particular “motifs” to be presented at the surface. It is at these motifs in which adsorbates are observed to preferentially adsorb.

A continuation of this observation leads to the hypothesis that any successive deposited elements will act to recreate the clusters that have been terminated. Using Scanning tunnelling Microscopy (STM), this has been recently shown on i-Ag-In-Yb in a display of a single element 3-dimensional Pb QC (whereas previous research demonstrates 2D thin films) [7]. The research carried out was on the 5-fold surface in order to reconstitute this structure as single element. In order to more comprehensibly complete the research, the same is attempted on the 3-fold surface of the same i-Ag-In-Yb QC.

Data so far suggests that the Pb adsorbs according to the 3-fold symmetry of the substrate. Further deposition leads to growth of tetragonal Pb islands with approximately 1nm base edges (as seen in Fig. 1), in preference to completion of the previous monolayer. careful analysis of Fast Fourier Transforms (FFTs) of these islands reveals that they are quasicrystalline in nature.

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An analysis of the physical properties of $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ – the first high-entropy alloy superconductor

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High-entropy alloys (HEAs) [1] are a modern alloy design strategy that utilizes the disorder of solid solution phases to stabilize new and unique structures. As HEAs are random mixtures consisting of four or more principal elements (elements in similar concentrations, from 5% to 35% each) the entropic term in the Gibbs free energy $G = H - TS$ is sufficiently large to stabilize simple structures (bcc, fcc, simple hex) with randomly filled sites rather than more complex intermetallics. Technologically favourable structural and mechanical properties have been found in HEAs [1], but no particularly interesting physical properties (low electrical and thermal conductivity and standard para- or ferromagnetism) [2].

$\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ and its physical properties have, however, turned out to be quite fascinating [3] as **this alloy is the first HEA known to exhibit a transition to a superconducting (SC) state**. Our sample had composition $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ (EDS spectroscopy) and average body-centered cubic structure with lattice parameter $a = 3.36 \text{ \AA}$ (determined by powder XRD). Since the lattice properties – namely, the lattice parameter and Debye temperature – conform to Vegard’s rule of mixtures, we have interpreted the mixing to be completely random. The measured electrical resistivity, heat capacity and magnetic measurements indicate that $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ is a type II superconductor with a critical temperature of $T_c \approx 7.3 \text{ K}$, a lower critical field $\mu_0 H_{c1} \approx 32 \text{ mT}$ and an upper critical field of $\mu_0 H_{c2} \approx 8.2 \text{ T}$. Further analysis of the specific heat gives us an energy gap in the electronic density of states (DOS) at the Fermi level of $2\Delta \approx 2.2 \text{ meV}$ and an indication that $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ is close to a BCS-type phonon-mediated superconductor in the weak electron-phonon coupling limit. Moreover, due to the large amount of disorder we are tackling with a “dirty” superconductor. While the transition from normal to SC state lowers the energy, this decrease is not sufficient to compensate the weakening of entropic stabilization at low temperature and stabilize $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ – therefore we predict that $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ is metastable (albeit extremely long-lived).

Open questions regarding superconductivity in HEAs remain: How wide (or narrow) is the composition range for HEA superconductors and does it enable us to optimize their properties? What is the mechanism behind this superconductivity?

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Crystallization in rapidly quenched Fe-B-Si system with additions of C and Cu

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Glass formability and phase transformations in rapidly quenched ferromagnetic nanostructured $(\text{Fe}_{85}\text{B}_{15-x}\text{Si}_x)_{98-y}\text{C}_2\text{Cu}_y$ (where $x=0; 5$ and $y=0; 1$) systems have been investigated by different methods. The consecutive crystallization stages of bcc-Fe and borides were determined by resistometry, differential scanning calorimetry and by thermogravimetry, where the values of important transformation parameters were estimated and mutually correlated with the results from structure analysis by TEM and XRD. Morphology of nano-sized Fe grains in amorphous matrix and their transformation to borides matrix was observed by TEM in dependence on the chemical composition and thermal treatment. The effects of systematic alloying on the transformation process and on the resulting structure have been correlated with selected magnetic properties of the samples after suitable annealing.

Syntheses and crystal structure determination of quasicrystal approximants in the RE-Au-Si systems (RE = Gd, Tb, Dy, Ho and Yb).

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Tsai-type 1/1 approximant crystals in the RE-Au-Si systems (RE = Gd, Tb, Dy, Ho and Yb) have been synthesized using various approaches of high temperature solid state synthesis techniques. The chemical composition of the approximants could vary in the range: RE(13.64 to 15.29)Au(69.47 to 70.08)Si(14.63 to 16.9) in atomic percentages. Few millimeter sizes of faceted crystals were grown using Au(79)Si(21) binary alloy as a flux [1]. The atomic structures of the compounds have been determined by using single crystal and powder X-ray diffraction data. The approximants are essentially iso-structural and their atomic structures are described with concentric polyhedral cluster units made up of disordered tetrahedron, dodecahedron, icosahedron, icosi-dodecahedron and (defected) triacontahedron, from the inside to out [2]. Moreover, it is observed that an additional RE atom could partially or fully replace the inner most disordered tetrahedron [1-3]. The relative ratio of the central RE atom to the disordered tetrahedron have been controlled during the syntheses and consequently 1/1 approximants with different occupancy of the central RE atom have been synthesized. The occupancy of RE atom at the cluster center affects some physical properties even for approximants which have the same chemical components and close compositions.

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Influence of Ni on the magnetocaloric effect in $\text{Fe}_{84-x}\text{Ni}_x\text{Zr}_6\text{B}_{10}$ soft-magnetic amorphous alloys

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We have studied the influence of Ni on the magnetocaloric effect (MCE) in Nanoperm-type amorphous materials by investigating a series of $\text{Fe}_{84-x}\text{Ni}_x\text{Zr}_6\text{B}_{10}$ alloys with $x=0, 2, 4$ and 6 and if the results fit the proposed “master curve” for second-order magnetic transition (SOMT) alloys. As expected, the Curie temperature increased with the amount of Ni from 428K for $x=0$ to 482K for $x=6$. The maximum magnetic entropy change (ΔS_M^{PK}) for an applied field of 1.4 T also increased, reaching a value of 1.52 J/Kkg for $x=6$, which is an increase of 25% compared to the Ni-free alloy. We confirmed the proposed “master curve” behavior for the temperature dependence of ΔS_M for different alloy compositions of the same series. The refrigerant capacity first decreased for $x=2$ and then increased, reaching a maximum value of 67 J/kg ($\Delta H = 1.4\text{ T}$) for $x=6$. For a 5 T field change, the value increased to 245 J/kg , which is comparable to the value achieved with $\text{Gd}_5\text{Ge}_{1.9}\text{Si}_2\text{Fe}_{0.1}$.

DFT modeling and transport properties of palladium based intermetallic compounds

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Intermetallic compounds are innovative catalyst materials. Their potential lies in spatial separation of active sites which enables high activity and selectivity. [1] By tuning their chemical composition it is possible to change their electronic properties. Palladium based intermetallic compounds, particularly PdGa and PdIn have shown very good catalytical properties in partial hydrogenation of acetylene to ethylene and methanol steam reforming processes respectively. Although catalysis occurs on the surface, it is important to know properties of the bulk as well. In order to get a deeper insight into those systems we calculated their electronic and vibrational spectra within density functional theory. [2] Detailed analysis of their experimental transport properties with correlation to the electronic structure will be presented.[3] We extracted scattering rates of different bands by the use of experimental transport properties. From vibrational spectra and electrical resistivity we successfully estimated Debye temperature. [4]

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Structure and Properties of Equiatomic Fe-M-Nb-B (M=Co, Ni) and M-rich Metallic Glasses

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The structure and properties of equiatomic Fe-M-Nb-B (M=Co, Ni) and M-rich amorphous ribbons with varying content of B in as-cast and annealed states have been investigated with respect to the M/Fe ratio. The evolution of mechanical and electromagnetic properties has been correlated with the types of crystalline phases formed during crystallization. The results from high-resolution elemental mapping and correlation analyses have been used to discuss the mechanism of mass transport across the amorphous matrix/crystalline grain interface. Specific compositions of the investigated systems alloyed with atoms enhancing nanocrystal formation have been analyzed to assess the alloying effect.

The Aluminum-Iridium binary system and Al-Ir based ternary compounds

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The Al-Ir binary system was thoroughly studied in the aluminum rich area of the diagram. A new compound with a stoichiometry Al_7Ir_3 has been found at 70 at% Al with a melting point at around 1380°C. Its structure has not been resolved yet but the powder X-ray diffraction pattern of this phase is very close to that of Al_7Rh_3 compound, although there are some discrepancies among the intensities. This Al_7Rh_3 compound¹ has been reported to have a monoclinic structure with lattice parameters: $a=10.309\text{Å}$, $b=3.808\text{Å}$, $c=6.595\text{Å}$, $\beta=102.4^\circ$, but with no further information about the space group or the structure. It is likely that our compound Al_7Ir_3 has a similar structure with analogous lattice parameters.

A new ternary compound $(\text{Al},\text{Si})_2\text{Ir}$ was also identified in the Al-Ir rich part of the Al-Si-Ir ternary system. Wavelength-dispersive X-ray spectroscopy analysis revealed an average composition of $\text{Al}_{61.53}\text{Si}_{5.64}\text{Ir}_{32.83}$ with a very narrow homogeneity range and differential scanning calorimetry measurements indicated a melting point around 1450°C. This phase is isostructural to the orthorhombic Ga_2Ir phase² and has similar lattice parameters: $a=3.957\text{Å}$, $b=12.859\text{Å}$, $c=10.600\text{Å}$ (space group Cmc21).

Another ternary phase with a composition of Al_3AuIr has been found in the aluminum-rich area of the Al-Au-Ir system. Differential thermal analysis indicates a melting point of 990°C and single-crystal X-ray diffraction measurements reveal that this ternary phase adopts a Ni_2Al_3 structure type (space group P-3m1) with $a=4.2584(5)\text{Å}$ and $c=5.1991(7)\text{Å}$. This compound is isostructural to the $\text{Al}_3\text{Cu}_{1.5}\text{Co}_{0.5}$ phase also found in the Al-rich part of the Al-Cu-Co ternary diagram.

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Elaboration and study of the $\text{Sc}_{57}\text{Ru}_{13}$ 1/1 cubic approximant of icosahedral structures in the (Sc,Ru) system

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The $\text{Sc}_{57}\text{Ru}_{13}$ phase structure [1] is quite remarkable as almost a perfect example of a 1/1 cubic approximant made essentially of two almost identical atomic Mackay clusters, one centered at (0,0,0) and the other at $\frac{1}{2}(1,1,1)$ plus a few extra glue atoms. The Mackay clusters are connected to each other along the ternary axes by Sc octahedra.

Using these data [2], we have derived a simple 6D primitive model of a hypothetical icosahedral phase that would generate this 1/1 approximant as shown on Figure 1. The model being primitive in 6D, generates a $\text{Im}\bar{3}$ structure that is an ideal simplified structure of the actual cubic phase.

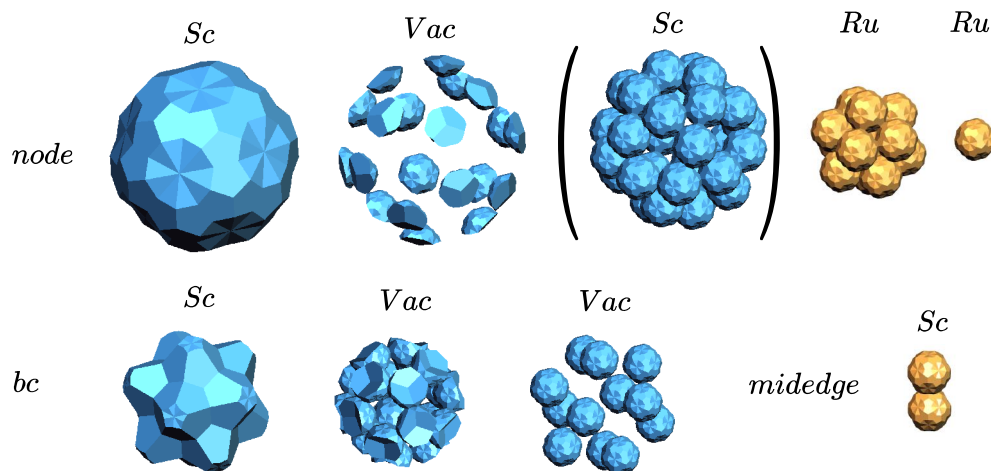


Figure 1: Atomic Surfaces defining the hypothetical icosahedral phase $\text{Sc}_{81.5}\text{Ru}_{18.5}$ in the (Sc,Ru) system: All atomic surfaces are located at special points (little groups $m\bar{3}5$ and $-5m$) in the 6D space

The comparison between the actual cubic structure and the predicted one of 1/1 cubic approximant issued from our 6D primitive model shows an excellent agreement.

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	Sunday 31 May	Monday 1 June	Tuesday 2 June	Wednesday 3 June	Thursday 4 June	Friday 5 June
9h– 10h30		<i>Thermodynamics C. Tassin</i>	<i>Introduction on the structure of CMA M. Mihalkovic</i>	<i>Coatings C. Vahlas</i>	<i>Transmission electron microscopy and SEM R. Portier</i>	<i>Nanostructures P. Svec</i>
10h30-11h				BREAK		
11h-12h30		<i>Thermodynamics (plus tutorial) C. Tassin</i>	<i>X-ray/neutron characterization M. de Boissieu</i>	<i>Coatings C. Vahlas</i>	<i>Transmission electron microscopy and SEM R. Portier</i>	<i>Nanostructures P. Svec</i>
12h30-14h00				LUNCH		
14h00-15h30		<i>Bulk materials preparation P. Gille</i>	<i>X-ray/neutron characterization M. de Boissieu</i>	<i>Transmission electron microscopy R. Portier (tutorial)</i>	<i>Tutorial Crystallography and X-ray diffraction M. de Boissieu R. Portier M. Mihalkovic</i>	EXCURSION
15h30-16h				BREAK		
16h-17h30	REGISTRATION	<i>Bulk materials preparation P. Gille</i>	<i>Thermodynamics C. Tassin (tutorial)</i>	<i>Crystal structure prediction M. Mihalkovic (tutorial)</i>	Lab visit	EXCURSION
17h30-19h	REGISTRATION		POSTER SESSION			
19h00 - 20h30	Welcome Party		POSTER SESSION		GALA DINNER	