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Poster Session Abstracts

Tuesday, December 9, 2014

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Formation of structurally complex phases during solidification of Al–Pd–Cr alloys

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Recently a great effort has been devoted towards studying microstructure, phase equilibria, and phase evolution in Al-base complex metallic alloys [1-3]. In this work, the formation of the less-known hexagonal ζ_b and the decagonal quasicrystalline approximant ε_n was investigated during solidification of alloys Al₇₁Pd₂₄Cr₅, Al₇₃Pd₂₀Cr₇, and Al₇₃Pd₂₃Cr₄. To perform the investigation, differential thermal analysis (DTA), synchrotron X-ray powder diffraction, and scanning electron microscopy coupled with the energy-dispersive X-ray spectroscopy were used. In all the investigated alloys structurally complex phases ε_n ($\varepsilon_6+\varepsilon_{28}$) and ζ_b , as well as the δ -phase were identified. Based on the results of DTA sequences of phase transformations were determined accompanying the alloy solidification. The Al₇₁Pd₂₄Cr₅ alloy was found to start to solidify at 1031.4°C through β . Primary dendrites of ζ_b were observed in Al₇₃Pd₂₀Cr₇ and Al₇₃Pd₂₃Cr₄ alloys. The peritectic reaction, liquid+ ζ_b + δ → ε_n + ζ_b + δ , leading to the formation of decagonal quasicrystalline approximant ε_n ($\varepsilon_6+\varepsilon_{28}$) took place in the final step of the solidification of all the investigated alloys at approximately 792°C.

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[3] B. Grushko, B. Przepiórżyński, D. Pavlyuchkov, S. Mi, E. Kowalska-Strzęciwilk, M. Surowiec. Complex intermetallics in Al–Cu–Cr system, *Journal of Non-Crystalline Solids*, 442 (2007), pp. 114–116

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Crystal growth and orientation of type-I clathrate single crystals

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Type-I clathrates possess promising thermoelectric properties, as they feature a high electric conductivity together with a low thermal conductivity. These properties are due to the specific crystal structure which contains two kinds of polyhedral cages, which host the cations or guest atoms. To unravel the origin of the thermoelectric properties high quality single crystals are necessary to study in detail the electrical and thermal transport, as well as the details of the crystal structure and the phonon dispersions at various temperatures.

Single crystals of the two clathrates $\text{Ba}_8\text{Ni}_{3.5}\text{Ge}_{42.1}[\]_{0.4}$ and $\text{Ba}_8\text{Au}_{5.25}\text{Ge}_{40.3}[\]_{0.45}$ have been grown by means of the crucible-free Czochralski pulling method and the Bridgman technique [1,2]. In this contribution, we present the details of the crystal growth and the orientation procedure to obtain various samples of different shapes and orientations for the different measurement techniques.

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[2] H. Zhang *et al.*, *Inorg. Chem.* **50**, 1250 (2011).

Electromagnetic properties of DBSA-doped polyaniline: from fundamentals towards application with carbon nanotubes

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We have carried out a comparative experimental study of the dc electrical conductivity σ and magnetic susceptibility χ of own-made polyaniline (PANI) pellets doped with dodecylbenzene-sulphonic acid (DBSA), a long molecule with surfactant properties. For all samples, we find [1] that σ at low temperatures (T) is governed by the variable-range hopping (VRH) in a homogeneously disordered three-dimensional (3D) system of coupled one-dimensional (1D) chains. Depending on the doping and the corresponding disorder level, the VRH exponents are either 1/2, 2/5, or 1/4. At higher T , in all samples, we find an exponent 1 that signifies nearest-neighbour hopping. All these exponents are predicted in a model by Fogler, Teber, and Shklovskii [2] for the charge transport in quasi-1D Anderson–Mott insulators, and conditions for their appearance depend on disorder and T . We identified the presence of a soft Coulomb gap in our samples, which signifies a long-range Coulomb interaction.

Change from one exponent into another in $\sigma(T)$ appears at a crossover temperature T^* , where there are also noticeable features in $\chi(T)$. This coupling of charge and spin is discussed in the spirit of $k_B T^*$ being the thermal energy which causes an enhancement of the density of delocalised (Pauli) spins at the expense of localised (Curie) spins as T rises above T^* . Utilising the observed correlation between spin dynamics and electronic transport, we estimate the energy scales in the electronic structure of PANI–DBSA.

Utilising a property that both PANI–DBSA and multiwall carbon nanotubes (MWCNT) are soluble in chloroform, we have produced bulk blends of these two materials, the achieved mass fraction of MWCNT being up to 40 %. This is as remarkable as the accompanying effective loss of the temperature dependence of σ : it decreases by only 3 times from room temperature to 10 K, whereas this decrease for pure PANI–DBSA is by a factor of 10^6 . Thus, our blends simultaneously offer a solution to the problem of applications of MWCNT in bulk form, as well as to that of poor conductivity of PANI–DBSA at low T . It is also possible to make thin films, both of PANI–DBSA and of the blends, on a commercial plastic substrate (FR4).

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[2] M. M. Fogler, S. Teber, B. I. Shklovskii, *Phys. Rev. B* **69**, 035413 (2004)

The characteristic function for Fibonacci chain probability distribution with flips in LS sequence

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The moments' series expansion of the characteristic function of the atomic positions probability distribution in the Fibonacci chain with LS sequence flipped to SL is presented.

Fibonacci chain is well known model of 1D quasicrystal with units L and S arranged aperiodically. The diffraction diagram of the Fibonacci chain gives sharp peaks in discrete positions in the reciprocal space. It was shown [1], that expressing the atomic positions in a reference to the periodic lattice with lattice constant related to the wavevector in the Fourier space gives the probability distribution (AUC) characteristic for a particular structure. Due to necessity of using vectors \mathbf{k} and \mathbf{q} with norm relation $k/q=\tau$ to index diffraction pattern two lattices are required to obtain the probability distribution function: one for \mathbf{k} , and the second one for \mathbf{q} . The marginal distribution of variable related to shorter lattice constant is the AUC. The probability distribution function for quasicrystals is uniform with linear dependence $\mathbf{v}(\mathbf{u})$ [2, 3].

For quasicrystals the Fourier Transform of the probability distribution is both the structure factor and the characteristic function of the probability distribution. The characteristic function can be expanded in the power series with parameters being moments of the probability distribution function. Fitting the moments of the probability distribution allows recreating the distribution for the structure. The recreation correctness depends on the number of parameters taken to the fitting procedure (Fig. 1).

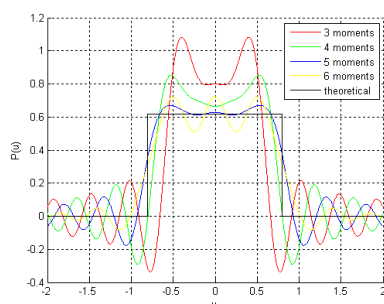


Fig. 1 The AUC recreated from diffraction pattern of the Fibonacci chain by reverse Fourier Transform of the characteristic function of the atomic positions probability distribution. Recreation depend on the number of moments in the power series expansion

In this work flips between sequences $LS \rightarrow SL$ are allowed which modify the shape of the probability function, but don't affect the quasicrystalline setting. Those flips can't be modeled with simple tiling model but, as it is shown in this work, statistical approach allows designating those flips in the structure.

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Atomic structure of selected phases of ϵ -family in Al-Pd-Co system

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Fine structures of phases of the ϵ -family in the Al_{73.8}Pd_{11.9}Co_{14.3} alloy were studied. In the investigation, scanning electron microscopy including energy dispersive X-ray spectroscopy, X-ray diffraction, transmission electron microscopy, and scanning transmission electron microscopy using high-angle annular dark-field detector were used. The near-equilibrium at 700 °C long-term annealed sample exhibited the structural (ϵ_{16}) and chemical homogeneity. In the microstructure of the as-cast sample, non-equilibrium phases ϵ_6 , ϵ_{16} , and ϵ_{28} were observed to transform mutually by cluster re-arrangement. The structures determined experimentally were compared with those calculated by VASP software.

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Investigation of decagonal quasicrystalline approximant ε_n in Al–Pd system

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Up to date many complex metallic alloys have been studied with the intention to search for quasicrystalline phases. Although many Al-Pd-TM (TM = transition metal) systems have been investigated [1-3], the results obtained head back to the Al-Pd system where the area of ε_n in related phase diagram has not been completely refined yet with regard to the experimental results [4,5]. This work deals therefore with the investigation of decagonal quasicrystalline approximant ε_n in the above binary system. The alloys Al₇₇Pd₂₃, Al₇₄Pd₂₆, Al₇₃Pd₂₇, Al_{72.4}Pd_{27.6}, and Al₆₇Pd₃₃ were long-term annealed at 500 or 700°C and then characterized by the scanning electron microscopy (SEM) including energy-dispersive X-ray spectroscopy (EDX), the transmission electron microscopy (TEM), the X-ray diffraction (XRD), and the differential scanning calorimetry (DSC). The results related to the phase evolution were used to propose new knowledge about ε_n .

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Adsorption properties of the $\text{Al}_{13}\text{Fe}_4(010)$ surface toward molecules involved in the semi-hydrogenation of acetylene: a DFT study

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The semi-hydrogenation of acetylene is an important chemical reaction involved in the industrial production of polyethylene: it is used to avoid the poisoning of the catalyst by reducing the possible traces of acetylene in the mixture. Traditional industrial catalysts are generally noble metal based alloys, like Pd-Ag alloys¹. The $\text{Al}_{13}\text{TM}_4$ (TM=Fe or Co) complex metallic alloys have recently been considered as a low cost alternative material for this reaction²⁻³.

To understand the reactivity of the promising $\text{Al}_{13}\text{Fe}_4$ catalyst, an investigation at the atomic scale is mandatory. Here, we focus on the $\text{Al}_{13}\text{Fe}_4(010)$ surface, whose structure has been previously determined by a combination of both experimental and *ab initio* methods⁴ (Fig. 1).

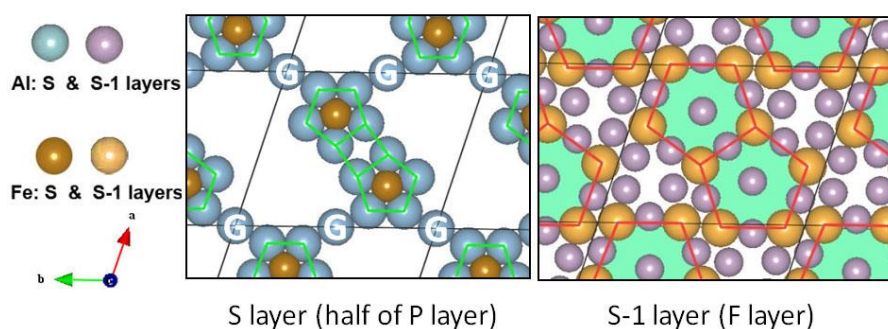


Fig 1. Structures of the surface (S) and subsurface (S-1) layers of the considered surface model. Two models are considered in this study. They differ by the number of surface Al-glue atoms (the glue atoms are identified by (G)): there are 2 surface Al-glue atoms per surface unit cell in model A while the B model do not contains surface Al-glue atoms. Green zones of S-1 layers are covered by atoms of S layer.

The considered surface models, which differ in the number of surface Al-glue atoms (Fig. 1) present about 50 non-equivalent possible adsorption sites. Our calculations show that few of them are favorable adsorption sites for molecules involved in the semi-hydrogenation of acetylene. Atomic hydrogen is more stable on surface Al-Fe bridge sites and directly above Fe atoms of the subsurface layer. The H_2 molecule is adsorbed only on Fe top sites with an activated bond distance equal to 0.92 Å. Hydrocarbon species also prefer to be bonded to Fe atom: C_2H_2 forms $2\sigma+1\pi$ bond toward 3-fold Al_2Fe site and C_2H_4 forms 1π bond on top iron Fe site.

In this work, the influence of the surface Al-glue atoms are discussed. For example, the absence of surface Al-glue atoms brings up new favorable adsorption sites for hydrocarbon species, located just above Fe-Fe bonds in the subsurface layer (Fig.1). Finally, the adsorption properties of this surface will be compared with the ones obtained for the $\text{Al}_{13}\text{Co}_4(100)$ surface^{5,6}.

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Adjusting the composition of InPd

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InPd (CsCl prototype structure [1]) is a possible catalyst for methanol steam reforming. According to the binary phase diagram [2] this intermetallic compound has a congruent melting point of around 1285°C and its stability region is quite broad reaching from 45 to 61.5 at% Pd. Determination of intrinsic bulk [3] and surface properties is the basis for a better understanding of the mechanisms of the catalysis. For this purpose single crystalline InPd samples of an appropriate size have to be available to enable a number of characterization methods with different requirements on the sample geometry.

It was shown earlier that cm³-sized crystals can be grown by the Czochralski technique [4]. The crystals were grown from In-rich solutions instead from congruent melts to reduce the vapor pressure of In. The composition of the crystals grown from a solution will follow the solidus line in the phase diagram. So InPd crystals prepared in this way at maximum growth temperatures of around 1100°C will always have a slightly In-rich composition. It was also described that the cross sections of the grown crystals show a compositional inhomogeneity with a smaller In content towards the rim of the crystals [4]. This was explained by evaporation of In from the surface of the already grown crystal during the ongoing growth process.

The In loss by evaporation can be used to adjust the composition of small InPd samples in the full range of the InPd stability region in a post-growth treatment. Therefore an ampoule inclosing a piece of InPd and filled with inert gas can be placed in a temperature gradient. The intermetallic compound in the hot part at temperatures below the original growth temperature will lose In by evaporation and the composition can be shifted towards the 1:1 composition or even further towards the Pd-rich side of the stability region. By this approach small single crystalline samples with different compositions could be prepared in post-growth annealing experiments which would enable composition-dependent measurements of physical properties.

- [1] E. Hellner, F. Laves, Z. Naturforsch. **A 2** (1947), 177-183.
- [2] H. Okamoto, J. Phase Equilib. **24** (2003), 481.
- [3] M. Wencka et al., Intermetallics **55** (2014), 56-65.
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Surface Structure of Ag-In-RE Approximants and Quasicrystalline Metallic Films on the Surface of *i*-Ag-In-Yb Quasicrystal

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Quasicrystals are metallic alloys, which show long-range order with lack of periodicity and translational symmetry and possess classically forbidden rotational symmetry such as fivefold and tenfold symmetry. [1] Crystalline approximants which have similar structure and chemical composition to parent quasicrystals can help to understand the structure of quasicrystals because their structure can be well understood using conventional surface analysis techniques.

To understand the influence of quasiperiodicity on physical properties of quasicrystals, it's worthwhile to have single element quasicrystals. For this purpose, quasicrystal surfaces have been used as template to produce artificial single element quasicrystals. [2-3] For example, recently multi-layered quasicrystalline lead (Pb) film has been successfully grown on the fivefold surface of *i*-Ag-In-Yb quasicrystal. [4]

In this work, the structure of (100) surfaces of Ag-In-RE 1/1 approximants (RE = Gd and Tb) has been studied. Moreover, the *i*-Ag-In-Yb surface has been used as template to grow metallic films. Scanning tunneling microscopy (STM) was employed to characterise the surface and thin film formation. We will also present the surface structure of various approximants related to Ag-In-Yb quasicrystal.

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Torque magnetometry as a sensitive probe for measuring magnetic anisotropy in paramagnetic and magnetically ordered states of magnetic systems

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Torque magnetometry is an experimental method that probes bulk magnetic anisotropy of a magnetic sample. Measured magnetic torque gives most informative results when single crystalline samples are available. In this work some advantages of torque magnetometry over standard magnetometry measurements will be presented.

An application of highly sensitive low-field ($H < 1\text{T}$) torque magnetometry is presented on several spin $S=1/2$ systems with small magnetic anisotropy which comes mainly from the anisotropy of the electron g factor. In the paramagnetic sample magnetic torque is proportional to the magnetic susceptibility anisotropy, and thus represents a much more sensitive method for measuring magnetic anisotropy than e.g. measurement of susceptibility by standard magnetometry methods. This turns out to be relevant in $S=1/2$ systems where anisotropic exchange interaction is present, such as 1D $S=1/2$ Heisenberg antiferromagnet with Dzyaloshinskii - Moriya interaction [1]. Torque magnetometry can routinely detect the rotation of magnetic axes with temperature and in combination with electron spin resonance (ESR) spectroscopy this rotation can be correlated to the temperature change of the g tensor [2].

Symmetry of the magnetically ordered states can also be determined by torque, as will be shown on examples of antiferromagnetically ordered systems with easy plane [3] and cubic [4] anisotropy and uniaxial ferromagnet [5]. In collinear uniaxial antiferromagnet reorientation of the spin axes influences angular dependence of torque in magnetic field H smaller than the spin flop field H_{SF} . This allows the determination of the value of spin flop field in $H < H_{SF}$, which gives torque magnetometry an advantage over standard magnetization measurements [6]. Probing magnetic symmetry with torque can be used as an alternative when standard methods such as e.g. neutron scattering cannot be employed.

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Discovery of a $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ Superconducting High-Entropy Alloy

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High-entropy alloys (HEAs) are multi-component mixtures of elements in similar concentrations, where the high entropy of mixing can stabilize disordered solid-solution phases with simple structures like a body-centered cubic or a face-centered cubic, in competition with ordered crystalline intermetallic phases. We have synthesized a HEA with composition $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ (in at. %), which possesses an average bcc structure of lattice parameter $a = 3.36 \text{ \AA}$. The measurements of the electrical resistivity, the magnetization and magnetic susceptibility and the specific heat revealed that the $\text{Ta}_{34}\text{Nb}_{33}\text{Hf}_8\text{Zr}_{14}\text{Ti}_{11}$ HEA is a type II superconductor with a transition temperature $T_c \approx 7.3 \text{ K}$, an upper critical field $\mu_0 H_{c2} \approx 8.2 \text{ T}$, a lower critical field $\mu_0 H_{c1} \approx 32 \text{ mT}$ and an energy gap in the electronic density of states at the Fermi level of $2\Delta \approx 2.2 \text{ meV}$. The investigated HEA is close to a BCS-type phonon-mediated superconductor in the weak electron-phonon coupling limit, classifying as a "dirty" superconductor. We show that the lattice degrees of freedom obey Vegard's rule of mixtures, indicating completely random mixing of the elements on the HEA lattice, whereas the electronic degrees of freedom do not obey this rule even approximately, so that the electronic properties of a HEA are not a "cocktail" of properties of the constituent elements. The formation of a superconducting gap contributes to the electronic stabilization of the HEA state at low temperatures, where the entropic stabilization is ineffective, but the electronic energy gain due to the superconducting transition is too small for the global stabilization of the disordered state, which remains metastable.

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: $a=10.309\text{\AA}$, $b=3.808\text{\AA}$, $c=6.595\text{\AA}$, $\beta=102.4^\circ$, 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: $a=3.957\text{\AA}$, $b=12.859\text{\AA}$, $c=10.600\text{\AA}$ (space group Cmcm).

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 $a=4.2584(5)\text{\AA}$ and $c=5.1991(7)\text{\AA}$. 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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Graphene and related 2d structures research unit of the CEMS center

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In early November 2014, minister of science, education and sports declared first seven Croatian scientific centers of excellence. Center of Excellence for Advanced Materials and Sensing Devices unites four key research units: photonics and quantum optics, new functional materials, physics and technology of ion beams, and graphene and related two-dimensional structures. First three units are led by scientists from Ruđer Bošković Institute: M. Stipčević, M. Ivanda and M. Jakšić.

The research unit focused at Graphene and related 2D Structures (G2D) is led by M. Kralj from the Institute of Physics. Graphene and its potential application are in the last 10 years in the focus of research interest of a large number of scientists. Moreover, discoveries of whole new classes of 2D crystals in the past few years intensifies this research direction even more. The potential of graphene and related 2D structures is recognized globally, e.g. through EU's 2013-2023 Graphene Flagship to develop future technologies based on graphene. Graphene and 2D materials are more often mentioned in the context of green technologies, e.g. as a platform for future ultra-efficient solar cells or cost-effective batteries.

The G2D core team of 12 researchers from the Institute of Physics (M. Kralj, D. Aumiler, T. Ban, A. Šiber, T. Vuletić, I. Živković), Ruđer Bošković Institute (M. Buljan, I. Bogdanović-Radović, A. Gajović, I. Halasz, P. Lazić) and Faculty of Natural Sciences (H. Buljan), recognized great potential of joint focused research. The G2D's mission is to set frame for the top-level research and competitiveness at international level aiming at the development of new 2D materials. The goal of the G2D research unit is to gather team of scientists capable to attract funding from the most competitive EU and other international funds, as well as to promote scientific research motivated, inter alia, by applications of direct interest for Croatian hi-tech and small and medium enterprises. This center of excellence will be presented by a poster.

Pd₂Ga/SiO₂ nanoparticles: a NMR and physical properties study**Mitja Krnel**^{1*}, M. Klanjšek¹, A. Jelen¹, S. Vrtnik¹, M. Wencka³ and J. Dolinšek¹¹Jožef Stefan Institute & University of Ljubljana, Jamova 39, 1000, Ljubljana, Slovenia²Center for Individual Nanoparticle Functionality, Department of Physics building 307, Technical University of Denmark, DK-2800, Lyngby, Denmark³Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznan, Poland

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The Pd₂Ga intermetallic compound is a highly selective and stable catalyst for the semi-hydrogenation of acetylene[1]. In this contribution, we present an experimental investigation of NMR properties of Pd₂Ga nanoparticles supported on SiO₂ and we compare these properties with properties of bulk Pd₂Ga.

Two powder samples were measured, containing 23 wt.% and 13 wt. % of Pd₂Ga.

Samples were characterized by X-ray diffraction and SEM microscopy. We measured the ⁷¹Ga NMR spectra for both samples in 9.4 T magnetic field by frequency sweep. We also tested the Korringa relation[2] by measuring the temperature dependence of ⁷¹Ga spin-lattice relaxation rate and temperature dependence of Knight shift in the temperature range from 9 K to 300 K for both samples and compared it with previously measured data for bulk Pd₂Ga. From the measurements of the temperature dependence of spin-lattice relaxation rate we can conclude that the amount of Pd₂Ga in the sample does not affect the Korringa constant. The Korringa constant for nanoparticles is slightly higher than for the bulk Pd₂Ga. The physical properties measurements show that Pd₂Ga is a diamagnet with metallic electrical resistivity and moderate thermal conductivity. The thermoelectric power is negative with complicated temperature dependence, indicating complexity of the Fermi surface.

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Synthesis of single grain Au-Sn-*R* (*R*=rare-earth) quasicrystals and their approximants

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Thanks to its binary character and the existence of 2/1 and 1/1 approximants (APs), structure information of icosahedral quasicrystal (*i*-QC) is now available in the Cd-Yb system^[1]. Isostructures of *i*-QC and approximants have been reported in Au-based system^[2], which showed interesting physical properties. However, so far, the large size of single crystal has not been obtained in the Au-based systems^[2]. In this work, we intended to search new *i*-QC phase and to synthesize single-grained crystals of 2/1 and 1/1 APs in the Au-Sn-*R* (*R*=rare earth elements) systems using self-flux technique.

High purity elements were placed in the Al₂O₃ crucible sealed in quartz tubes under an Ar atmosphere, followed by the compositional homogenization and the heat treatment using an electric furnace. Then, the single grained crystals were separated from the Au-Sn melt using a centrifuge. Phase identification of the samples was carried out using powder X-ray diffraction. The compositions were analyzed using SEM equipped with EDS and ICP-AES.

Figure 1 shows powder X-ray diffraction patterns of two Au-Sn-Yb samples. The peaks can be fully indexed with *i*-QC and 2/1 AP, respectively. In addition, the sample (a) has clear crystal shape of pentagonal dodecahedron (Fig. 2), which evidences that this phase is the *i*-QC. The Au-Sn-Yb *i*-QC was found for the first time. On the other hand, millimeter-sized single crystals of 1/1APs were obtained in the Au-Sn-*R* (*R*= Ce, Pr, Nd, Sm, Gd, Tb) systems. In this presentation, we will discuss the phase formation of *i*-QC, 2/1 and 1/1 APs in these Au-Sn-*R* systems in term of the atomic sizes of rare-earth elements.

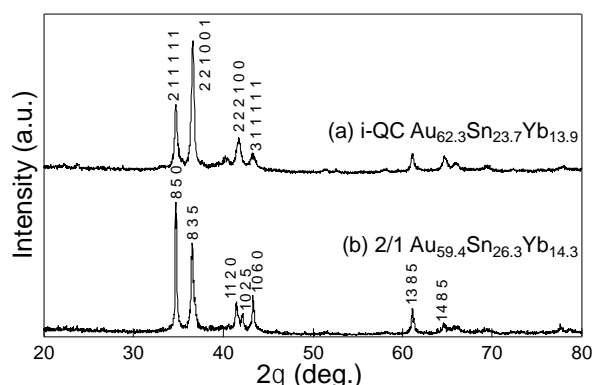


Fig. 1 Powder x-ray diffraction patterns of (a) *i*-QC and (b) 2/1 AP obtained in the Au-Sn-Yb.

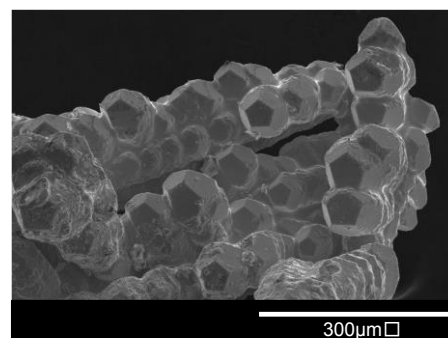


Fig. 1 SEM image of the single grained crystals of the Au-Sn-Yb *i*-QC.

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Evidence of 3D-Dirac dispersion in PbSnSe by the de Haas von Alphon oscillations

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Single crystals of mixed chalcogenide PbSnSe in composition $\text{Pb}_{0.83}\text{Sn}_{0.17}\text{Se}$ is predicted to be a 3D Dirac semimetal. Materials with a 3D linear band dispersion represent a novel class of material which is an extension of the well-known 2D Dirac dispersion in graphene. Recently predicted and discovered materials with the 3D Dirac dispersion are Cd_2As_3 , Na_3Bi and topological insulators at the topological phase transition, of which PbSnSe is an example.

By SQUID magnetometry up to 5T we have observed well-defined de Haas von Alphon oscillations. Temperature analysis of the dHvA oscillations allowed us to find microscopic parameters such as the scattering time, effective mass and charge concentration. Analyzing the phase of dHvA oscillations we observed the π -Berry phase shift which is a result of the linear band dispersion.

Magnetization dynamics reveals inhomogeneity in different systems: from amorphous alloys and agglomerated nanoparticles to multiferroic crystals

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Magnetic transitions in materials are often much more complicated than are the examples from the cook-books of magnetism. Therefore, additional measurements should always be performed in order to develop the realistic model of magnetic state of the system. One way of distinguishing between the magnetic states is via dynamics of the dc magnetization after change of outer conditions, i.e. the magnetic field or temperature.

Magnetic transitions in multiferroic family of $K_3Fe_5F_{15}$ and similar compounds motivated us to study the slow relaxation of magnetization of these materials on the hours time scale after change of magnetic field. This slow process was described by a logarithmic time dependence over a broad temperature and field range, similar to the behaviour of magnetic nanoparticles. The results were explained with thermal activation of magnetic moments of the magnetic nano-regions in crystal over the anisotropy barriers. Thus, from magnetization measurements the sizes of magnetic regions were estimated to be in the nanometre range, that should be of importance for the multiferroicity and magneto-electric coupling.

Conducted reasoning was enlighten knowing magnetic behaviour of the nanoparticles, where slow relaxation of the magnetization comes from the activation of their magnetic moments over the anisotropy barriers. Surprisingly, in our studied FeNiB amorphous nanoparticles, both coated in SiO_2 and uncoated, the relaxation of magnetization deviated from this simple picture. However, this deviation and comparison with the geometrically determined size distribution indicate that the magnetic units responsible for the observed dynamics consist of several physical nanoparticles.

Similarly, the slow magnetic relaxation appeared in system of $Hf_{100-x}Fe_x$ metallic glasses. For $35 \leq x \leq 43$, which is above the paramagnetic regime and below the onset of the ferromagnetic state, observed behaviour was explained with the self-assembled magnetic nano-clusters embedded within a paramagnetic matrix. This reveals uniquely the development of the chemical order showing that the clusters grow rapidly with increasing x . In this way, magnetic method showed as very convenient in indicating the evolution of chemical order on nanometre scale.

In three presented cases applicability of slow magnetic relaxation method teaches us how to use it for study of the nano-magnetic inhomogeneities in wide class of different materials with the non-trivial magnetic behaviour.

Physical and structural properties of incommensurately modulated Fe_{2-x}Ge intermetallic

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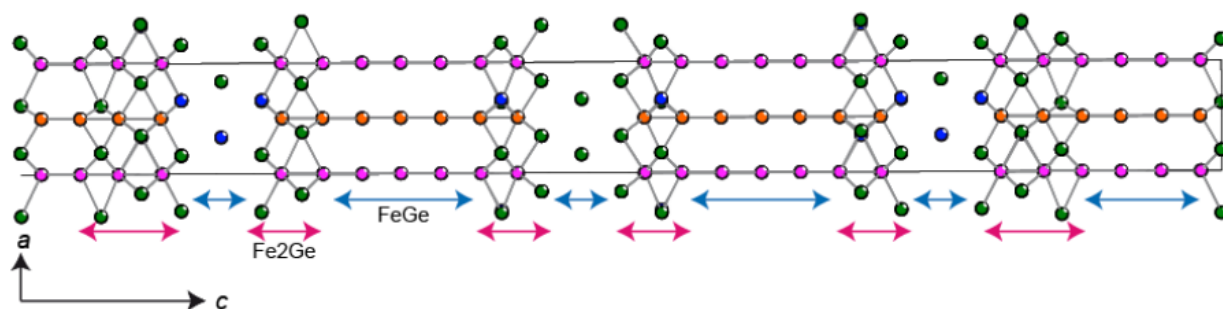
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Iron-germanium system has very rich phase diagram hosting variety of phases and compounds. One of them (FeGe) recently attracted much attention. In thin film form of this compound skyrmions were reported near room temperature (at 260K) [1]. Authors found that when thickness of crystal becomes greater than distance between skyrmions, more ordinary ferromagnetic phase starts to dominate. This discovery pushed further investigations of iron-germanium system in context of spintronic applications.

Here we report on investigation of Fe_{2-x}Ge phase that has bulk ferromagnetic transition at 420 K. Transport properties show typical behavior of complex metallic alloys. Detailed structural analysis revealed that crystal structure can be described by incommensurately modulated distribution of vacancies in all six Fe sites of the Fe_2Ge structure, while all Ge sites are fully occupied. Using the satellite reflections, the structure solution has been obtained in the superspace group $P-6m2(00\gamma)000$. In the modulated structure, layer blocks of the FeGe and Fe_2Ge composition aperiodically alternate along the hexagonal c-axis.



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Crystal structure and stability of Y family of phases in Al-Co system

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The contribution is focused on experimental investigation of the Y-Al₁₃Co₄ in Al-Co system. The investigated Al_{75.5}Co_{24.5} alloy was prepared by induction melting and after casting sectioned into several samples. The samples were annealed for 330 h at temperatures 1080, 1090, and 1110°C and subsequently rapidly cooled to fix their high-temperature microstructures. In the investigation X-ray diffraction, differential scanning calorimetry, and scanning electron microscopy including both energy dispersive X-ray spectroscopy and electron backscatter diffraction were used. The microstructure corresponding to the Y-Al₁₃Co₄ area was found as morphologically heterogeneous comprising of light-grey needles inserted into the dark-grey matrix. It was found out that the needles are formed by orthorhombic Y₂-Al₁₃Co₄ and the matrix corresponds to monoclinic Y₁-Al₁₃Co₄. Crystal structures of both the phases were refined. Decorative, symmetrical, and structural similarities between them are discussed in the contribution.

The authors wish to thank to the European Regional Development Fund (ERDF) for financial support of the project ITMS:26220120014 “Center for development and application of advanced diagnostic methods in processing of metallic and non-metallic materials” funded within the Research & Development Operational Programme, to the Slovak Academy of Sciences for the support in the frame of the “Center of Excellence for functional multiphase materials” (FUN-MAT, I/2/2011), as well as to the Grant Agency VEGA for the financial support under contracts 1/0143/12 and 1/0811/14, and to the Slovak Research and Development Agency for the financial support under contract APVV-0076-11.

The Effects Of Deposition Conditions And Annealing Temperature On The Structure And Morphology Of Ta-N Thin Films

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Tantalum nitride (Ta-N) thin films were prepared by reactive magnetron sputtering at room temperature and at various partial pressures of the reactive gas N₂. The films were subsequently annealed in the temperature range up to 950°C. The crystal structure and the nanomorphology of films were investigated with grazing incidence X-ray techniques: specular reflectivity (XRR), diffraction (GIXRD) and small angle scattering (GISAXS). Structural features in films depend on the nitrogen partial flow rate (pN₂); as pN₂ increases the crystal structure changes: from amorphous Ta-rich (pN₂ = 10%), to fcc-TaN (pN₂ = 20-40%), to amorphous N-rich (pN₂ > 40%), to cubic-Ta₂N₃ (pN₂ > 80%); the density of the films is correspondingly affected. Upon annealing, amorphous films crystallize into fcc-TaN, while as deposited fcc-TaN and cubic-Ta₂N₃ films are stable up to 950°C with releasing stacking fault deformations. The loose homogenous structure of the films deposited at high pN₂ > 60% anneals into particulate nanostructure with the average grain size increasing from 3 nm (annealing @ 550°C) to 15 nm (annealing @ 950°C).

Templated quasicrystalline molecular layers

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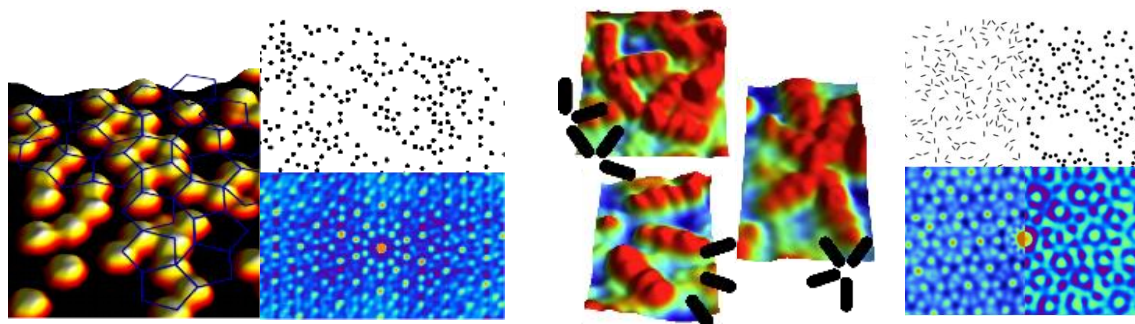
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Quasicrystals are materials with long range ordering but no periodicity. We report scanning tunneling microscopy (STM) observations of quasicrystalline molecular layers on five-fold quasicrystal surfaces. The molecules adopt positions and orientations on the surface consistent with the quasicrystalline ordering of the substrate. Carbon-60 adsorbs atop sufficiently-separated Fe atoms on icosahedral Al-Cu-Fe to form a unique quasicrystalline lattice whereas further C₆₀ molecules decorate remaining surface Fe atoms in a quasi-degenerate fashion. Pentacene (Pn) adsorbs at tenfold-symmetric points around surface-bisected rhombic triacontahedral clusters in icosahedral Ag-In-Yb.



Left: STM data of C₆₀/Al-Cu-Fe with Penrose P1 tiling superimposed and autocorrelation of C₆₀ positions extracted from larger-scale STM image (shown above the autocorrelation function)

Right: High-resolution STM data of Pn/Ag-In-Yb with specific motifs shown to aid the eye and autocorrelation of Pn positions (with and without orientation information)

MOCVD of Fe and Al coatings under compatible conditions: towards intermetallic catalyst coatings.

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The intermetallic compound $\text{Al}_{13}\text{Fe}_4$ is an active and selective catalyst for the semi-hydrogenation of acetylene in the production process of polyethylene [1]. Its crystallographic structure shows a high average Fe-Fe interatomic distance and a low coordination of iron atoms which follows the concept of “site isolation”. This compound is also interesting because of its low cost (e.g. no noble metals) and low toxicity compared to industrial catalysts. However, it has been produced in powder form which limits its use in catalytic engineering. In this context, our work ultimately aims at developing $\text{Al}_{13}\text{Fe}_4$ as supported films and/or nanoparticles by metal-organic chemical vapor deposition (MOCVD) from suitable molecular precursors.

This communication concerns the first step towards this objective, namely the development of the unary deposition of Al and Fe in compatible conditions. The dimethylethylamine alane precursor (DMEAA, $[\text{AlH}_3(\text{NMe}_2\text{Et})]$) is selected for Al deposition. Films are deposited on silicon substrates at 10 Torr between 139°C and 241°C. The deposited films are found to be free of heteroatoms but show a rough microstructure which could be smoothed by in situ pretreatment of the substrate surface by plasma. We determined the Arrhenius plot of the global deposition reaction. The growth rate varies slightly between 167°C and 227°C, and decreases sharply above. The activation energy of the surface reaction is 1.098×10^8 J/kmol. A chemical kinetics model is currently under development that will ultimately determine the appropriate conditions for the co-deposition with Fe. Iron pentacarbonyl, $\text{Fe}(\text{CO})_5$, as well as original molecular precursors based on nitrogen ligands (triazinates, amidinates, guanidines ...) will be presented as potential candidates.

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The influence of surface domains on magnetization of very soft magnetic ribbons

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The influence of surface fields H_p (generated by core currents) on the parameters of M-H loops (the coercive field H_c , the maximum magnetization M_m , etc.) of amorphous and nanocrystalline $Fe_{73.5}Cu_1Nb_3Si_{15.5}B_7$ ribbon and amorphous VITROVAC 6025Z ribbon has been investigated. In amorphous $Fe_{73.5}Cu_1Nb_3Si_{15.5}B_7$ ribbon H_c decreases with H_p with unchanged M_m , whereas in nanocrystalline $Fe_{73.5}Cu_1Nb_3Si_{15.5}B_7$ and VITROVAC 6025Z ribbons H_c increases with H_p and M_m decreases with H_p . This unusual increase of H_c with H_p is ascribed to the influence of H_p on the surface domain structure (SDS) and strong interaction between SDS and inner (main) domain structure (MDS) in these materials.

Transport in high quality decagonal quasiperiodic monocrystals $d\text{-AlCoNi}$ vs $d\text{-AlCoCu}$ Petar Popčević^{1*}, **Kristijan Velebit**¹, Ante Bilušić, Peter Gille³ and Ana Smontara¹¹Institute of Physics, Zagreb, Croatia²Ludwig-Maximilians-Universität München, München, Germany

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Decagonal quasicrystals offer unique opportunity to investigate differences of physical properties of periodically and quasiperiodically ordered structures on the same crystal [1]. That is due to unique structure of decagonal quasicrystals that is periodic along one spatial direction and quasiperiodic (with decagonal symmetry) in plane perpendicular to the periodic direction.

Detailed investigations of transport properties of high quality single crystals of $d\text{-AlCoNi}$ and $d\text{-AlCoCu}$ revealed that, contrary to some earlier work [2], electrical resistivity shows positive temperature coefficient (PTC) of electrical resistivity in quasiperiodic plane as well as that in periodic direction but with much higher residual resistivity [3]. Maximum in electrical resistivity along quasiperiodic directions indicates crossover from Boltzman like to non-Boltzman like electronic transport regime.

Minimum in electrical resistivity at low temperatures is most likely due to spikiness of the density of state near Fermi energy that is positioned near very narrow local minimum.

Differences in thermopower among different directions suggest strong anisotropy of quasi Fermi surface.

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**Femtosecond laser techniques for investigation of novel 2D materials
at CEMS Center of Excellence**

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Two-dimensional (2D) materials have historically been one of the most extensively studied classes of materials due to the wealth of unusual physical phenomena that occur when charge and heat transport is confined to a plane. Recent progress in the exfoliation of layered materials and the nanofabrication of functional structures has revived the interest in 2D materials such as the layered metal dichalcogenides (MDCs), copper oxides, iron pnictides and graphene. True potential of such materials lies in combination of their unique optical and electronic properties which determines their optoelectronic and energy harvesting functionalities, making them ideal candidates for interdisciplinary research approach.

The functional properties of any material are determined by its response to external stimuli, which drive it out of equilibrium. Hence, fundamental understanding is gained from studying relaxation processes. Here, femtosecond optical spectroscopy combined with an optical microscope to investigate the local excited state dynamics in novel 2D materials is presented. This tool enables us to combine nanoscale spatial resolution and sub-picosecond (ps) time resolution. It provides many advantages over the standard transient absorption techniques because it directly investigates the excited state dynamics at a local scale.

Statistical approach to the analysis of singular continuous diffraction pattern

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The 1D Thue-Morse sequence is the example of well-defined aperiodic (not periodic or quasiperiodic) structure. Its diffraction pattern consists of two parts - classical atomic Bragg component and a singular continuous part.

Statistical approach using Average Unit Cell (AUC) concept allows calculating the so-called envelope function. It gives the intensity values of Bragg peaks and their satellites. However, for each scattering vector k separate envelope function is needed.

The satellite peaks are splitted into three classes of peaks depending on the index labelling the scattering vector. For each class, thanks to the known probability distribution in the AUC, scaling factor of intensity of peaks can be find. These scaling factors are fractional and consistent with those obtained in mathematical considerations.

The same scaling properties are obtained for the decorated Thue-Morse sequence.

Degradation and surface protection of thermoelectric materials based on CoSb_3

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Cobalt triantimonide based materials are used as components of thermoelectric devices at temperature not exceeding 450 °C. Its application is limited due to the poor thermal and chemical stability, however this deficiency can be overcome by means of a suitable protective coating. Such coating should block the diffusion of antimony and oxygen. Two different coating systems were investigated: magnetron sputtered Cr-Si layers and enamel coatings. The quality of the protective layers was evaluated on the basis of oxidation tests in air up to 600 °C. The surfaces, fractures and cross-sections of specimens were analyzed to assess integrity and adherence of the deposited layer as well as the extent of reaction and diffusion phenomena at interfaces. The Cr-Si thin layers appeared oxygen-tight at 500 °C while the amorphous layers - even at 600 °C.



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Centre for Advanced Laser Techniques (CALT)

We will present Centre for Advanced Laser Techniques - CALT (<http://calt.ifs.hr>), which is a key infrastructural project of the Institute of Physics selected by the Ministry of Science, Education and Sport of Republic of Croatia to the indicative list of projects to be funded through the EU Structural Funds (ERDF) in the 2014-2020 period.

The main goal of the project is to **improve, upgrade and develop new research infrastructure based on advanced laser techniques** at the Institute of Physics.

CALT will be located at the Institute of Physics in Zagreb (IPZg), the only research institution in Croatia to have several larger laser/optical systems and relevant expertise, which are the basis for laser-matter interaction studies. The location at IPZg is in the focus of scientific developments in Croatia. CALT therefore bears strong synergic potential which could bring together researchers from various fields of science & technology.

CALT will be set as a collection of state-of-the-art laboratories that will be open to users, where both the infrastructure and the expertise will be at service to the RDI community. CALT's activities; which comprise research, education, and providing access to laser facilities; will address socially important issues through planned research activities regarding the environment (laser spectroscopy for detecting and tracking ozone formation/chemistry), food safety (plasma diagnostics/treatment), health (bio-imaging, laser and plasma treatment, magnetometry), energy (graphene-based devices, light sources), and security (optical sensors). In addition, specific professional training will be available which will give boost to Croatian science and innovation capacities in general.

