CMAC Days Abstract booklet.

Abstracts are arranged in alphabetical order of the presenting author.
Characterisation of the corrosion resistance of new Al-Cr-Fe Complex Metallic Alloys (CMA) in relation to surface properties

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Al-Cr-Fe Complex Metallic Alloys (CMA) are Al-based crystalline intermetallic phases that show high corrosion resistance with good electrochemical thermodynamic stability for pH’s ranging from 0 to 14[1]. Nevertheless, the influence of the passive oxide on the surface properties of Al-Cr-Fe CMA still needs to be deeply understood. These remarkable corrosion properties can be combined with the additional low friction coefficient and reflectivity and could be exploited in resistant “multifunctional” coatings.

Recently, single phase large grain single- or polycrystals of the orthorhombic Al₈₀Cr₁₅Fe₅ (unit cell dimensions a = 12.5006 Å, b = 12.6172 Å and c = 30.6518 Å and 306 atoms) were prepared. In this contribution, recent results on the behaviour of the Al-Cr-Fe CMA in acidic condition (pH 0-2) will be reported. Electrochemical characterisations in pH 0 (H₂SO₄) and pH 2 (HCl) on single crystalline materials allowed determining the intrinsic thermodynamic stability of the passive oxide[2]. The passive oxide layer has been studied by conventional XPS depth profile analysis and for the first time, by means of Hard X Ray Photoelectron Spectroscopy (HAXPES), a non-destructive synchrotron technique particularly suited for the study of buried interfaces. In order to probe different depths, two excitation energies, 3 keV and 6 keV and different electron escape angles (30°, 45°, 78°) were used, exploiting the highest resolution possible (up to 350 meV) Excitation energy of 6 keV was adequate to probe the oxide/metal interface and allowed us to propose a model for the oxide.

In addition to that, preliminary results on an in situ electrochemical experiment combined with surface x-ray diffraction characterisation study will be presented.


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Oral
Plasticity in complex crystals

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The study of plasticity in brittle materials is complicated by the need to suppress cracking. Conventionally this is done either by applying very high confining pressures or by using indentation. However, the former is experimentally difficult, while the latter does not allow different types of slip system to be studied. An alternative approach is to make the samples sufficiently small, reducing the energy available in the sample to drive cracking. It has been shown [1, 2] that, by compression of micron-sized specimens, brittle materials can be deformed plastically even at room temperature to yield information on how plasticity occurs over a range of temperatures [3] and strain-rates, while also allowing the deformed samples to be studied by techniques such as transmission electron microscopy or electron-backscattered diffraction. The plastic flow behaviour of a range of materials has been studied, including intermetallics of the Nb-Co system, one of which, NbCo₂, is completely brittle and the other, Nb₂Co₇ which shows plasticity on one slip system, as well as the complex metallic alloy, Al₁₃Co₄, at room temperature and other brittle materials such as semiconductors [4].


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INVITED
Describing complex intermetallics

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Complex compounds can be found in a large variety of intermetallic systems. They are usually categorised according to the number of atoms per unit cell, which amounts to hundreds or even thousands in some cases [1]. Highly symmetric lattices seem to be preferred by these compounds, so we started our systematization with the face-centered cubic (fcc) structures [2]. The largest group of complex fcc intermetallics consists of structures with approximately 400 atoms per unit cell and contains more than 40 structures. These compounds do not only crystallize mainly in the same space group, but can also be assigned to one common structural aristotype. Chemically, however, they are very diverse, with compositions of Li$_{81.0}$Sn$_{19.0}$, Zn$_{90.5}$Ir$_{9.5}$, Na$_{86.3}$Tl$_{13.7}$, Mg$_{86.3}$Rh$_{13.7}$ and Al$_{63.6}$Ta$_{36.4}$, among others.

On the other hand, chemically very similar compounds can assume quite different geometries: in the Al-Ta-Cu system, at least three complex structures can be found within a very narrow compositional range. Two of them belong to a series of fcc structures: Al$_{56.6}$Ta$_{39.5}$Cu$_{3.9}$ and Al$_{55.4}$Ta$_{39.1}$Cu$_{5.4}$ with approximately 6000 and 23 000 atoms per unit cell, respectively [1,3]. The third one is a new hexagonal compound Al$_{57.4}$Ta$_{39.0}$Cu$_{3.5}$, which was recently investigated and can in the following be compared to the already known phases in the system.

In order to better understand complex intermetallics, we describe their structures in different ways, for example in terms of the cluster approach, as superstructures or as layered compounds. When these compounds are interpreted as cluster packings, two recurring structural motifs are most prominent: multiple-shell fullerene-like clusters packed closely in different ways and blocks of smaller polyhedra (mainly Friauf polyhedra and similar clusters) filling the remaining gaps. Another general property of complex intermetallics is a complex diffraction pattern, which contains a small subset of strong reflections indicating that the structure can be regarded as a superstructure. The periodicity of the underlying basic structure corresponds also to the number of flat and puckered layers, which can be regarded as building the structure by simple stacking.

By comparing geometrically similar but chemically different structures, as well as geometrically diverse but chemically similar compounds, we hope to reveal the building principles responsible for the formation of highly complex intermetallic structures. In order to do this, we juxtapose the mentioned complementary methods of structure description.


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Oral
Co-deposition of Al and Cu by metalorganic chemical vapour deposition (MOCVD) is a relevant process for the direct formation of Al-Cu coatings of pin point targeted phases, and noticeably for the formation of the complex metallic alloy γ-Al₄Cu₉ [1]. Despite its simplicity, such process suffers from the occurrence of competitive phenomena occurring on the growing surface during co-deposition. This results for example in reduced growth rate and consequently it may hamper process characteristics and penalize the readiness level of the MOCVD-based technology. Alternatively, sequential deposition of Al and Cu, followed by post deposition annealing is less restrictive; it takes advantage of the high individual growth rates of the unary films and allows operation at different processing conditions for the deposition of each sublayer.

However, the introduction of an annealing step implies a need for a thorough investigation of the as-processed bilayers, of the phase transformation path, and of the final microstructure. For this purpose, we employ different characterization techniques, including glow-discharge optical emission spectroscopy (GD-OES) for elemental depth profiling, and high-temperature X-ray diffraction (HT-XRD) and high-temperature resistivity measurements for phase transitions determination. A brief recall is made about GD-OES, while an entire part of the presentation is dedicated to the presentation and use of a newly-patented high-temperature resistive meter for the monitoring of microstructure evolution and phase transitions in Al/Cu samples [2-3].

The obtained results show that MOCVD associated with post deposition heat treatment is a valid way to obtain films of intermetallic alloys, paving the way to conformal deposition of this type of materials for numerous application fields.


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Oral
Dynamical Peculiarities in Complex Metallic Alloys

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High structural complexity is one of the key features of CMAs. Its consequences are manifold and give rise to a variety of surprising physical properties in these phases. In this talk the influence that structural complexity may exert on the lattice dynamics of CMA systems will be presented.

This is exemplified for two different CMA phases, which evidence peculiarities in their dynamical behavior, clearly having their origin in the respective structural building blocks. While for the clathrate system Ba-Ge-Ni the dynamics of the Ba guest atoms and the Ge-Ni host framework is discussed, in ScZn₁₆ the dynamics of the innermost, tetrahedral shell in the constituting Tsai-type cluster will be addressed. For both systems experimental results from inelastic neutron scattering are analyzed and interpreted by means of ab-initio and molecular dynamics simulations.

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Oral
The various forms of Bi islands formed on the (100) surface of the Al13Co4 complex metallic alloy.

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The growth and stability of Bi thin films on the (100)-Al13Co4 surface has been investigated from submonolayer to high coverage regime by scanning tunnelling microscopy (STM/STS) and low-energy electron diffraction (LEED) for temperatures ranging from 30 K to 633 K. Initially, Bi adsorption leads to the formation of a pseudomorphic monolayer, which is followed by the formation of islands of different heights with increasing coverage. The inplane structure, islands height and morphology indicate that these islands have either pseudo-cubic (110) or (111) orientation normal to the surface. The (110) oriented islands correspond to bilayer stackings (either 2 or 4 ML in height) while the (111) oriented islands correspond to a trilayer stacking. The in-plane orientation of (110) islands with respect to the substrate is random while (111) islands adopt one of 4 possible orientations. In addition, the (111) islands show a moiré structure. The fact that Bi islands grow either with (110) or (111) structure simultaneously on the same substrate is rather unexpected and has never been reported before. It must be related to a subtle energy balance between both orientations, allowing both structures to co-exist. Other phenomena like island reshaping at room temperature, strong influence of the deposition temperature and flux on island density and their most frequent structure type have also been observed. Above 5 ML coverage, the hexagonal (111) morphology is stabilized and the film further grows in a layer-by-layer mode. Height specific features appear in STS spectra recorded on islands of various types, consistent with confined electronic states. Finally, the islands entirely desorb around 523 K while the pseudomorphic Bi monolayer seems to be stable up to 633 K.

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Poster
The Intermetallic Compound ZnPd: Chemical Bonding and Catalytic Properties in Methanol Steam Reforming

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The intermetallic compound ZnPd is reported to exist in two structural modifications. Single-phase samples of the intermetallic compound ZnPd (CuAu-type) were prepared with different bulk compositions. The existence of the hypothetic cubic CsCl-type high-temperature phase at the equiatomic composition could not be proven experimentally. Furthermore, quantum chemical calculations of the total energy reveal, that the cubic 1:1-phase is highly unfavourable. Analysis of the chemical bonding applying the electron localizability approach results in charge transfer from zinc to palladium and proves direct Pd–Pd interactions in the (001) plane to be the main reason for the tetragonal distortion of the cubic CsCl-type structural pattern for ZnPd [1].

In methanol steam reforming (MSR), the formation of ZnPd on an initial Pd/ZnO catalyst is made responsible for the drastic increase in CO₂ selectivity compared to Pd/MₓOᵧ (M = Al, Si, Zr). But the roles of ZnPd and ZnO are still under debate. MSR experiments on unsupported, intermetallic Zn₁₀₀₋ₓPdₓ (x = 46.8–59.1) samples (CuAu-type) proved that Pd-rich catalysts showed limited activity and very low selectivity to CO₂, while Zn-rich catalysts possessed good activity and CO₂ selectivity up to 99.4%. XP spectra of the near-surface region were recorded on as-prepared and reduced samples, showing significant variations in Pd:Zn surface ratios, Pd3d binding energies and the amount of oxidized Zn species on the surface. These properties were correlated to the Pd-content of the bulk. In-situ XPS studies revealed that only Zn-rich samples exhibited oxidized Zn species and intermetallic ZnPd on the surface. The catalytic properties correlate strongly with the electronic structure, i.e. the valence band which is determined by the bulk composition. All ZnPd samples still revealed a partially intermetallic near-surface region under MSR conditions. The use of well-characterized intermetallic compounds allows a rational development of highly selective catalysts in methanol steam reforming [2].

References:

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Oral
Low-temperature structures of $\varepsilon$-Al-Pd-Mn phases optimized by *ab initio* methods

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We have studied and resolved occupancy correlations in the existing average structure model of the complex metallic alloy $\xi'$-Al-Pd-Mn [1], which has approximately 320 atoms in the unit cell and many fractionally occupied sites. Model variants were constructed systematically in a *tiling-decoration* approach and subjected to simulated annealing by use of both density functional theory and molecular dynamics with empirical potentials. We reproduce the Al-Pd-Mn phase diagram at $T = 0$ K and derive an enthalpy of formation for each experimentally known stable structure. This yields a direct measure for thermodynamic stability for our structure models with respect to competing phases.

Our optimal structure resolves a cloud of fractionally occupied sites in pseudo-Mackay clusters. In particular, we demonstrate the presence of rotational degrees of freedom of an Al$_9$ inner shell, which is caged within two icosahedrally symmetric outer shells Al$_{30}$ and Pd$_{12}$. Outside these clusters, the chemical ordering on a chain of three nearby sites surprisingly breaks the inversion symmetry of the surrounding structure, and couples to a nearby Al/vacancy site.

The tiling representation allows to extend structure models for the $\xi'$-phase to structure models of other $\varepsilon$-phases. Our refined tiling-decoration model applies to any structure within the $\varepsilon$-phases family, including the metastable decagonal quasicrystalline phase, and will serve as a starting point for an accurate microscopic modeling of the *metadislocations* [2].


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**Poster**
Reconstruction on the $\text{Al}_2\text{Cu} (001)$ surface mediated by covalent bonding

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Surface reconstructions are generally observed on covalently bonded materials, but are not frequent on metal surfaces. Recently, quantum calculations on the $\text{Al}_2\text{Cu}$ metallic alloy identified covalent-like Al-Al bonds [1]. In this study, we show that these covalent bondings are at the origin of a surface reconstruction for $\text{Al}_2\text{Cu}(001)$.

The bulk structure of the $\text{Al}_2\text{Cu}$ intermetallic compound is described as interpenetrating graphite-like aluminium $6^3$ nets with copper atoms positioned in the channels between the nets [2]. Along the [001] direction, the bulk structure consists in a stacking of pure Al and pure Cu planes.

Experimentally, it is observed that only one of these two possible terminations occurs at the (001) surface. The combination of both experimental methods (STM, STS, LEED, UPS, XPS) and ab initio computational methods (atomic relaxations, STM simulations, electronic structure calculations) gives many arguments to match the surface plane with a bulk truncated surface model terminated by incomplete Al planes, with Al missing rows oriented along two directions rotated by 90 degrees from each other. Ab initio calculations highlight the influence of the covalent-like interaction on the surface reconstruction. The energetic cost associated with the removal of pairs of Al atoms is found to be the lowest for the two nearest surface Al atoms, the remaining atomic rows being oriented according to the graphite-like Al $6^3$ nets used to describe the $\text{Al}_2\text{Cu}$ bulk structure [2]. We also discuss the contributions of configurational and vibrational energies on the stability of this reconstructed surface.

Fig.1: STM images. Left: Experimental image (L=17.0 Å, M= 12.8 Å). Right: Simulated image (the structural model used leads to L rows).


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Single crystal growth in the Ga-Pd system: First results and problems to be solved

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Some not really complex binary phases in the Ga-Pd system, namely Ga\textsubscript{7}Pd\textsubscript{3} (Pearson symbol: cI\textsubscript{4}0), GaPd (cP\textsubscript{8}), and GaPd\textsubscript{2} (oP\textsubscript{12}) have recently been explored as highly selective heterogeneous hydrogenation catalysts in the semi-hydrogenation of acetylene [1]. Compared to pure Pd or alloyed catalysts, intermetallic compounds with well defined crystalline structures and fixed sites of the catalytically active element have a considerably higher long-term stability. This has been explained according to the active-site isolation concept [2].

Although the technical application of catalysts made from intermetallic phases will be based on ultra-fine powders or even nanoparticles, single crystals of these compounds are needed to study their intrinsic properties, e.g. their anisotropic surface structures, and basic processes of catalysis. That is, why we try to grow cm-size single crystals of these Ga-Pd phases each of them requiring very specific conditions for crystallization that can be derived from the binary phase diagram [3].

GaPd can be grown either from a congruent melt or from Ga- or Pd-rich high-temperature solutions. The same options principally exist for growing GaPd\textsubscript{2}, but quite high liquidus temperatures and accordingly a high Ga vapour pressure suggest to prefer crystallization from a Ga-rich melt. Contrary, Ga\textsubscript{7}Pd\textsubscript{3} is only stable at temperatures lower than 460°C and crystal growth is limited to a crystallization from a Ga-rich solution at relatively low temperatures making materials transport and the preparation of inclusion-free single crystals the main problem.

We have grown first examples of single crystalline samples of Ga\textsubscript{7}Pd\textsubscript{3}, GaPd and GaPd\textsubscript{2} by the Czochralski method from off-stoichiometric melts. The obtained GaPd single crystals show a fairly high structural perfection [4] and offer a wide scientific playground based on the complexity of enantiomorphism and the polarity of specific faces. GaPd\textsubscript{2} is characterized by a broad stability region with retrograde solubility of the excess component. Thus, precipitation may occur during post-growth cooling depending on the growth temperature. With Ga\textsubscript{7}Pd\textsubscript{3} the inclusion of liquid solution droplets during growth is the most severe problem that can even destroy the already grown crystal because of density changes occurring during the low-temperature peritectic reaction.


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Poster
Crystal growth of the type-I clathrate $\text{Ba}_8\text{Ni}_{3.5}\text{Ge}_{42.1}\square_{0.4}$ by Czochralski pulling method.

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The substance $\text{Ba}_8\text{Ni}_{x}\text{Ge}_{46-x}$ has been selected to explore the guest-host interactions and bonding feature in the crystal structure of cage compounds. Those have attractive attention because of their intriguing properties, i.e. high thermoelectric efficiency, which is very promising for future applications. To be able to relate the physical properties to the structural aspects, single crystals of sufficient size (suitable for neutron scattering) are necessary. A crucible-free Czochralski pulling method was used for the growth of $\text{Ba}_8\text{Ni}_{3.5}\text{Ge}_{42.1}\square_{0.4}$ [1].


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Poster
Single crystal growth of InPd by the Czochralski method
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The structurally simple intermetallic compound InPd (CsCl type of structure) could be a promising catalytic material for methanol steam reforming. For some studies of the physical and chemical properties well defined and crystallographically oriented single crystalline samples are essential.

Crystal growth of InPd was done with the Czochralski technique from In-rich solutions. Earlier this method has been applied successfully for the preparation of GaPd crystals from Ga-rich solutions [1]. Due to the retrograde solubility of the stability region of the InPd intermetallic compound crystallized in an off-stoichiometric way, precipitations of In$_3$Pd$_2$ can occur during cooling down. To avoid second phase inclusions during growth the pulling speed has to be limited. Furthermore the relatively high vapor pressure of Indium is an important feature only just tolerated by the existing Czochralski system.

We will present the first results of the grown InPd single crystals and will discuss the quality of the crystallized material. Because of a lack of native seeds the very first crystal had to be obtained by new experimental configurations that will be shown as well.


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Oral
Covalent bonding induced by chemical decoration of close-packed structures in intermetallic compounds

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The Hume-Rothery (HR) idea has been applied for quasicrystals(QCs) and related compounds since the very beginning and widely accepted. On the other hand, there have been several arguments that covalent bonding plays more important role in QC-related systems. Covalent nature in the electronic states of intermetallic compounds is of great interest because it leads to novel properties, which are very different from simple pure metals. Recently we have discussed formation mechanism of a deep pseudogap in the electronic density of states of the Al-Li Bergman and Zintl compounds with an emphasis on the differences among isostructural Al-Mg compounds [1]. Since Li scatters electrons very weakly in comparison with Al and Mg, the potential landscape for electrons in Al-Li compounds is not that of the entire close-packed structure but that of the Al sublattice, which is a rather porous network like a diamond lattice. The porous network structure enhances the covalent nature of electronic structures, hence the deep pseudogap in the electronic density of states in the Al-Li compounds. This concept of chemically-decorated close-packed network provides a novel picture, which is alternative to the HR one, in the electronic structures in complex intermetallic compounds.

A family of intermetallic compounds with tetrahedrally close-packed structures is known as Frank-Kasper alloys [2]. Among the Frank-Kasper alloys, the chemical decoration of closed-packed structures modifies the electronic structure significantly in several systems. In this talk, we show some further examples and try to discuss roles of covalent bonding on physical properties and stability of the chemically-decorated close-packed networks.


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INVITED
Structural impact of Pt on a γ-brass related composite structure in the Zn-Pd system: a guided view by (3+1)-dimensional space description

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The γ-brass Hume-Rothery [1] phases which adopt at vec values near about 21/13 presently attract most attention due to their structural complexity and challenge for the understanding of the underlying stabilization mechanism. Morton, by electron microscopy studies, revealed that the γ-brass regions of Cu-Zn [2], Ni-Zn [3] and Pd-Zn [4] do not only accommodate the γ-brass phase but also a bundle of structurally related, complex phases with lower symmetry than that of the γ-phase.

A bundle of γ-brass related phases in the Zn-rich region of the Pd-Zn phase diagram is investigated using single crystal X-ray diffraction. In the course of a preliminary investigation of the Pd-Zn system, a γ-brass related composite structure (a = 1292.9(3) pm, b = 911.2(4) pm, c = 33.32(1) pm, Cmc21, oC276), Pd\textsubscript{24.3}Zn\textsubscript{75.7} has been refined from single crystal X-ray diffraction data in the conventional 3D space group using supercells [5]. It can be refined with the (3+1) dimensional space description as well by considering as commensurate modulated structure [6].

In order to gain an insight into expressions, cause and mechanism and structure-property relationship for such phases, we studied the impact of substitution of zero-valent palladium and bi-valent zinc by zero-valent platinum on the evolution of the structure of ternary derivatives of Pd\textsubscript{24.3}Zn\textsubscript{75.7} by the use of (3+1) formalism.

This presentation will discuss about the understanding of the complexity of the atomic arrangement through the various modulation which correlates with the variation of composition of the ternary phases.


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Oral
Cell geometry, short range order and phase stability of ternary Laves phases \( A(B'_1,B''_x)\_2 \) by first-principles calculations

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Laves phases [1] crystallize with an ideal composition \( AB_2 \) in one of the three polytypes C14 (hexagonal), C15 (cubic) or C36 (hexagonal). The high abundance and the small number of atoms per unit cell make these compounds suitable candidates to study phase formation and structural details by first-principles calculations (VASP) [2,3]. This contribution will compare theoretical with experimental results for a number of ternary Laves phases of type \( A(B'_1,B''_x)\_2 \) with extended homogeneity ranges. Here, the \( B' \) and \( B'' \) atoms substitute each others on the crystallographic sites, 2\( a \) and 6\( h \), influencing the thermodynamic stability, the cell geometry and the type of short range order in these compounds.

For example, computations of the enthalpies of formation and Gibbs free energies for \( \text{Nb}(\text{Cr}_{1-x}\text{Co}_x)\_2 \) and \( \text{Ta}(\text{V}_{1-x}\text{Fe}_x)\_2 \) Laves phases along the sections \( \text{NbCr}_2–\text{NbCo}_2 \) and \( \text{TaV}_2–\text{TaFe}_2 \), respectively, predict the homogeneity ranges for the C14 and C15 phases in good agreement with the experimental results. Furthermore, the phenomenon preferential site occupation as well as lattice geometries will be discussed.


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Oral
Acetylene hydrogenation on surface of AlPd (B20) compound: *ab-initio* DFT study

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The acetylene hydrogenation on the pseudo-fivefold surface of AlPd (B20) has been studied using *ab initio* density-functional-theory (DFT) method. Our *ab initio* study has been motivated by recent experimental works on catalytic properties of isostructural GaPd compound, e.g. [1]. We have found a detailed atomistic scenario for the hydrogenation process catalyzed by the pseudo-five-fold AlPd surface. Binding energies for adsorption and coadsorption of H\(_2\) and C\(_2\)H\(_x\), x=2-5, molecules at various sites on the surface were calculated. The hydrogenation is a complex multi-step process. We have searched for and explored an optimal reaction pathway of the hydrogenation by the Langmuir-Hinshelwood mechanism. The energetic barriers of the reaction steps were calculated by the nudged-elastic-band method. We have identified two different kinds of the reaction centers. Our results demonstrate that the active sites are not the Pd atoms alone, but triangular PdAl\(_2\) or rectangular Pd\(_2\)Al\(_2\) clusters. The energetic barrier of any reaction step of the optimal reaction pathway does not exceed 70 kJ/mol. This value is lower than the height of the energetic barrier at the acetylene to ethylene hydrogenation over the Pd catalyst where for the rate determining step the barrier heights between 78 kJ/mol and 85 kJ/mol were reported. The desorption energy of ethylene of is by more than 10 kJ/mol lower than the barrier to further hydrogenation to ethyl. This confirms that AlPd (and GaPd) can be an efficient as well as selective hydrogenation catalyst.


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Oral
Complex Metallic Alloy Phases in the Al-Mg-Zn System


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The elements Al, Mg and Zn are major components for a large number of light and high strength alloys, such as the Al-based alloys of the 7xxx series. In addition, the Al-Mg-Zn system has attracted much interest because four complex metallic alloy phases, called $\tau_1$, $\tau_2$, $\Phi$ and $q$, formed as ternary intermetallic compounds. The experimental phase diagram data of the Al-Mg-Zn system was assessed by Liang et al. [1,2], by Petrov et al. [3] and by Raghavan [4]. The assessment of Petrov includes the four intermetallic compounds while those of Liang and Raghavan disregard the $\tau_2$ and $q$ phases due to insufficient experimental data. The aim of the work was to redetermine the homogeneity ranges of the $q$, $\tau_2$ and the $\Phi$ phases and to determine the crystal structure of the $\Phi$ phase. Samples were prepared by furnace-controlled melting and annealing in Ta ampoules or by centrifugation from the self-flux and characterized by XRD, SEM, EDXS, WDXS and DSC.

While reinvestigating the Al-Mg-Zn phase equilibria in the vicinity of the subsystem Mg-Zn, a number of new ternary phases were discovered. Single phase material could be obtained for the known $\Phi$ and $\tau_2$ phases and for four new intermetallic compounds. The crystal structures for the $\Phi$ phase and three of the new intermetallic compounds were solved and the crystal structure of the $\tau_2$ phase was reinvestigated. While $\tau_2$ ($Pa-3$, $a = 23.065(1)$ Å) is an approximant of the icosahedral quasicrystalline phase $q$, the $\Phi$ phase ($Pbcm$, $a = 8.9374(2)$ Å, $b = 16.812(3)$ Å, $c = 19.586(4)$ Å) and one of the new phases ($Imm2$, $a = 5.2546(2)$ Å, $b = 40.240(2)$ Å, $c = 25.669(1)$ Å) turned out to be decagonal approximants.

The low temperature phase of the latter is a Laves block type structure with $P6_3$ (173), $a = 22.5943(7)$ Å, $c = 59.578(2)$ Å. Surprisingly, we have also found one phase ($Fd-3m$, $a = 27.5987(9)$ Å) isotypic to Samson’s phase $\beta$-$Al_3Mg_2$ at Zn rich composition.


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Poster
The structure of Al-Cu-Me (Me = Co, Rh, Ir) quasicrystals

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We present a real space structure refinement of three decagonal phases: Al-Cu-Co, Al-Cu-Rh, Al-Cu-Ir. The structure factor, which was used for the modelling process, was calculated using a statistical method [1], which allows a purely 3-dimensional, real space optimization of a quasicrystalline structure. Such an approach has already been successfully used for structure refinement of various modifications of the Al-Ni-Co quasicrystal [2,3,4]. This is the very first attempt of quantitative structure optimization of Al-Cu-Ir and Al-Cu-Rh quasicrystals based on high resolution, synchrotron diffraction datasets. Up to now the only structure investigation of an Al-Cu-Rh quasicrystal was based on electron microscopy, the structure of the Al-Cu-Ir quasicrystal has not been studied before and the Al-Cu-Co structure was refined only based on a rather limited, in-house diffraction dataset. The current refinement gives much more details about the structure.

All three decagonal phases show ~4 Å periodicity (two atomic layers per period). Their space group is centrosymmetric P10₅/mmc. While the Al-Cu-Co phase shows a significant amount of diffuse scattering in the interlayers of the diffraction pattern, the Al-Cu-Ir and Al-Cu-Rh phases exhibit no diffuse scattering. This fact is well-reflected in the structure of Al-Cu-Ir and Al-Cu-Rh phases, i.e. they are well-ordered, the Cu/Ir and Cu/Rh positions can clearly be distinguished and the only disorder present is the partial occupation of several Al positions. All decagonal quasicrystals are ternary alloys based on Al and two transition metals. This is the very first structure refinement of a decagonal phase distinguishing the positions of two different transition metal atoms. The initial model for all phases was the same and based on the rhombic Penrose tiling. The initial decoration of the rhombuses was derived based on a structure solution obtained from charge flipping. The refined structure gives reasonable R values, and the chemical composition agrees well with the EDX measurements.


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Poster
Surfaces of AlCu alloys: structure and reactivity with oxygen

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Complex metallic alloys (CMAs) are defined as intermetallic compounds characterized by large unit cells - unit cell of infinite dimensions in the case of quasicrystals - and the occurrence of well-defined atomic clusters. In order to explore the influence of the structural complexity on the surface reactivity, we studied theoretically several AlCu phases, from simple ordered models to the more complex Al$_3$Cu$_4$ and Al$_4$Cu$_9$ compounds. This work was carried in the framework of the density functional theory, which is at the moment the most adapted ab initio method to deal with the structural and electronic properties of these systems.

We first investigated, in a slab geometry, in plane copper segregation at the (111) Al surface for various Cu compositions in an Al layer and at various positions close to the surface. Calculated segregation energies show that there is a tendency to segregation, not at the surface, but close to it, in the sub- and sub-sub-surface planes. Similar results are observed for the first stage of formation of (100) GP zones, modelled by doping Al (100) planes with Cu clusters. However this segregation does not happen at the (100) surface: a full copper (100) monolayer is much stable deep in the bulk. Our results fit clearly into a picture of energetics and geometrical properties dominated by preferential tendency to Cu-clustering close to the (111) Al surface [1].

The zeta$_1$- and zeta$_2$- Al$_3$Cu$_4$ phases are approximants of the i-AlCuFe quasicrystal. From the only available experimental study (X-ray diffraction [2]) it is known that the large primitive cells are characterized by some of their sublattices having a random fractional occupation of their atomic sites. We constructed substitutional periodic models of these partially disordered phases using the Special Quasirandom Structure method. Based on these SQS structures, our DFT calculations have shown that the zeta$_2$ phase is 50 meV/at. more stable than the zeta$_1$ phase.

We studied also the first oxidation stages of model AlCu alloys at low Cu concentration. In the presence of copper, there is a reduction of the oxygen adsorption energy which results mainly from the competition between the electronic transfers towards the copper and the oxygen atoms of the aluminum surface electrons.

In the case of the g-Al$_6$Cu$_9$ complex metallic alloy, we find that the adsorption properties are again strongly modified by the presence of copper in the surface and subsurface regions. The adsorption energy decreases when the shortest O-Cu distance is reduced.


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Oral
Formation of pseudomorphic Pb thin films on Al$_{13}$TM$_4$ (=Co, Fe) approximant surfaces

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We have investigated the adsorption of Pb atoms on the orthorhombic Al$_{13}$Co$_4$ (100) and the monoclinic Al$_{13}$Fe$_4$ (010) surfaces for various substrate temperatures. Both complex metallic alloys are approximant to the decagonal quasicrystals. For the Al-Co system, Pb adatoms remain highly mobile at 300K and adsorb preferentially within the hollow site situated in between adjacent Al pentagonal clusters present at the surface. These experimental findings are supported by ab initio calculations based on density-functional theory (DFT). For two temperature regimes (300K and 573K), Pb adsorption leads to the formation of pseudomorphic monolayers above which the high adsorbate mobility prohibits the growth of additional layers. For the high temperature deposition, we propose a structural model for the Pb film and discuss its relationship with the underneath substrate. For the Al-Fe system, we have characterised Pb adsorption at 300K from submonolayer to multilayer regime. While the initial stages of adsorption differs to the Al-Co system, the deposition leads to the formation of a pseudomorphic monolayer. The resulting atomic structure of the Pb film will be discussed in relation to the arrangement of the substrate bipentagonal motifs.


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Poster
Monoclinic $\text{Al}_{13}\text{Fe}_4$ is a complex metallic alloy that has a unit cell containing 102 atoms. The structure can be described as the stacking along the $[010]$ direction of two types of layers, flat (F) having 17 Al and 8 Fe atoms, and puckered (P), having 22 Al and 4 Fe atoms per unit cell. There are two types of each plane, producing a stacking sequence $\text{F}_1\text{P}_1\text{F}_2\text{P}_2$.

We present a quantitative LEED study of the surface structure of the $\text{Al}_{13}\text{Fe}_4$ CMA using LEED data that were measured at room temperature. The procedure for structure determinations using LEED involves the assumption of a model structure, computation of the intensity spectra for that model structure, and comparison of the calculated spectra to the experimental spectra using a reliability factor ($R$-factor). These calculations were performed using the SATLEED suite of programs [1].


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Poster
Chemical Bonding in Ba and Ge based Type-I Clathrates

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In the crystal structure of type-I inorganic clathrates $A_8E_{46}$, the $6c$ site of the space group $Pm-3n$ (no. 223) is the preferred site for most of the substituting atoms, $X$, especially at low substitution levels of less than 6 $X$ atoms per formula unit. Much of the interest has focused on clathrates with $A = Ba$, $E = Si$ or Ge and $X$ a late transition metal from groups 9-12, mainly due to their potential use in thermoelectric applications. For example, recently a thermoelectric figure of merit of 0.9 at 680 K was reported for an SPS-treated Ba$_8$Au$_{5.3}$Ge$_{40.7}$ specimen [1]. Our present theoretical study investigates how the nature of chemical bonding changes as we choose different $X$ in the hypothetical Ba$_8X_6$Ge$_{40}$ clathrates where all six $X$ atoms are assumed to occupy the $6c$ positions. The elements considered are $X = Li, Mg, Ga, Ge$ and transition metals of groups 9-12. The analysis is based on the electron localizability indicator – electron density approach, and the aim is to elucidate the role of $X$-Ge and $X$-Ba interactions in the physical properties.


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Oral
Structure solution of decagonal ZnMgDy quasicrystal

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Here we report the first structure solution in the ZnMgRE family of decagonal quasicrystals (d-ZnMgDy) based on single crystal X-ray diffraction data. Samples with the composition (Zn$_{57.6}$Mg$_{40.8}$Dy$_{1.6}$) were prepared by induction melting followed by annealing at 375°C for 10 months and quenching to room temperature. The resulting samples consist mainly of a hexagonal phase with the d-ZnMgDy existing as the secondary phase. The morphology of the decagonal phase is needle-like with grains of 50 µm in length and approximately 15 µm in diameter. X-ray diffraction experiments were carried out both in-house (Oxford Xcalibur PX diffractometer, CCD detector, Mo Kα radiation) and at the Synchrotron facility in Swiss-Norwegian Beam Line, ESRF, Grenoble (λ=0.6980 Å).

The Laue group is specified as 10/mmm and no systematic extinctions were observed. The direct space quasilattice parameters are $a_1 = 4.626(8)$ Å and $a_5 = 5.214(5)$ Å. SUPERFLIP program package [1] (based on charge flipping and low density elimination algorithms) was used for structure solution. Reconstructed electron density shows structural motifs similar to previous HRTEM studies [2]. Rhombic parts inside the decagonal clusters, reported earlier [2], exist in several orientations, causing the appearance of split positions in the structure. Based on the reflection conditions and the electron density, the most probable space group is $P10/mmm$.

Composition as measured by SEM/EDX is 59.8(4) at% Zn, 38.5(4) at% Mg and 1.7(2) at% Dy.


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Oral
Low hysteresis losses in a first-order magnetic transformation

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Magneto-calorics are materials that heat up, or cool down, when exposed to an external magnetic field. This is called the magnetocaloric effect. This effect can be used in magnetic refrigeration which is more efficient than conventional gas compression technology.

Gd$_5$Si$_2$Ge$_2$ is known for its giant magneto-caloric effect near room temperature, because of a simultaneous magneto-structural transformation that is occurring when exposed to an external magnetic field. [1] But this is accompanied by large hysteresis losses. With small additions of iron into Gd$_5$Si$_2$Ge$_2$ its $T_C$ increase to room temperature and lowers the hysteresis losses when substituting for Ge, because of the suppression of the structural transformation. [2] We focused on the reduction of the hysteresis losses almost to zero without a large reduction in the magnetocaloric effect, e.g. keeping the first order magnetic transition. We found out that with the right thermal conditions one can achieve a unique microstructure, which has a pronounced effect on the magnetic properties of the sample. With our treatment we could obtain a very dynamic microstructure, with lots of precipitates and small grain sizes. This affected the properties in such a way that the hysteresis losses were reduced to a minimum while keeping the high magnetic entropy change, e.g. magnetocaloric effect, while cycling though a magnetic field. The Arrott plot of the magnetic measurements showed that the transition is still of a first order. This suggested that the structural transformation that is occurring usually at already lower fields is shifted to higher fields and is not effecting our measurements at low fields. It is possible that the unique microstructure hinders the easy structural transformation, making this a hysteresis free magnetocaloric material at lower magnetic fields. This increases the refrigerant capacity of the material. It is possible that this can be applied also in other magnetocaloric systems.


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Oral
Structure of the orthorhombic $\text{Al}_{13}\text{Co}_4(100)$ surface using LEED

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Orthorhombic $\text{Al}_{13}\text{Co}_4$ is a complex metallic alloy that is an approximant of the decagonal Al-Co-Ni quasicrystal, and its (100) surface is an approximant of the 10-fold quasicrystal surface. $\text{Al}_{13}\text{Co}_4$ has a unit cell containing just 102 atoms, and it contains the same basic pentagonal bipyramidal structure elements as the decagonal quasicrystal. The structure can be described as the stacking along the [100] direction of two types of layers, flat (F) having 17 Al and 8 Co atoms, and puckered (P), having 22 Al and 4 Co atoms per unit cell. There are two types of each plane, producing a stacking sequence $F_1P_1F_2P_2$ and a separation between planes of about 2 Å.

The results of a Low-energy electron diffraction (LEED) study [1] of the surface of $\text{Al}_{13}\text{Co}_4(100)$ show that after annealing to 1165 K, the surface structure is consistent with a dense Al-rich plane with surface Co atom depletion. Various structure models were considered, and the best agreement was found with a model that consists of Al-rich terminating planes with no Co atoms, and otherwise a structure similar to the bulk puckered layers.

The LEED measurements were carried out for a sample temperature of 80 K, and the final dataset consists of 69 symmetry-nonequivalent beams, with a total energy range of 19 640 eV. The acquisition of such a large data set was possible due to the high density of diffraction beams (from the large unit cell), the relatively low symmetry of the structure, and by acquiring the data at low temperature to minimize thermal scattering.

The procedure for structure determinations using LEED involves the assumption of a model structure, computation of the intensity spectra for that model structure, and comparison of the calculated spectra to the experimental spectra using a reliability factor (R-factor). These calculations were performed using the SATLEED suite of programs [2].


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INVITED
Effective potentials for phonon dynamics in clathrates

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Intermetallic clathrates are currently actively investigated due to their special thermoelectric properties. They are composed of periodically arranged cages, formed by host atoms, which enclose single guest atoms. The low thermal conductivity of these structures has been attributed to the interaction of the phonons with local vibration modes (“rattling”) of these guest atoms inside the host framework.

For computational studies of dynamic properties long simulation times and large samples are required. This makes first principle calculations of these structures, even with very fast computers, very unfeasible. Classical molecular dynamics, however, can easily handle large systems and long simulation times. The potentials needed for these MD simulations can be obtained from ab-initio calculations with the force-matching method. It uses large numbers of reference data to fit an effective potential that can reproduce the forces, energies and stresses of the ab-initio calculation.

To model the strongly directional atomic interactions in clathrates, angular dependent potentials are required. An analytic potential will be presented to model these systems. The phonon dynamics of clathrates was studied with these potentials and will be compared with ab initio results.

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Oral
First steps of oxygen adsorption on different Al-TM metallic alloys

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While the high resistance of quasicrystals to oxidation has been well documented over the years [1], information on the reactivity of complex metallic alloys remains scarce. It is then reasonable to postulate that several CMA systems, approximant phases to parent quasicrystal for instance, should also exhibit a high oxidation resistance.

Here, we report the adsorption of oxygen diatomic molecules on the surfaces of several Al-TM based intermetallic compounds. These systematic experiments aim at underlining if the surface structural complexity may affect the oxygen-surface reactivity. Consequently, we have investigated the initial steps of oxidation on the Al₂Cu(100), Al₁₃Fe₄(010), Al₉Co₂(001) and Al₁₃Co₄(100) surfaces. The O₂ adsorption has been characterized experimentally using STM, LEED and XPS for different sample temperatures.

The adsorption of O₂ leads to a disordered surface layer with the disappearance of the LEED patterns. However, particular adsorption sites have been identified on two systems at low coverage. When adsorbed on the Al₁₃Fe₄ (010) surface, oxygen nucleates initially in between the bi-pentagonal motifs present on the surface. From our proposed surface model and STM observations, we believe that the adsorption site for oxygen is on-top of the glue atoms. For the Al₉Co₂ (001) system, we observe two different adsorption sites B3 and T1 (labelled on Fig.1) which give different contrasts in the STM images: dark and bright spots respectively. Ab initio calculations of the different possible adsorption sites for atomic oxygen agree with the B3 adsorption site obtained in our STM results.

Fig. 1: Oxygen adsorption on Al₉Co₂ (001) surface: (a) STM image (7.3 x 9.6 nm²) of 0.5L of oxygen and (b) schematic representation of the possible adsorption sites that have been calculated.


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Oral
Thin film growth on icosahedral Ag-In-Yb quasicrystal

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We will present thin film growth of various elements and molecules on surfaces of a recently available icosahedral Ag-In-Yb quasicrystal [1-3] studied by various surface science techniques, including scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). STM reveals that Pb grows pseudomorphically up to second layer. Higher coverage yields fivefold-twinned hexagonal Pb islands with (111) surface orientation. The islands are of specific heights (magic heights), which correspond to the stacking of four-six atomic layers of the bulk Pb, possibly due to the confinement of electrons in the islands. Sb and Bi yield quasicrystalline monolayer but show different growth behaviour than Pb at higher coverage. The structure of the quasicrystalline films can be described in terms of substrate structure and is in good agreement with first-principles calculations. The growth of molecules, e.g., C₆₀ and pentacene on the same surface will be also discussed.


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Oral
Anisotropy of transport properties in the single d-Al-Co-Ni quasicrystals

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We have continued to study the anisotropy of transport properties of some complex metallic alloys based on aluminum [1-3], by investigating the anisotropy and temperature dependence of transport coefficients on single crystals of d-Al70Co10Ni20 quasicrystals. So far, our results for the anisotropic transport properties of the approximants to decagonal quasicrystals (d-QC) are correlated with data from literature for d-QC obtained from polycrystalline ingots of questionable quality, and underparameterized structure. For these systems only approximate dependence of the anisotropy directions and the length of periodicity were known. During the past few years phase diagrams of aluminum based alloys have been more fully investigated. On the basis of these investigations, appropriate parameters of preparation have produced a good quality d-QC single crystals suitable for investigating the structure by neutron diffraction as well as accurate transport measurements. Our results for the first Al70Co10Ni20 quasicrystals are given in which the measurement of electrical resistance, thermopower, thermal conductivity and Hall effect have been obtained using the same single crystals [4].


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Oral
Magnetic and transport properties of $\delta$-Zn$_{10}$Fe

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We have studied magnetic susceptibility, electrical resistivity, thermoelectric power, thermal conductivity, specific heat and Hall coefficient of a phase ($\delta$) that exists in Zn-rich part of Zn-Fe system. This phase crystallizes in hexagonal space group $P\bar{6}_3$mmc with unit cell parameters $a=12.787(3)$ Å, $c=57.222(7)$ Å and 556 atoms in unit cell [1]. The sample was a single crystal and magnetic susceptibility measurements reveal that it is a paramagnet without any hysteresis in magnetization curve. The electrical resistivity amount to about 190 $\mu$Ωcm at the room temperature. It is a metallic like with relatively large residual resistivity at low temperatures and positive temperature coefficient, but tends to saturate at room temperature. Low-temperature specific heat in $C/T$ versus $T^2$ plot shows an increase in $C/T$ below 8 K, that is frequently observed in heavy fermion systems. The thermoelectric power is small (<4 $\mu$V/K) and negative with complicated temperature behaviour (local minimum around 70 K and maximum around 150 K). The thermal conductivity is anomalously low (<10 W/mK) for an alloy of metallic elements. Hall coefficient is positive and increases significantly with temperature at lower temperatures, while exhibiting a tendency to saturate at temperatures above the room temperature. Such temperature behavior could be attributed to the anisotropy of electron scattering times [2].


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Poster
Application of the Average Unit Cell concept to the 3D aperiodic Ammann-Kramer Tiling

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Ammann-Kramer tiling is a 3D generalization of the Penrose tiling. It consists of two kinds of structure units: prolate and oblate rhombohedra with all edge lengths equal. All faces of the structure units are identical rhombuses. The ratio of the face diagonals is equal to τ, and the acute angle amounts to arctan(2) = 63.44°. The volume ratio of the unit tiles as well as the ratio of their frequencies in the tiling also equals τ. Ammann-Kramer tiling reveals an icosahedral symmetry, thus it can be used as a quasilattice for building a model of an icosahedral quasicrystal.

One can generate the set of points of the Amman-Kramer tiling by projecting a 6D hypercubic lattice via 3D window—the so called atomic surface. In case of the tiling the atomic surface has the shape of a rhombic triacontahedron.

We present a derivation of the structure factor of the Amman-Kramer tiling on the basis of the average unit cell concept [1], which allows a structure factor calculation in physical space only. This method has been successfully used to perform a structure refinement of the decagonal basic Ni-rich Al-Ni-Co phase [2,3].

Any point of the tiling can be written in the so called reference lattice: \( r_i = n_i \lambda_i + u_i \), \( \lambda_i = 2\pi/k_i \), where: \( i=x,y,z \), \( n_i \) is an integer, \( \lambda_i \) is a reference lattice constant for a given direction and \( u_i \) is a position in the reference lattice. The reference lattice constant is related to a scattering vector \( k_i \) which is observed in the diffraction pattern. The position distribution of Amman-Kramer tiling points \( P(u_x,u_y,u_z) \) is called an average unit cell. Because of the aperiodicity of the tiling the distribution \( P(u_x,u_y,u_z) \) should be related to another one \( P(v_x,v_y,v_z) \), whose lattice constants are elongated by τ. A 6D distribution \( P(u_x,u_y,u_z,v_x,v_y,v_z) \) is only nonzero along lines: \( v_i = -\tau^2 u_i \). This is a characteristic feature of quasicrystalline lattices. One can show that there is a linear relation between the shape of the distribution and the shape of the atomic surface. A structure factor for any scattering vector can be calculated as a Fourier transform of this distribution. It is important to see that because of the characteristic relation between \( v_i \) and \( u_i \), the Fourier transform actually reduces to a 3D integral.

The comparison between structure factors obtained with three methods (numerical calculations, in the perpendicular space and with average unit cell concept) will be presented to show the perfect agreement.


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Poster
Thermoelectric properties of melt spun Ba$_8$Ga$_{16-x}$Ge$_{30+x}$ clathrates and promising oxides

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Ba$_8$Ga$_{16}$Ge$_{30}$ is the clathrate with the highest thermoelectric figure of merit known to date. We will present p- and n-type materials of Ba$_8$Ga$_{16-x}$Ge$_{30+x}$ (-0.1 < x < 0.1) prepared by the time and cost-effective melt spinning technique [1]. Temperature dependent measurements of the electrical resistivity, Hall effect, Seebeck coefficient, and thermal conductivity will be presented and discussed in terms of a two-band model.

The second part of the talk will introduce promising thermoelectric oxides with focus on Ca$_3$Co$_4$O$_9$ [2]. The high Seebeck coefficient in Ca$_3$Co$_4$O$_9$ is due to the spin entropy term, confirmed by magnetotransport measurements using a modified fitting based on the molecular field model, and due to strong electronic correlations in this material, confirmed by a high Sommerfeld coefficient.


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Invited
Icosahedral shape of viruses capsid: a mathematical investigation

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Viruses display symmetry for reasons of genetic economy \cite{1}: By packaging their genomic material into protein containers arranged with icosahedral symmetry, they maximize container volume while minimizing the portion of the genomic sequence needed to code for this container. From a mathematical point of view, this implies that techniques from group theory can be used to predict virus architecture. We show here that via an affine extension of the icosahedral group a library of point arrays can be generated that can be used to predict the material boundaries in viruses \cite{2,3,4}. In particular, this theory is able to account also for the genome organization in simple RNA viruses, and reveals geometric constraints on the capsid proteins that could not be predicted previously \cite{5}. By construction, these point arrays correspond to vertex sets of quasi-lattices such as those occurring in the study of quasicrystals, and we show that extra information on virus architecture can be obtained from these associated tilings \cite{6}. We also discuss how these structural results imply new insights into the infection process \cite{7}.

\begin{thebibliography}{9}
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\textbf{Invited}
Effect of intergranular interaction and lattice rotation on predicted residual stress and texture for polycrystalline metals

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Rotation of grain crystal lattice is the basic mechanism of texture formation and of anisotropic behavior of metals during plastic deformation, e.g. residual stress. Two definitions of crystal lattice rotation are taken into account [1]:

**Classical definition**

Lattice rotation, $\delta \omega_{ij}^{\text{CL}}$, has to compensate the plastic rotation (rigid body rotation):

$$
\delta \omega_{ij}^{\text{CL}} = - \delta \omega_{ij}^{\text{P}} = - \frac{1}{2} (m_i n_j - m_j n_i) \delta \gamma
$$

where $m$ and $n$ are slip direction and slip plane, respectively.

**Preservation Condition definition**

If the orientations of specified sample directions/planes are assumed to be constant in the sample reference frame, then corresponding shear components ($kl$) of the displacement gradient have to be compensated: $\delta e_{kl} = 0$. This involves:

$$
\delta \omega_{kl}^{\text{PR}} = - \delta e_{kl} = - m_k n_l \delta \gamma
$$

In the case of deformation by rolling this requirement leads to:

$$
\begin{align*}
\delta \omega_{21}^{\text{PR}} &= - \delta e_{21} = - m_2 n_1 \delta \gamma \\
\delta \omega_{31}^{\text{PR}} &= - \delta e_{31} = - m_3 n_1 \delta \gamma \\
\delta \omega_{32}^{\text{PR}} &= - \delta e_{32} = - m_3 n_2 \delta \gamma
\end{align*}
$$

The classical definition of crystal lattice rotation leads in general to different texture and residual stress predictions than the definition based on the orientation preservation of selected sample planes and/or directions. Also the intensity of grain-matrix interaction plays an important role in the prediction of the above quantities. These problems were studied using elasto-plastic deformation model of polycrystalline materials. Examples of austenite and ferrite steels were considered, i.e., metals with low and high stacking fault energy.


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Poster
Scaling of the structure of quasicrystals

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Quasicrystals are aperiodic structures and there are no unit cells for them in physical space. Recently it was shown that structure of quasicrystals can be successfully described in physical space by statistical approach. The normal unit cell is replaced by an Average Unit Cell (AUC) [1,2], where atoms occupy the positions with some probabilities. Knowing the probability distribution one can calculate the structure factor and use it for the structure refining procedure [2-4]. It is shown that the structure refinement of quasicrystals can be done in physical space only.

For all crystalline structures (including quasicrystals) one can define an appropriate scaling factor. After scaling of all the distances by such factor the self-similar structure is obtained. The same holds in reciprocal space. When scattering vector of any diffraction peak is multiplied by the scaling factor, another diffraction peak is reached. For ordinary crystals the scaling factors are the integer numbers, which leads to the periodic lattice. For modulated structures the scaling factors can be either rational or irrational numbers leading to the commensurate or incommensurate structures. For the model quasicrystals, like the Fibonacci chain, Penrose tiling or 3D Amman-Kramer tiling, the scaling factor is equal to the golden mean value $\tau \approx 1.618$. The irrational value of the scaling factor results in an aperiodic structure. One can approximate this value by rational numbers which leads to some approximants.

In the AUC approach the scaling properties of quasicrystals give a particular probability distribution of atomic positions. The distribution is no-zero only along a line and such linear relation for perfect quasicrystals essentially simplify the complicated calculations of the corresponding structure factor. For some rational approximation of $\tau$ the non-zero distribution becomes broader which effects the intensity of the diffraction peak at the inflated position of scattering vector. The width of the distribution at AUC approach can be used as an order parameter for the description of the critical behaviour of diffraction pattern for different approximants when the scaling factor approaches the golden mean value.


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Oral
Low plateau pressure Laves phase type hydrogen storage alloy

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It is known that hydrogen storage in metal hydrides is one of the attractive and softer modes for storing gaseous hydrogen. The Laves phase stabilized either as C14 or C15 type usually shows higher hydrogen storage capacity, rapid kinetics and relatively longer electrochemical charge-discharge cycle life than the well known AB₅ type storage materials. In addition to their technological potential, such materials raise questions of fundamental interest concerning the effect of hydrogen absorption on their structural, electrical, and magnetic properties.

In this work, we describe and discuss the synthesis, structural-microstructural and hydrogen storage behavior of three AB₂ type storage materials namely (a) ZrFe₂, (b) Zr(Fe₀.₇₅V₀.₂₅)₂ and (c) Zr(Fe₀.₅V₀.₅)₂ and Ti₀.₈₅ₓV₀.₉₅Fe₀.₁₅Zr₀.₀₅ (x = 0.02, 0.03, 0.04, 0.05 and 0.06) C14 and C15 Laves phase materials. These alloys were synthesized by radio frequency induction melting in argon atmosphere. X-ray diffraction and transmission electron microscope have been employed for structural and microstructural characterization. The Surface morphology and elemental composition of these alloys were investigated by scanning electron microscope and energy dispersive X-ray analysis. The pressure composition isotherms of these alloys were investigated at room temperature to 200 °C and pressure ranges of 0-100 respectively, using a fully computerized PCI apparatus. The yet another interesting feature observed in our present study is that the plateau pressure remains well below 1 atmosphere for all the composition.


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Oral
Epitaxial growth of pentacene on quasi-periodic substrates

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We present the surface characterisation of the adsorption of pentacene and the resulting thin film structure at quasi-periodic surfaces. Pentacene is a poly-cyclic, aromatic hydrocarbon which tends to adsorb intact, in a planar geometry on metallic surfaces [1]. STM and LEED are utilised to study local and long range order at the intricate surfaces.

At the clean, fivefold surface of the i-AgInYb quasicrystal [2] all the pentacene molecules align along high symmetry directions of the substrate. It forms many cluster features with pentagonal symmetry (see figure a)) leading to the propagation of five-fold order up to monolayer coverage. This contrasts growth at the i-AlPdMn surface where there are no local, repeating cluster features (see figure b)) resulting in a disordered layer.

The complexity of the substrate is reduced by the formation of a one-dimensionally aperiodic Cu multilayer at the i-AlPdMn surface [3][4]. This surface offers rows for the linear molecules to align along; acting as an effective barrier to the rotation of the molecules. A periodic film is imaged from sub-monolayer (see figure c)) up to multi-layer coverage. The inter-molecular interaction is evidenced to dominate over the influence of the aperiodic rows.

The presentation will provide detailed descriptions of the adsorption and growth. The results will be compared to similar systems involving quasicrystalline and periodic surfaces.


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