

**Workshop of the European Network of Excellence
Complex Metallic Alloys**

Frontiers in Complex Metallic Alloys

CMA-Zagreb '08

Institute of Physics, Zagreb, Croatia
October 1-4, 2008.

Program and Abstracts

cma2008@ifs.hr
<http://cma2008.ifs.hr>

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Frontiers in Complex Metallic Alloys

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Editor:

Ana Smontara

Laboratory for the Study of Transport Problems

Institute of Physics, Zagreb, Croatia

Reaching the Institute

Institute is easily reachable from the bus station near the main town square – Ban Jelačić square. See the map on the cover page. Busses depart every 10-20 minutes.

Computer and Internet Service

Two desktop computers will be available in the multimedia room near to the lecture hall. The room will also be equipped with a number of Ethernet cables for the connection directly to laptops.

Conference Proceedings

The workshop proceedings will be published in a regular issue of the international journal *Croatica Chemica Acta*.

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Dear Colleagues,

Welcome to the Institute of Physics and Workshop "Frontiers in Complex Metallic Alloys" - CMA-Zagreb'08, organized by the European Network of Excellence *Complex Metallic Alloys* (CMA) and supported by the Croatian Academy of Sciences and Arts.

The main scope of the workshop is to provide comprehensive information on the most recent results in the field of complex metallic alloys giving plenty of time for discussions on various aspects of the field. Due to the interdisciplinary of the field, the invited and contributing speakers include physicists, chemists and material scientists, members as well as non-members of the CMA network.

Contributions cover the areas of CMA studies including, but not limited to, preparation and synthesis, electron transport and DOS, lattice dynamics, thermal transport, thermoelectricity, and surface physics in ultrahigh vacuum of cluster-based complex metallic alloys and related materials.

We wish you a stimulating workshop and a pleasant stay in Croatia.

Workshop chairs and Local Organizing Committee.

Professor Leontić Anniversary

The workshop will take the opportunity of celebrating Prof Leontić, one of the most prominent scientists of Croatia.

Boran Leontić was born August 3 1928 in Split (Croatia), where he finished the Primary School and five grades of the Secondary School (Gymnasium). Continued his education in London (G.B.) where he graduated from the Secondary School and the first year of Physics and Chemistry at the University of London. He graduated (B.Sc.) in physics at the Faculty of Natural Sciences (FNS) and Mathematics of the University of Zagreb in 1951. He obtained a PhD degree in Physics at the University of Manchester (GB) in 1954. From 1954 to 1957 he was an assistant professor at the Department of Physics at FNS (Zagreb). From 1957 to 1963 he worked at CERN in Geneva (CH) and from 1963 to 1968 at Brookhaven Natl. Lab. (BNL) in Upton (USA). Since 1968 he is professor at FNS, University of Zagreb where he acted as head of the Experimental Physics Division until 1978. During the same period he was Director of the Institute of Physics of the University (IFS) where he also led the Section of the Physics of Metals II.



Together with his collaborators he developed the method of continuous rapid solidification (R.Q.) and discovered localised spin fluctuations in the samples obtained by R.Q. Together with E. Babić he shares the Ruđer Bošković Prize (1974). Since 1986 he has done research on high-temperature superconductors and transport properties of amorphous and disordered systems.

In 1998 the University of Zagreb nominated him Professor Emeritus of Physics. He was awarded the Order of "Danica hrvatska" with the image of Ruđer Bošković. In 2000 he received the State Prize for lifetime work.

Timetable and Program

Wednesday, October 1 – Arrival

17:00 -19:00

REGISTRATION

19:00 -

Welcome Party

Thursday October 2 – morning

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I - An invited lecture
C - A contributed lecture

Thursday October 2 – afternoon
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- | | | |
|-------|---|----|
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| 15:30 | D. Babić (I) , M. Baćani, M. Novak , I. Kokanović
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17:00-17:20

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chair J.-M. Dubois

- | | | |
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Abstracts of Lectures

Open Theoretical Problems in the Physics of Aperiodic Materials

Anuradha Jagannathan

Laboratoire de Physique des Solides, Bât.510, Université Paris-Sud, 91400, Orsay, France

Quasicrystals have been around for more than twenty years, and a lot of conceptual and technological advances have occurred during this time. It is however clear that many challenges remain, firstly, as regards improvement of experimental measurements, where the role of extrinsic factors such as instrumental resolution, or of contaminants often remains unclear. Secondly, many challenges remain in the development of theoretical models describing these materials. Two main lines of approach have been followed: on the one hand ab-initio calculations based on ansätze for the real structures, which are necessarily heavily numerical, due to the complexity of the models, and on the other hand, simplified models based on quasiperiodic tilings, which can be regarded reference templates for building real structures.

In this survey of quasicrystal physics, I will review some selected interesting physical properties and go on to focus on some of their novel electronic and magnetic properties that pose a challenge for theorists in this field. One would like, for example, to define a relatively simple model containing the basic elements that characterize the quasicrystal, and arrive at robust predictions that do not depend on fine tuning the parameters of the model. Conventional methods, for example based on the existence of Bloch states, that work reasonably well in predicting the electronic structure in periodic solids will clearly no longer apply, and new theoretical approaches are necessary for aperiodic solids.

I will outline some theoretical approaches, both numerical and analytical, to electronic, magnetic and vibrational properties of aperiodic solids. Whereas the DC electrical conductivity, an averaged quantity, is generally anomalously small in quasicrystals, local responses can be anomalously large or small depending on the location of the probe, and will show singular properties due to aperiodicity. Similarly, the magnetic response will have complex nonanalytical variations in real space. I will show how “perpendicular space” provides a compact and elegant way to characterize such spatial properties of such solids. Since disorder can be expected to be inherent in these materials – whether temperature induced or quenched-in – I will discuss the effects of various kinds of disorder. Examples will be shown to illustrate how the behavior in quasicrystals contradicts expectations based on the conventional wisdom.

Keywords: quasicrystals, transport, electronic and magnetic properties

Synthesis and crystal growth of complex metallic alloys

Peter Gille

Ludwig-Maximilians-Universität München, Department of Earth and Environmental Sciences, Crystallography Section, Theresienstr. 41, D-80333 München, Germany.

Single crystal growth of complex metallic alloys in Al-based systems means solidification from Al-rich solutions that is driven by the special needs of solution growth as well as possible features of giant unit cell materials that consist of large clusters. These two reasons limit crystal growth to extremely low solidification rates.

The Czochralski method may be regarded as the most versatile technique to meet the conditions necessary for growing a series of different complex metallic alloys. Single crystal growth has been achieved in various binary and ternary metallic systems yielding large single crystals of e.g. $\text{Al}_{13}\text{Co}_4$, Al_9Co_2 , $\text{Al}_{13}\text{Fe}_4$, $\text{Al}_{13}\text{Ru}_4$, $\text{Al}_4(\text{Cr,Fe})$, $\text{Al}_4(\text{Cr,Ni})$, $\text{Al}_{13}(\text{Co,Ni})_4$, $\text{Al}_{13}(\text{Fe,Cr})_4$, $\text{Al}_{13}(\text{Fe,Ni})_4$ and decagonal quasicrystals of the AlCoNi and AlCoCu phases making basic research on surface properties, on catalysis, and on bulk electronic and thermal properties possible.

A detailed description of all decisive steps of the Czochralski growth procedure will be given with particular emphasis to seeding from a native phase as well as spontaneous nucleation if no seed crystal from a preceding experiment is available.

Single-Crystal Growth of Complex Metallic Alloys in Aluminium-Based Systems

Michael Feuerbacher

IFF-IMF, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

Complex metallic alloys (CMAs) represent a novel field in materials science. Due to their salient structural features, e.g. large lattice parameters and icosahedral local coordination, these materials potentially possess novel physical properties and hence are also of interest for technological application.

Currently, the investigation of the physical properties of CMAs attracts high scientific attention. However, in order to reach an understanding of the intrinsic physical properties of a given CMA phase, i.e. the properties of the ideal material, undisturbed by grain boundaries, foreign phases, etc., sample materials of high structural quality are required. For CMAs, this is not always straightforward the phases often solidify incongruently, their primary solidification area in the phase diagrams is frequently small, and inconvenient elements may be involved. Therefore, advanced growth methods have to be applied.

In the present communication we report on the development of single-crystal growth routes for various CMA phases in Al-based alloy systems employing Czochralski-, Bridgman,- and self-flux growth techniques. The spectrum of phases produced covers different types of global structure, local order and elemental constituents and represents a solid materials basis for the experimental exploration of the physical properties of this class of materials. We will show various examples, with an emphasis on Taylor phases in the systems Al-Mn-(Pd, Fe) and hexagonal phases in the system Al-Mn-(Ni) and Al-Cr.

Keywords: complex metallic alloys, single-crystal growth, Al-based alloys

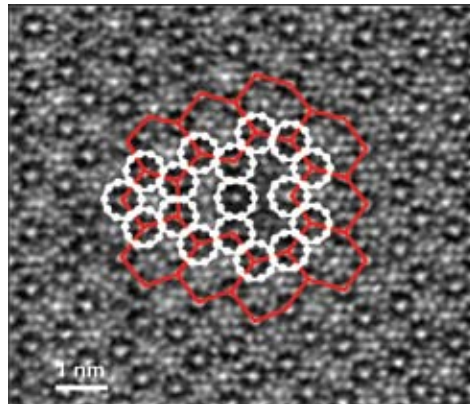


Figure 1. HAADF –STEM micrograph of a metadislocation in ξ' -Al-Pd-Mn with a superposed tiling representation and cluster distribution.

1. K. Urban and M. Feuerbacher, *J. Non Cryst. Sol.* **334 – 335** (2004), p.143.
2. H. Klein, M. Feuerbacher, P. Schall and K. Urban, *Phys. Rev. Lett.* **82** (1999), p. 3468.

**Chemical Vapor Deposition of Metallic Coatings:
From Single Elements to Complex Metallic Alloys**

Constantin Vahlas

Institut Carnot CIRIMAT, Toulouse, France

Processing of metallic thin films by chemical vapor deposition (CVD) has been rapidly developed during the past few years, mainly due to numerous potential applications in the microelectronics industry but also for the purposes of protection, reflectance, conductivity and/or decoration. Due to its high throughput and to the conformal coverage of the processed films, CVD of metals favorably competes with physical vapor deposition techniques in particular application fields. The talk will be based on a comprehensive introduction of the steps involved in the metalorganic CVD (MOCVD). Their influence on the physicochemical characteristics of the films and ultimately on their properties of use will be exemplified through selected processes of single element metallic films (aluminium, copper, iron, nickel, platinum or ruthenium). MOCVD of binary or ternary alloys is actually in its infancy. The state of the art in this field will be presented and this will allow pointing on the challenges to be met in order to achieve robust MOCVD processes for the deposition of Complex Metallic Alloy coatings.

Melt Spinning and Melt Centrifugation as Preparation Methods for Ag-Mg and Mg-Pd Complex Metallic Alloys

G. Kreiner¹, C. Kudla¹, J.P.A. Magongo¹, M. Mihalkovic²

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The objective of this contribution is to discuss two frequently encountered problems in phase diagram studies. The first problem is the sluggish formation of phases at low temperatures via a solid state reaction. Often, these phases have been overlooked in older studies. In principle, melt spinning offers an additional and advantageous route in alloy preparation, especially when it comes to the synthesis of the low temperature phases. An example is the Ag-Mg system. The phase diagram was reinvestigated using X-ray powder and single crystal diffraction, thermal analysis, optical and electron microscopy. In addition to the previously reported phases ϵ -Ag₇Mg₂₆, ϵ' -Ag₁₇Mg₅₄ and γ -AgMg₄, two low temperature phases, κ -Ag₂Mg₅ and γ' -Ag₉Mg₃₇ have been prepared by annealing melt spun samples. γ' is a CMA phase and crystallizes in P6₃ with $a = 12.490(1)$ Å and $c = 14.448(1)$ Å. A model of the crystal structure could be obtained by using an adaptive Metropolis Monte Carlo algorithm based on Ag-Ag, Ag-Mg and Mg-Mg pair interactions.

The second problem is the cascade-like formation of a large number of phases by peritectic reactions if the window to the melt is small. Here, melt centrifugation is a valuable tool for crystal growth. An example is ζ -Mg₆₄Pd₁₇, a CMA with 1944 atoms per orthorhombic face-centred unit cell with $a = 28.053(2)$ Å, $b = 27.986(3)$ Å and $c = 48.573(2)$ Å. The melt centrifugation technique has been used to grow specimens of optimal size for single crystal structure analysis and for TEM investigations. In the latter case thin slices have been obtained from hexagonal bar-shaped specimens of 30 µm diameter by focused ion beam (FIB) milling. TEM studies reveal a high density of planar defects by 60° nano twin domains. In combination with X-ray structure analysis it was possible to propose a model for the defect-free crystal structure.

Complex Interfacial Layer between Periodic and Quasicrystalline Materials

T. Duguet^{1,2}, S. Kenzari^{1,2}, E. Gaudry^{1,2}, V. Demange^{2,3}, T. Deniozou^{1,2,4}, J. Ledieu^{1,2}, T. Belmonte^{2,3}, J.M. Dubois^{1,2} and V. Fournée^{1,2}.

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The problem of adherence of quasicrystalline materials is seldom reported in the literature although it represents one of the major issues in developing functional coatings. As a result, it is frequently observed that quasicrystalline coatings delaminate spontaneously from the substrates. The present work is an attempt to solve this issue by introducing an interfacial layer and by forming a complexity gradient between the two aperiodic and periodic half-crystals. We use two model surfaces to study such an interface: the fivefold surface of the icosahedral (*i*-)Al-Pd-Mn quasicrystal and the Cu(111) surface. We demonstrate the possibility of growing the same γ -Al₄Cu₉ as a surface alloy by adsorbing and annealing Cu/*i*-Al-Pd-Mn and Al/Cu(111), respectively. This compound shares similar electronic and structural features with quasicrystals and can be considered as an approximant phase. Clear orientation relationships with both substrates are demonstrated by LEED and STM, according to $[110]_{\gamma} // A5_{ico}$ and $[110]_{\gamma} // [111]_{Cu}$. Using this knowledge, we go one step further toward the 'real world' and form polycrystalline γ -Al₄Cu₉ on both steel and the fivefold surface of the *i*-Al-Pd-Mn sample by magnetron sputtering. Transmission electron microscopy is performed on a cross section of the latter and these investigations demonstrate the orientation relationships between the approximant and the quasicrystal. We postulate that structural similarities together with the locking of common dense axis favour the adherence.

**Physics and NanoEngineering of CMAs:
From Disordered Alloys to HeteroEpitaxy of Functional Multilayers**

Davor Pavuna

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I will briefly summarize some of the physics and materials insights that I gained by studying rapidly quenched alloys (1975-1990): ferromagnetic or superconducting ribbons, microcrystalline broad metallic sheets and striking quasicrystals. The challenges of preparation, metastability, characterization of these materials and tailoring of their properties by chemically varying the alloy composition turned out to be very useful later when I addressed the challenges of the band-gap engineering in III-V optoelectronics and eventually the basic physics and nano-engineering of high-Tc cuprates and related materials. I will illustrate how seemingly unrelated concepts guide the basic science and controlled functionality of multilayer heteroepitaxy of correlated electron systems. Specifically, I will overview our systematic work on *Direct* ARPES (=DARPES) on *in-situ* grown, non-cleaved, ultra-thin (<25nm) cuprate films and how do we tailor the properties of advanced heteroepitaxies by controlling the growth parameters, interfaces, doping, strains, (local) energy dispersion and electronic structure and properties [1]. Recent results on the determination of Fermi surface topology obtained from the observed wavevector quantization in ultrathin cuprate films (< 18 units cells) [2] will also be discussed.

Keywords : Rapidly Quenched Metals, Physical Properties, Films, Superconductivity, Ferromagnetism, Nanoengineering, Heteroepitaxy, ARPES, Transport.

1. D. Pavuna et al. :

http://www.iop.org/EJ/article/1742-6596/108/1/012040/jpconf8_108_012040.pdf

2. D. Ariosa et al. Appl. Phys. Lett. **92**, 092506 (2008)

New aspects of variable-range-hopping conductivity in doped polyaniline

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Temperature (T) dependence of the electrical conductivity σ of own-made polyaniline pellets, highly doped either by HCl or by dodecyl benzene sulphonic acid, is measured and discussed. For the both dopants, the variable-range-hopping exponent equal to $2/5$ is found below $T^* \sim 200\text{-}250$ K. This result can be understood on the basis of a recent theory by Fogler, Teber and Shklovskii, which takes into account Coulomb correlations in a three-dimensional network of chain-like conductors and predicts a power-law density of states for charge excitations around the Fermi energy. At $T > T^*$, $\sigma(T)$ increases faster than at lower T , implying a tendency towards nearest-neighbour hopping by a reduction of the average hop length.

Keywords: doped polyaniline, electrical conductivity, hopping transport, Coulomb interaction

Phase transition in diluted, disordered magnetic alloys

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The number of amorphous magnetic alloys from amorphous series $\text{Fe}_x\text{Ni}_{80-x}\text{B}_{18}\text{Si}_2$ with compositions around the one of ferromagnetic threshold ($x \approx 2.5$) were investigated by measuring the ac susceptibility.

First, it is shown how to extract nonlinear components of susceptibility from measured higher harmonics and then their dependence on driving ac field is given.

The three types of the measurement of initial and differential ac susceptibility were used to investigate the phase transition from ordered to the disordered phase. The parameters of the FM – PM transition (T_C , critical exponents γ , β and δ) were independently obtained. The dependence of critical parameters on the concentration of magnetic component (Fe) is given and correlation with some theoretical models is discussed.

Correlation Between Electronic Structure, Mechanical Properties and Stability of TE-TL Metallic GlassesRamir Ristić¹, Emil Babić², Mirko Stubičar², Ahmed Kuršumović³¹Department of Physics, Osijek, Croatia²Department of Physics, Faculty of Sciences, Zagreb, Croatia³Department of Materials Science, Cambridge University, United Kingdom

We show that mechanical properties (stiffness and hardness) of TE - Ni,Cu (TE = Ti, Zr and Hf) amorphous alloys increase approximately linearly with Ni, Cu content, x , over a wide composition range ($x \leq 66$ at%). This correlates with the observed increase of the Debye temperatures with x and shows that the strength of interatomic bonding increases with x in these alloys. The thermal stability (e.g. the crystallization and glass transition temperatures) of these alloys also increases with x , thus with increasing interatomic bonding. Since in all these alloys the electronic density of states at the Fermi level, $N(E_f)$, decreases linearly with x within the same x -range, a very simple relationship exists between the electronic structure and mechanical and thermal properties. We also estimate the mechanical properties of hypothetical amorphous TEs (by extrapolating the properties of alloys to $x = 0$) and compare them with those of stable crystalline phases of TEs.

Keywords: metallic glasses, mechanical properties, hardness

The texture of the zinc alloys obtained by “the mill for the ultra-rapid quenching”

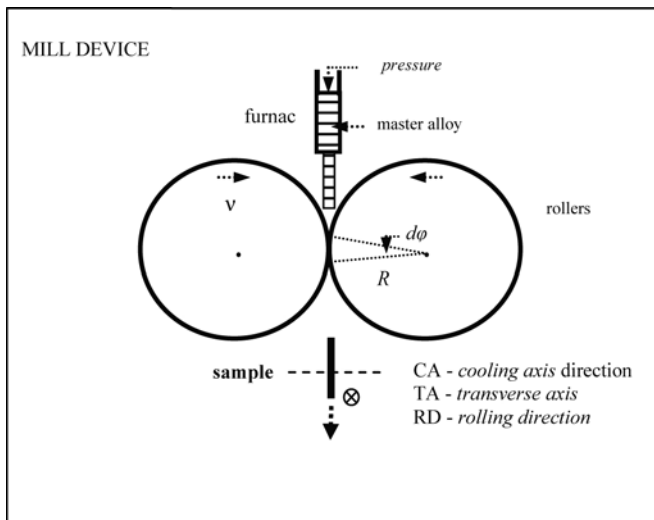
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We report on the investigation of the texture of the Zn(Fe, Co, Ni) alloys obtained by “the mill for the ultra-rapid quenching”⁽¹⁾. It is noticed a certain difference of the texture and of the grain size in the samples depending on the different kind and different concentrations of the impurities dissolved in the zinc matrix. The discussion and tentative explanation of these effects lead us to still one important conclusion: the cooling process of the samples during the contact to the metallic rollers determines the texture of the samples, but not the rolling, which is inherent to the method of quenching used.

Keywords: texture, ultra-rapid quenching, Zn alloys

1. Diploma work, Zagreb, 1971.



Stability of icosahedral quasicrystals

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Stable icosahedral quasicrystals (*i*-Qc) have been discovered in a number of alloys. Stability of the *i*-Qc has been interpreted in terms of Hume-Rothery rules *i.e.*, atomic size factor and valency electron concentration, e/a . The *i*-Qcs are electron compounds having strict value of e/a , which have been verified in most of alloy systems. Stable *i*-Qcs are classified into three groups according to their structures of icosahedral clusters and they basically obey the criterion of e/a but slight difference in constrain of atomic size factor.

Electron mobility in Quasicrystals, approximants and complex metallic alloys

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Transport properties related to electron mobility in quasicrystals, quasicrystalline approximants and complex metallic alloys exhibit a rich variety of phenomena. Electrical resistivity can vary between regular metallic with a positive temperature coefficient (PTC) to semiconductor- or insulator-like with a negative temperature coefficient (NTC). For some compounds, a temperature-independent resistivity is observed. Thermoelectric power can be positive, negative or it changes sign with temperature. For compounds exhibiting a narrow pseudogap in the strongly reduced electronic density of states (DOS) at the Fermi energy, the high resistivity (several 1000 micro-ohm-cm) with a NTC and the thermopower that changes sign occur naturally from the temperature-dependent changes of the chemical potential and the associated shift of the Fermi-Dirac distribution with respect to the position of the pseudogap minimum on the energy scale. However, NTC resistivity can also occur in compounds where the DOS value at the Fermi energy is metallic-high and does not exhibit any pseudogap. In such cases, the resistivity is low, of the order 100 micro-ohm-cm, but exhibits a pronounced NTC and sometimes also a maximum in the resistivity. The reason is slow velocity of charge carriers due to dispersionless electronic bands in the frequency–wave vector relation. For single-crystalline samples, the resistivity, thermopower, Hall coefficient and thermal conductivity exhibit anisotropy along different crystalline directions. This anisotropy emerges naturally from the anisotropy of the electronic band structure, as a consequence of the anisotropy of the atomic structure. The anisotropic Hall coefficient can be positive hole-like for some crystalline directions and negative electron-like for other directions on the same crystal. The above phenomena will be discussed for the single-crystalline samples of icosahedral *i*-Al-Cu-Fe, *i*-Al-Pd-Mn and *i*-Al-Pd-Re quasicrystals, decagonal *d*-Al-Ni-Co quasicrystal and decagonal approximant phases $Al_4(Cr,Fe)$, Y-Al-Ni-Co and $Al_{13}Co_4$.

Pseudo-gaps and electronic densities of states

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Investigation of the atomic structure of complex stable crystalline intermetallic alloys has pointed out that atoms are arranged in complex packing and clusters with often partial occupancy of all atomic sites. How is the electronic structure of such a complex intermetallic compounds? We present and discuss here the results of an investigation of the electronic structure of the valence band of such systems, carried out using the X-ray emission spectroscopy technique. This allows one to gain insight separately on the energy distributions of occupied states averaged around the various chemical species in the specimen. Basically Al or Mg based compounds are studied here. It is shown that the electronic structure is also quite complex in these compounds. Emphasis is put on the presence of a pseudogap at the Fermi level in the electronic distribution of Al or Mg states as well as electronic interactions in the vicinity of the Fermi level.

Keywords: electronic structure, pseudo-gap

Magnetic Resonance Studies of Hydrogen Mobility in Metallic Alloys

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In last decades, several metallic alloys which also form quasicrystalline or CMA phases, have shown promising potential for the hydrogen storage applications. Here we review several magnetic resonance-based methods that we've used in last few years to inspect the mobility of hydrogen in different metallic alloys.

Specifically, we used the following magnetic resonance experiments:

- Direct measurement of hydrogen diffusion using nuclear magnetic resonance in large magnetic field gradients of the fringe field of superconducting magnet
- Proton spin-lattice relaxation time dispersion measurements using fast field-cycling relaxometer
- Measurements of deuteron linewidths and relaxation time in deuterated metallic alloys.

In the studies, we have used several samples of Ti-Zr-Ni and Zr-Cu-Ni-Al alloys, both in icosahedral quasicrystalline (QC) form and in complex metallic (CMA) and bulk metallic glass (BMG) forms. The combined approach allows for a comprehensive study the influence of alloy structure and hydrogen loading percentage on the hydrogen mobility in these alloys.

Keywords: quasicrystals, CMA, crystalline, magnetic resonance, diffusion, hydrogen storage

Lattice dynamics of complex metallic alloys.Marc de Boissieu¹ and Marek Mihalkovic²

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We will review some of the recent results obtained in the study of the lattice dynamics of complex metallic alloys. After a brief introduction on lattice dynamics we will show that a joint experimental and theoretical study of the lattice dynamics can now be carried out. Indeed on one hand detailed understanding of the atomic structure of CMA is now emerging, even for quasicrystals [1], and on the other hand tractable Hamiltonian have been developed. This will be illustrated on the Zn-Mg-Sc alloy where this procedure was applied to the quasicrystal and its 1/1 approximant [2]. Some recent results on the dynamics of skutterudites will also be presented. We will finally outline some of the challenging and open questions in this field.

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Computer modeling of lattice dynamics in complex metallic alloys

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Complex metallic alloys challenge computer modeling of lattice dynamics as the system sizes are often prohibitive for direct ab-initio harmonic-approximation method based on direct construction of dynamical matrix from forces responding to individual atom displacements. Secondly, the complexity inherently tends to produce certain frustrated local atomic motifs where harmonic approximation becomes problematic. Finally, apart from the typically just few meV wide standard acoustic regime of propagating phonons, the character of the vibrational modes beyond the propagating phonon acoustic regime depends on the particular structure. The talk illustrates the situation on the examples of few complex intermetallic alloys from Al--Mg--Zn, Sc--Zn, Al--Co and other systems, discusses diagnostic techniques available for characterizing vibrational modes, and points out outstanding exceptional cases with peculiarities

Vibrational Properties of ZnMg Phases – Probing Zn_2Mg and $Zn_{11}Mg_2$

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We present and compare results on the vibrational properties of two complex ZnMg phases, the relatively simple Frank-Kasper type hexagonal Zn_2Mg Laves phase, and the cubic $Zn_{11}Mg_2$ phase.

For both structures we performed measurements and simulations of the dynamical structure factor and the vibrational density of states. The experimental studies were carried out using inelastic neutron scattering. In the simulations, ab-initio forces were calculated and then the dynamical matrix was obtained within the harmonic approximation. A comparison of the density of states of the two phases shows an excess of low energy modes in $Zn_{11}Mg_2$. These unusual low energy modes, which were seen in the measurement, could also be reproduced in our simulations.

Keywords: density of states, dynamical structure factor

Theoretical Aspects of Thermal Transport

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The "complex metallic alloy" notion embraces different classes of materials including giant-unit-cell intermetallics, quasicrystalline phase approximants and quasiperiodic crystals. All of them exhibit complex structures that contain some hundred up to several thousand atoms in their basic structural units. A basic feature of CMAs is the presence of two competing physical length scales: one defined by the structural unit parameters and the other determined by the long-range order of these units through the space, which can be either periodic (translation symmetry) or quasiperiodic (inflation symmetry). Accordingly, one expects the emergence of a peculiar lattice dynamics stemming from the competition between transport mechanisms acting on different scales in these systems. In addition, the emergence of some transport anomalies is also related to chemical bonding effects, giving rise to some fine features in the electronic structure close to the Fermi level due to electronic states hybridization (short-range). The relative importance of short-range versus long-range order effects on the transport properties will generally depend on the type of elementary excitation being considered (i.e., charge carriers or phonons). This dynamical asymmetry may then have a significant impact on the range of validity of the Wiedemann-Franz law in these compounds. In this lecture we will discuss these issues within the framework of a unified phenomenological approach.

Heat Conduction in Complex Metallic Alloys

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Complex metallic alloys (CMA) are pure thermal conductors, with thermal conductivity comparable to those of amorphous materials. Two heat-carrying channels contribute to the thermal conductivity of the CMA: free electrons and lattice vibrations. According to Wiedemann-Franz law, at room temperature electron contribution can reach 50% of the total thermal conductivity. Lattice thermal conductivity is obtained by subtracting the electron contribution from the total thermal conductivity. Unit cells of complex metallic alloys contain many atoms, giving a complicated vibrational density of states. Nevertheless, for energy less than ~ 5 meV (i.e., $T \lesssim 50$ K) it is well described by Debye model, which is used for calculation of the lattice thermal conductivity. Above approximately 100 K the total thermal conductivity is larger than that given by the sum of Wiedemann-Franz and Debye contributions. We discuss an additional contribution to the thermal conductivity in two terms: (i) thermally activated propagation of localized lattice vibrations, and (ii) bipolar diffusion of conducting electrons due to presence of pseudogap in electron density of states.

Keywords: thermal conductivity, Wiedemann-Franz law, Debye model, localized lattice vibrations, bipolar diffusion

Modeling the transport properties of Taylor-phase and decagonal $\text{Al}_3(\text{Mn,Fe})$ complex intermetallics

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Transport properties of many quasicrystals can be explained and analytically calculated from the spectral conductivity function:

$$\sigma(E) \sim e^2 \sum | \langle i | v | j \rangle |^2 \delta(E - E_i) \delta(E - E_j).$$

The spectral conductivity can be regarded as the density of states multiplied by the diffusivity, $D(E)$. The *ab initio* calculations [1] of the spectral conductivity, but also an elaborate analysis[2] of the transport properties of some icosahedral quasicrystals indicate existence of the two deeps in the vicinity of the Fermi level that are modelled with Lorentzian peaks in the spectral resistivity.

However, this model cannot be applied for the transport properties of Taylor-phases of the complex intermetallics $\text{Al}_3(\text{Mn,Fe})$. The low temperature behaviour of the conductivity reveals a non-analytical, $|E|^{1/2}$ -like term in the spectral conductivity. Term like that has been already anticipated theoretically. In this presentation we describe a new method to analyze experimental data in order to extract spectral conductivity. The extracted spectral conductivity fits well the low temperature behaviour of the conductivity and the thermopower. This also provides a reliable method to separate the electronic and phonon contributions in the thermal conductivity.

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Keywords: complex intermetallic, T-phases of transition metals, spectral density, transport properties

NMR spectroscopic study of complex compounds

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Cage compounds as CMA: present and future

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Crystal structures of intermetallic clathrates and skutterudite derivatives are formed by the 3D host frameworks with the differently sized, filled or non-filled cavities. As for CMA, the basis structural motifs have relatively small unit cells with 34 to 150 atoms. The complexity of the crystal structures increases rapidly by partial ordering of the constituents and/or defects [1]. The resulting unit cells may contain several hundreds of atoms being in agreement with the usual structural features of CMA [2].

A variety of emerging physical behaviours attract recently the worldwide attention to these materials. One of the key problems for the cage compounds is the discovery of the new representatives and developing of the new ways of their preparation, e.g., oxidation of chemically active intermetallic precursors for clathrate synthesis. Depending on the processing it may lead to a non-filled clathrate [3], or to metastable variants of clathrate-I. By oxidizing monosilicides A_4Si_4 of alkali metals as starting materials, the defect clathrates $A_{8-x}Si_{46}$ are formed [4]. First clathrates with mixed boron-silicon framework, e.g. $K_{8-x}B_7Si_{39}$ ($x = 1$), were obtained by conventional preparation techniques. They follow the Zintl rule in the composition, are diamagnets and show non-metallic behaviour in electronic transport [5].

The novel families of compounds with the filled-skutterudite crystal structure were prepared with the elements of the group 14 in the framework. The rare-earth (RE) representatives of the $REPt_4Ge_{12}$ family show, i.e., superconductivity at relatively high temperatures [6], also found for the alkaline earth (AE) filled $AEPt_4Ge_{12}$ skutterudites [6,7]. The tin-filled skutterudite $Sn_xPt_4Sn_ySb_{12-y}$ is the first representative of this group with the filler atoms located not in the centres of the cavities, but bonded covalently to the framework wall [8].

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A high field Mössbauer investigation on iron containing skutterudites

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Fe-containing ternary skutterudites show a large variety of magnetic ground states depending on the type of filler atom [e.g. 1-7]. For example in case of rare earth elements we observed no magnetic order, at least down to 2 K, for La, magnetic order with presumably some kind of antiferromagnetic spin alignment for Pr, ferromagnetism for Nd, complex magnetic properties, with possibly mixed valent behaviour for Eu, and Curie-Weiss dependence with large effective but low saturation moments for the non-magnetic filler atoms $M = \text{Na, K, Ca, Sr, Ba, Tl}$ and Yb, pointing to an itinerant character of the magnetic order. For compounds with monovalent filler atoms weak band ferromagnetism is proposed, whereas for those with divalent fillers strong spin fluctuations are expected to exist.

In this work we report on a systematic high field (up to 13.5 T) ⁵⁷Fe Mössbauer investigation of $\text{MFe}_4\text{Sb}_{12}$ with $M = \text{Na, K, Ca, Sr, Ba, La, Pr, Nd, Eu, Yb, and Tl}$.

Although crystallographically only one Fe site is present in the structure, in some compounds at least two subspectra are necessary for the analysis, because of the asymmetry of the spectra. For the compounds with Pr, Nd, and Eu a correlation with the concentration of voids on the rare earth site is in fair agreement with the obtained spectral ratio. But this interpretation does not hold for the di- and monovalent filler atoms. The values of the induced hyperfine fields at 4 K are much too small to explain directly the large effective moments deduced on the Fe sites from susceptibility measurements at high temperatures. Band structure calculations point to an at least partly compensation of core and valence contributions of the induced hyperfine fields on the ⁵⁷Fe nucleus.

Surprisingly centre shift and quadrupole interactions are practically independent of the valence of the filler atom. Possible reasons will be discussed.

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Thermoelectric Properties of Cage Compounds

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Complex Metallic Alloys (CMAs) with cage structure such as intermetallic clathrates or skutterudites have large potential for thermoelectric applications. In these inclusion complexes atoms (or molecules) of one type (guest) are enclosed in cavities formed by atoms of another type (host or framework). The belief is that the guest atoms are loosely bound in the cavities and undergo large, essentially localized oscillations ("rattling") which strongly scatter the heat carrying (acoustic) phonons, leading to low and "glass-like" thermal conductivities. At the same time the rattling does not significantly affect the electronic properties since the charge carriers are confined to the framework. This concept is usually referred to as "phonon glass - electron crystal" (PGEC) [1].

The potential of a material for thermoelectric applications is determined by the material's dimensionless thermoelectric figure-of-merit $ZT = TS^2\sigma/\kappa$ where S is the thermopower, σ the electrical conductivity, κ the total thermal conductivity (which contains electronic and lattice contributions, $\kappa = \kappa_e + \kappa_l$), and T the absolute temperature. In a PGEC the ratio σ/κ is large and therefore the ZT value is enhanced with respect to a situation without cage structure. Traditional thermoelectric materials (Bi-Sb-Te alloys) currently in use in commercial devices have room temperature ZT values of approximately unity [2]. For clathrates and skutterudites promising ZT values have so far been achieved at elevated temperatures, e.g., $ZT = 1.1$ for the clathrate $\text{Eu}_8\text{Ga}_{16}\text{Ge}_{30}$ at 750 K [3], $ZT = 1.35$ for the clathrate $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$ at 900 K [4], or $ZT = 1.4$ for the skutterudite CeFeCoSb_3 at about 900 K [5] and $ZT = 1.7$ at 575 K in $\text{In}_{0.2}\text{Ce}_{0.2}\text{Co}_4\text{Sb}_{12}$ [6].

Our investigations into the synthesis and characterization of various materials with cage structure and their thermoelectric properties will be presented.

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MR Evidence for Molecular Groups Trapped in Cages of $\text{Co}_4\text{Al}_{13}$ and $\text{Fe}_4\text{Al}_{13}$

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Orthorhombic $\text{Co}_4\text{Al}_{13}$ with layered structure and pentagonal channels [1] has been for a long time considered as an approximant for decagonal quasicrystals. Moreover, with 102 atoms per unit cell, cluster arrangement of atoms and inherent disorder [1], it has been treated as a member of complex metallic alloys [2]. Recent X-ray investigation in combination with an analysis of the chemical bonding based on quantum mechanical calculations revealed the structural resemblance of $\text{Co}_4\text{Al}_{13}$ and clathrates [3]. Co-Al-Co molecular groups are considered as guests trapped in cages formed by other Al and Co atoms. According to this model a unique bonding situation for the Al atoms in the Co-Al-Co molecular groups in comparison with the other Al atoms is expected.

Since nuclear magnetic resonance (NMR) as a local probe has been proven to give insight into the local arrangements of the atoms of intermetallic compounds [4,5], ²⁷Al NMR measurements on powder samples and a single-crystal were done to get independent support for this model. Two ²⁷Al signals were identified in $\text{Co}_4\text{Al}_{13}$. First one originates from Al atoms forming cages. The second signal corresponds to Al sites with exceptionally large almost axially symmetric quadrupole coupling, in perfect agreement with isolated Co-Al-Co molecular groups. Similar structural features were found in quasihomologous monoclinic $\text{Fe}_4\text{Al}_{13}$ [6].

Keywords: ²⁷Al NMR; complex metallic alloys; approximants; clathrate structure; $\text{Co}_4\text{Al}_{13}$, $\text{Fe}_4\text{Al}_{13}$

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**Electronic Structure of Complex Metallic Alloys and
Quasicrystals: Experimental Studies**

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Complex metallic alloys and quasicrystals share structural motifs such as clusters, and as approximants the alloys bridge the gap between materials with translational periodicity and aperiodic solids. Since the origin of the structural properties of these materials lies in their electronic structure, i.e. the nature and arrangement of the electronic states at the Fermi level and over the entire range of valence level energies, an investigation of the density of states, and, more importantly, of the dispersion of electronic bands is required. The question of the presence of a band structure $E(\mathbf{k})$ in the conventional sense, which is not immediately obvious in quasicrystals, is of special interest. In the talk, I will present experimental studies of the electronic structure of several quasicrystals, approximants and other complex metallic alloys, with a view to identifying the relative importance of localized and itinerant states and the presence of a pseudogap in the density of states at the Fermi level. Similarities and differences between complex metallic alloys and quasicrystals will be discussed. Special emphasis will be laid on the interpretation of photoelectron spectroscopy data, since this method, in particular in its angle-resolved variant, has developed from a surface-related spectroscopy to a most powerful method of analyzing the electronic structure of solids, from 3D bulk to low-dimensional systems and nanostructures. An outlook will be given on problems in analyzing complex metallic alloys using surface-related spectroscopies, and on interesting experimental approaches to the study of the electronic structure of complex alloys.

* Work carried out in collaboration with the group of E. Rotenberg, Advanced Light Source, Lawrence Berkeley Laboratory, USA, CNRS Nancy, France, Forschungszentrum Jülich, Germany, and EMPA Thun, Switzerland.

Photoemission from supported 2D metallic systems

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Most of the noble metals grow on low index transition metal surfaces in form of well defined films. The ultraviolet photoemission spectroscopy revealed that these very thin metallic films in many cases exhibit spectral features that are not present in their bulk counterparts. In this talk I will present results of our experimental investigation of ultra thin metallic films that show quantum size effect that occurs due to the strong localization of electrons within the overlayer film. I will discuss quantization conditions, formation of quantum well states (QWS) and resonances (QWR), dependence of the QWS; binding energy on the supporting surface and film thickness, different aspects of interaction with supporting surfaces, oscillatory behaviour of some physical properties e.g. electron/phonon coupling. I will also discuss epitaxial growth of graphite monolayer on metal surfaces as an promising route to produce high quality graphene

Ag-Based Quasicrystal: Novel Template for Pseudomorphic Films

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The recent success in growing large single-grain samples of the Ag-based quasicrystal [1] has opened up the opportunity to carry out thin film growth studies on this new template. We studied the fivefold surface of icosahedral $\text{Ag}_{42}\text{In}_{42}\text{Yb}_{16}$, which is isostructural to the binary icosahedral Cd-Yb quasicrystal, using various experimental techniques, including scanning tunneling microscopy (STM), low-energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS). The surface can be prepared with large terraces suitable for the thin film growth study. Both the step height distribution and terrace structure are found to be consistent with bulk truncations at Yb-rich dense atomic planes.

Pb deposited on the surface forms a quasicrystalline network of pentagons in the first layer and of decagons in the second layer. This pseudomorphic film now can be used as a model system to investigate the impact of quasicrystallinity on the associated physical properties, independently of chemical composition of the bulk.

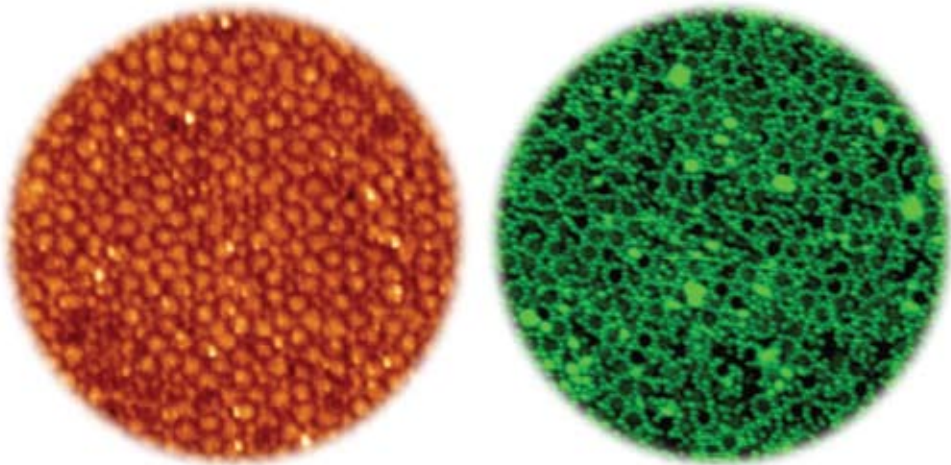


Figure 1: STM image of the clean fivefold i-Ag-In-Yb surface (left, 50nm x 50nm) and after Pb deposition (right, 60nm x 60nm).

[1] S. Ohhashi, J. Hasegawa, S. Takeuchi, et al., *Phil. Mag.* **87**, 3089 (2007)

[2] H. R. Sharma, M. Shimoda, S. Ohhashi and A. P. Tsai, *Phil. Mag.* **87**, 2989 (2007)

Scanning tunnelling spectroscopy of quasicrystals and complex metallic alloys

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The advances in crystal growth and surface preparation techniques of complex metallic alloys (CMA) and quasicrystals (QC) have opened the possibility to investigate the local valence electronic structure by means of low temperature scanning tunnelling microscopy and spectroscopy (STM/STS) at 5 K. This allows measuring the surface local density of states (LDOS) with sub-nm spatial resolution and high energy resolution in the meV regime. Of particular interest for these materials is the question to what extent the small 1st Brillouin zone for CMA or the absent translational symmetry in QC lead to localization of the valence electronic states in these materials.

We will discuss STM/STS investigations on the 5-fold and 2-fold surface of the icosahedral AlPdMn QC and show that indeed states localized in energy (30-70 meV) and space (< 2 nm) can be observed. These states are however superimposed to a large (1 eV) Hume-Rothery like pseudo-gap and averaging of the STS spectra on surfaces larger than typical 10x10 nm² leads to a disappearance of peaks corresponding to localized states in the averaged spectra. This observation clearly indicates the importance of measuring the DOS on a nanometer level. As we will show, the complexity of the surface structure and of the spectroscopic signatures make it very difficult to reach a quantitative conclusion on the nature of the localized states. A possibility to reduce this complexity is to investigate QC surfaces with a simpler structure like, the 2-fold surface of the decagonal AlCoNi QC, which exhibits simultaneously a periodic and an aperiodic crystal direction (which are perpendicular to each other). This allows to check if the observed states repeat themselves in a periodic way along the periodic direction and therefore one can exclude that the states are due solely to structural disorder, which is very often present on QC surfaces. The results from the QC investigations will then be compared to surfaces of complex metallic alloys that have similar local atomic arrangements as the QC but are periodic.

Friction anisotropy on decagonal quasicrystal surfaces

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Quasicrystals are peculiar in many aspects: the unusual transport properties, their high hardness and low friction. These have prompted applications as anti-stick and low friction coatings. Recent tribological studies on quasicrystal surfaces indicate that there is an intrinsic relationship between the aperiodic atomic structure of quasicrystals and their low friction. In this talk, I outline the recent investigations on the atomic scale friction properties of quasicrystal surfaces using a combination of atomic force microscopy and scanning tunneling microscopy in ultrahigh vacuum. This combination permits a variety of in situ measurements, including atomic-scale structure, friction and adhesion force, and indentation. Friction anisotropy was revealed at different length scales (macroscale and nanoscale) on the twofold surface of the Al-Ni-Co decagonal quasicrystal where atoms are arranged periodically along the tenfold axis and aperiodically in the perpendicular direction. I discuss the role of the surface oxide and the nature of mechanical contact in determining friction and adhesion properties.

Quantum Size Effects in Thin Films on Complex Aluminides

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We have investigated by scanning tunnelling microscopy the growth of Bi and Ag thin films on the fivefold surface of Al-Cu-Fe and Al-Pd-Mn quasicrystals [1]. For both systems, we observe the formation of islands with ‘magic’ height, corresponding to the stacking of a specific number of atomic layers. We interpret the special stability associated with a specific film thickness in terms of quantum size effects, arising from the confinement of the electrons within the film. In the case of Ag thin films, we have recently investigated in details the formation of quantum well states as a function of film thickness and for various conditions of the deposit. The film morphology is monitored by STM and the electronic structure by photoemission spectroscopy. It is found that the deposition temperature is critical for the appearance of quantum well states and the formation of magic islands.

[1] V. Fournée, H. R. Sharma *et al.*, Phys. Rev. Lett. **95** (2005) 155504.

Medium Energy Ion Scattering Studies of Complex Metallic Alloy Surfaces

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Medium energy ion scattering (MEIS) has long been applied to both amorphous materials to obtain depth profiles and also crystalline materials, where in addition, structural information can be obtained. Recently, work has been carried out at the UK national facility to investigate the composition and structure of aperiodic quasicrystalline complex metal alloys and thin metallic films grown on them. Initial studies revealed sensitivity to the unusual symmetries, with distinct blocking dips in the in-plane angular scattering spectra. Simulating this data using the VEGAS code is complicated by the aperiodic nature of the materials, but can be achieved using either a large slab of truly aperiodic structure of an 'approximant' model.

For $i\text{-Al}_{70}\text{Pd}_{21}\text{Mn}_9$, MEIS data indicate that Argon ion sputtering gives rise to Mn depletion and the formation of a thick five-domain AlPd(110) layer. Annealing to 450°C restores the Mn content and icosahedral structure. However, further heating to increasingly higher temperatures was seen to cause Mn enrichment above the ideal composition for the icosahedral structure, with larger amounts of disorder becoming apparent in the sample. For the highest temperature anneals, the surface showed low apparent roughness and exhibited blocking patterns consistent with a contraction of the outermost layer of atoms in line with previous structural studies of this material [*Gierer et al, Phys. Rev. Lett. 78 (1997) 467, Capitan et al, Physica B 283 (2000) 79*].

The deposition of Cu onto the five-fold surface of $i\text{-Al}_{70}\text{Pd}_{21}\text{Mn}_9$ gives rise to a one-dimensionally aperiodic film [*Ledieu et al, Phys. Rev. Lett. 92 (2004) 135507*], which on annealing transforms into a periodic structure. MEIS measurements reveal a pure Cu film for the aperiodic structure, whereas for the periodic structure, the surface is composed of a quaternary $\text{Al}_{65}\text{Mn}_{16}\text{Pd}_{11}\text{Cu}_8$ alloy. Simulations of the structure of the periodic film showed that it is composed of 5-domains of (110) oriented cubic material. Analysis of the aperiodic structure indicated nanoscale strips, with a Fibonacci arrangement of long and short widths, each having fcc(100) structure.

MEIS data for films grown by depositing Au on $i\text{-Al}_{70}\text{Pd}_{21}\text{Mn}_9$ at room temperature, both with and without In surfactant, indicate the formation of a stoichiometric AuAl alloy, which transforms to an AuAl₂ alloy on annealing to 315°C. However, the angular spectra revealed no structure in the films regardless of either annealing or pre-deposition of the In surfactant, contrary to previous studies of this system [*Shimoda et al, Jap. J. Appl. Phys. 40 (2001) 6073*]. The films were seen to be amorphous or at best polycrystalline, with a high degree of surface roughness.

The deposition of Bi on an icosahedral substrate has previously been shown to give rise to a monolayer film with additional material forming islands of predominantly 4 ML height due to quantum size effects [*Fournée et al, Phys. Rev. Lett. 95 (2005) 155504*]. MEIS energy spectra confirm similar behaviour for Bi on $i\text{-Al}_{70}\text{Pd}_{21}\text{Mn}_9$. Additionally, the angular spectra reveal the island structure to be similar to bulk Bi but with a slight distortion of the normal rhombohedral arrangement.

Adsorption Studies on Quasicrystal and Approximant Surfaces

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Much of our understanding of condensed matter and surface science is based on studies of periodic crystals. In recent years, this has been extended through the study of quasicrystals and their surfaces, which, although well ordered, are aperiodic. Now, the growth of approximant systems, which are large unit cell complex metallic alloys structurally related and close in composition to quasicrystalline phases, allows the direct comparison of structural and growth phenomena on related periodic and aperiodic surfaces. The use of CMAs as templates for adsorption studies should bring new understanding on several key questions. For instance, it is known that in a “classical” crystal, the lattice parameter is the relevant length scale for physical properties of a solid and dictates at the surface the growth mode of adsorbates. However, for approximants the relevant length scale for growth properties should best correspond to inter-cluster distances. Hence one may ask for instance what is the influence of a “giant” unit cell on thin film growth. Similarly, the growth of pseudomorphic mono-element thin films (with reduced chemical complexity) on CMA surfaces should allow us to probe the influence of aperiodic ordering and/or of large periodicity on the film electronic structure. One approach to answering these questions is to be performed simultaneous deposition on related CMA surfaces with or without lattice periodicity. Here we report our recent work of adsorption studies on icosahedral, decagonal and approximant surfaces. The formation of nano-sized islands, the nucleation at preferential adsorption sites, the electronic structure of the film and the overall growth mode of adatoms on these surfaces will be reviewed.

Abstracts of Posters

NMR Study of YbCu_{4.5} Complex Metallic Alloy Compound

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YbCu_{4.5} is a complex metallic alloy (CMA) with a giant unit cell which contains 7448 atoms. This is still an alloy with the largest unit cell observed. It has a monoclinic structure which derives from AuBe₅-type structure (space group $F43m$) via the introduction of planar defects parallel to $\{hhh\}$. The cell parameters are $a = 4.896$ nm, $b = 4.899$ nm, $c = 4.564$ nm and $b = 91.240$.

We studied the NMR spectra of ⁶³Cu at temperatures from 270 K to 4 K. We measured the position of the central peak, its width and relaxation time T_1 as a function of temperature. We found that above 80 K the behaviour of the peak position and T_1 is normal Curie-Weiss and Korringa, respectively. However, below 80 K we observed a change in behaviour and even more sudden (Kondo-like) changes below 20 K.

Deuterium dynamics in the icosahedral and amorphous phases of $\text{Ti}_{40}\text{Zr}_{40}\text{Ni}_{20}$ hydrogen-absorbing alloy studied by ^2H NMR

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The $\text{Ti}_{40}\text{Zr}_{40}\text{Ni}_{20}$ hydrogen-absorbing alloy was prepared in the icosahedral and amorphous phases by controlling the rotation speed of the melt-spinning method of sample preparation and the deuterium dynamics was investigated by ^2H NMR dynamic line shape and spin-lattice relaxation. The results were analyzed by the line-shape and relaxation models that assume deuterium thermally activated hopping within a manifold of different chemical environment. The observed 7 % larger activation energy for the deuterium hopping over the interstitial sites and the 10 % larger static spectrum width of the amorphous phase, as compared to the icosahedral phase, can be accounted for by the larger deuterium content of the investigated amorphous sample. From the deuterium dynamics point of view, the icosahedral phase is not special to the amorphous modification of the same material.

Hall effect of the triclinic $\text{Al}_{73}\text{Mn}_{27}$ and $T\text{-Al}_{73}\text{Mn}_{27-x}\text{Pd}_x$ ($0 \leq x \leq 6$) complex metallic alloys

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The Hall coefficient R_H of the triclinic $\text{Al}_{73}\text{Mn}_{27}$ and Taylor-phase $\text{Al}_{73}\text{Mn}_{27-x}\text{Pd}_x$ ($x = 0, 2, 4$ and 6) complex metallic alloys has been measured from 90 to 400 K. The Hall coefficients of all the samples are positive and they decrease strongly with the increase of temperature T . The shape of R_H vs. T curves indicates that, in the explored temperature interval, the samples are paramagnetic, and that the anomalous magnetic contribution to the Hall effect is dominant. For the separation of the normal R_0 and anomalous R_S Hall coefficient, the results for the paramagnetic susceptibility $\chi(T)$ and electrical resistivity $\rho(T)$, have been used. There it was assumed that in the approximate relation $R_H = R_0 + \chi \cdot R_S$, R_S is proportional to the square of resistivity. The well defined linearity of the R_H vs. $\chi(T) \cdot \rho^2(T)$ plots for all the alloys confirms the above assumption, and indicates that in these materials R_S is dominated by spin-orbit interaction and the side-jump effect. The values deduced from the R_H vs. χ and R_H vs. $\chi \cdot \rho^2$ plots in TAIMnPd phases, fall between $2 \times 10^{10} \text{ m}^3\text{C}^{-1}$ and 0 for R_0 , and are about $5 \times 10^7 \text{ m}^3\text{C}^{-1}$ for R_S . The values deduced from the R_H vs. $\chi \cdot \rho^2$ plots in the triclinic $\text{Al}_{73}\text{Mn}_{27}$ alloy are about $15 \times 10^{10} \text{ m}^3\text{C}^{-1}$ for R_0 , and about $1.5 \times 10^5 \text{ m}^3\text{C}^{-1}$ for R_S . The conduction electron densities estimated from R_0 are characteristic for metals and are of the order 10^{23} cm^{-3} in the TAIMnPd samples, and of the order 10^{22} in the triclinic $\text{Al}_{73}\text{Mn}_{27}$ sample. The fact that the anomalous Hall coefficient of all the investigated alloys is very large, is certainly due to the high resistivity of these alloys.

Keywords: Complex metallic alloys, Hall effect

The Influence of Thermal Treatment on Structural Order and Magnetic Properties of *i*-Al-Pd-Mn Quasicrystals

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The influence of thermal treatment on structural order and magnetic properties of icosahedral *i*-Al-Pd-Mn single-crystalline quasicrystals was studied by investigating a large set of samples prepared by the Czochralski and Bridgman techniques. By subjecting the samples to different thermal annealing sequences differing in annealing times, annealing temperatures and cooling rates the structural order was systematically changed by varying the concentration of thermal vacancies, thermal strains and secondary phase precipitates. These three effects represent a disorder which exists on the short scale of near-neighbor atoms and is believed to be an intrinsic property of the *i*-Al-Pd-Mn quasiperiodic structure ensuring the electronic or entropic stabilization of the structure. As the effective magnetic moment of Mn atoms is influenced by the structural order on the scale up to 5 – 10 Å around the atoms, the disorder can be studied indirectly by measurements of the electronic magnetization. A Quantum Design MPMS-XL-5 SQUID magnetometer equipped by a 5 T magnet was used to perform the magnetization measurements. The results show equal importance of all three effects – the change in the thermal vacancy concentration, the thermal strains due to the cooling rate selection and the presence/absence of secondary phase precipitates – on the size of the mean effective magnetic moment per Mn atom. The magnitude of the paramagnetic magnetization of the same *i*-Al-Pd-Mn material, subjected to different thermal treatments, was found to vary up to a factor of 30. Furthermore, it was found that long-term annealing at 800°C followed by slow cooling yields *i*-Al-Pd-Mn samples of the highest structural perfection, whereas rapid cooling and annealing at 600°C accompanied by the *T*-phase precipitate formation both result in an increase of the disorder on this scale. Employing water quenching procedure after the annealing period, one instantly reintroduces some disorder and corrupts the painfully achieved high temperature relaxed structure.

Lattice Dynamics Calculations of the High-pressure Phase Transition in CdTe

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The study of pressure induced phase transitions has been rapidly expanding field of research during the past few decades. It was discovered that many semiconductors have a rich phase diagram, as a function of pressure and temperature, with a number of phases, which were not known before.

The understanding of the mechanism of high pressure phase transitions at microscopic level is far from complete and more theoretical models are required.

We investigated the stability of the metallic rocksalt structure with respect to the high pressure Cmcm structure for II-VI semiconductor CdTe. The lattice dynamics calculations, based on density functional perturbation theory (DFPT), reveal that the rocksalt structure is unstable with respect to transversal acoustic mode at the Brillouin zone boundary. The phase transition is of the second order (zero volume change), associated with cell doubling in the high pressure Cmcm phase with frozen in deformation.

The present calculation gives the transition pressure more accurately then classical common tangent method. Since the volume change at the transition is very small or zero, the transition was estimated from the pressure at which the frequency of zone boundary transversal acoustic mode goes to zero.

The observed pressure of the phase transition in structural measurements was reproduced more accurately then in previous calculations and the difference between observed and calculated transition pressure is well below 10%.

Keywords: lattice dynamics, DFPT, phase transition, metals

**Anisotropic transport properties of the orthorhombic complex
metallic alloy phase $\text{Al}_{13}\text{Co}_4$**

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We have investigated anisotropic transport properties (electrical resistivity, thermoelectric power, Hall coefficient and thermal conductivity) of the orthorhombic $\text{Al}_{13}\text{Co}_4$ complex metallic alloy phase. The unit cell contains 102 atoms and the main structural features are pair-connected pentagonal-prismatic channels extending along the [100] direction [1]. In this sense $\text{Al}_{13}\text{Co}_4$ is structurally related to a group of other CMAs [2] of which orthorhombic $\text{Al}_{13}\text{Fe}_4$ is the most prominent. The crystalline-direction-dependent measurements were performed along three orthogonal directions [100], [010] and [001] of the $\text{Al}_{13}\text{Co}_4$ unit cell. Anisotropic electrical resistivity is low in all crystalline directions, decreases in the order $\rho_{[001]} > \rho_{[010]} \gg \rho_{[100]}$ and shows positive temperature coefficient typical of electron-phonon scattering mechanism. Anisotropic thermal conductivity appears in the order $\kappa_{[100]} \gg \kappa_{[010]} > \kappa_{[001]}$, so that [100] is the most conducting direction for both electricity and heat transport. The Hall coefficient R_H exhibits pronounced anisotropy. Magnetic field in a given direction yields the same R_H irrespectively of the direction of the current in the perpendicular plane. These anisotropies are analyzed in terms of the anisotropic structure of the $\text{Al}_{13}\text{Co}_4$ phase and compared to the literature-reported anisotropy of the transport properties other CMA's and related materials [3].

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Keywords: transport properties, approximants, $\text{Al}_{13}\text{Co}_4$

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The solidification path of the complex metallic Al-Mn-Be alloyBoštjan Markoli¹, Tonica Bončina² and Franc Zupanič²¹Naravoslovnotehniška fakulteta, Univerza v Ljubljani, Slovenija²Fakulteta za strojništvo, Univerza v Mariboru, Slovenija

The solidification path of $\text{Al}_{86.6}\text{Mn}_{2.5}\text{Be}_{11.4}$ and $\text{Al}_{84}\text{Mn}_{5.1}\text{Be}_{10.9}$ alloy melt spun, cast into copper mould and controlled cooled (during DSC) was investigated by means of light-optical microscopy (LOM), differential dynamic calorimetry (DSC) combined with thermogravimetry (TG), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD) line in Elletra Trieste, Italy. The constitution of samples from both alloys, were examined in all three states i.e. after melt spinning, casting into copper mould and differential dynamic calorimetry. It has been established that in the cast and controlled cooled specimens alloys consisted of aluminium rich α_{Al} -matrix, $\text{Al}_{10}\text{Mn}_3$ and Be_4AlMn phase. The amounts, shape and distribution of phases established varied depending on the solidification conditions and parameters, which were particular to each process i.e. melt-spinning, casting and DSC. In the case of casting and DSC the primary crystallization began with precipitation of Be_4AlMn phase followed by what could most likely be characterized as a univariant binary eutectic reaction $L \rightarrow (\text{Be}_4\text{AlMn} + \text{Al}_{10}\text{Mn}_3)$. The solidification process continued with what could be characterised as an invariant ternary eutectic reaction where the remaining melt (L) formed the heterogeneous structure ($\alpha_{\text{Al}} + \text{Al}_{10}\text{Mn}_3 + \text{Be}_4\text{AlMn}$) or ternary eutectic. Although this structure lacked typical shape and distribution of constituting phases, which is usually found in eutectics in general. This is not surprising since both phases containing manganese are metastable meaning that departure from equilibrium set in even at slow cooling rates. Nevertheless, based on the results of the extended metallographic examination we were able to conclude that the composition of the investigated alloys is obviously located in the area of the three-cornered reaction plateau where the eutectic reaction ended because the whole of the remaining melt was consumed by this reaction. When extremely high cooling rates were employed as it is in the case of melt-spinning the constituting phases of both alloys were precipitated in a very small form and the Be_4AlMn phase was completely absent in a form of primary polygonal particles and replaced by icosahedral quasicrystalline phase or the i -phase. There was also no evidence of the $\text{Al}_{10}\text{Mn}_3$ phase. Furthermore, XRD, SEM, TEM and AES confirmed such constitution of melt-spun ribbons. The distribution, size and shape of all constituents in the melt spun alloys also varied from the contact surface towards the free surface of ribbons. The smallest constituents were established at the contact surface measuring less than one-tenth of a $1 \mu\text{m}$ to $0.5 \mu\text{m}$ at the free surface. The grains of the aluminium rich matrix had mean diameter less than $20 \mu\text{m}$ close to the free surface down to $1 \mu\text{m}$ at the contact surface.

Keywords: complex Al-Mn-Be alloys, metallography, solidification

Comparison of molecular adsorption on quasiperiodic and periodic substrates

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Molecular interactions with surfaces are determined by the chemistry of the interactions between the adsorbing molecular and the substrate, and the inter-molecular interactions. It is of much interest to consider whether changes in the structure of the substrate, independently of changes in the chemistry, can have an influence of adsorption. In this work we compare the adsorption behaviour of C_{60} on Cu(111) and on a quasiperiodically modulated Cu film grown on the five-fold surface of the Al-Pd-Mn quasicrystal. Differences in the adsorption behaviour are discussed in terms of the strength of the molecule-substrate interactions and the availability of adsorption sites.

Transport properties of a YbCu_{4.5} complex metallic alloy compound

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Experimental results of electrical (σ) and thermal conductivity (κ) and thermoelectric power (S) of a polycrystalline sample of YbCu_{4.5}, in the temperature range 1.5 to 300 K, are present. In contrast with the divalent YbCu₂ compound, YbCu_{4.5} shows properties typical of an intermediate valence compound: low electrical conductivity and large thermoelectric power. The electrical conductivity shows the typical $\sigma(T)$ dependence of Kondo lattice systems with a room temperature value $\sigma(300\text{ K}) \approx 5 \times 10^6 (\Omega\text{m})^{-1}$, while thermoelectric power $S(T)$ is negative and shows the distinct temperature dependence which is attributed to the Kondo interaction. To our best knowledge, this is the first measurements of the thermal conductivity of YbCu_x compounds. The room temperature value of the thermal conductivity of YbCu_{4.5} is $\kappa \approx 21\text{ W/mK}$. A pronounced maximum in thermal conductivity at low temperatures, which is frequently found in simple nonmagnetic and rather pure samples, is absent. The absent of a maximum in $\kappa(T)$ is related to a larger contribution of residual scattering processes and a considerable weak coupling of electrons with phonons. Another intriguing feature of this alloy is that thermal conductivity increases monotonically with temperature above 100 K. The results are compared to the reported transport properties of the Ce-Cu and Yb-Cu systems [1, 2].

Keywords: transport properties, intermetallics, YbCu_{4.5}

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High pressure study of transport properties of CMA

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An important question, in the field of giant-unit-cell complex metallic alloys (CMA), is which of the two coexisting physical length scales, the large (defined by the crystal periodicity) or the short (characterized by the distances between icosahedrally ordered atoms), plays the dominant role in determining the electrical properties of those materials [1]. An insight into this problem can be achieved by applying external hydrostatic pressure to the material sample and measure the temperature dependence of the electrical resistivity. Because the pressure brings the atoms closer, the overlap of the atomic potentials increases and the potential barriers between neighboring atoms are reduced. Consequently, one expects the enhancement of the electrical conductivity due to the reduction of the inter-atomic distances. In order to check this assumption, we conducted resistivity measurements on the $A_{75}Pd_{20}Fe_2$ sample varying pressures from 1 bar to 18 kbar, in the temperature range 4-300K. The sample was mounted into a self-clamped pressure cell, using petroleum as the pressure medium. The pressure was monitored *in situ* by a calibrated InSb pressure gauge. The relative change in volume ΔV as a function of the pressure change Δp is estimated by evaluating $\Delta V/V = \Delta p/E$, where E is the material's elastic modulus. For a typical metal E is of the order 100 GPa, yielding $\Delta V/V \approx 2\%$ at 18 kbar. We observe that the resistivity drops significantly with pressure (from $\rho_{300K}(1\text{bar}) = 306 \mu\Omega\text{cm}$ to $\rho_{300K}(17.8\text{kbar}) = 284 \mu\Omega\text{cm}$. This is 7 % relative to the $p=1\text{bar}$ value, whereas this reduction amounts to 8.5 % at 4 K). This behavior is consistent with the consideration that the resistivity of a CMA material is governed by the smaller of the two coexisting physical length scales. It can be thus concluded that the inter-atomic distances determine the electrical properties of CMA's, which is also valid for regular metals and alloys.

Keywords: transport properties, pressure, complex metallic alloys

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Anisotropic thermal conductivity of the Y-Al-Ni-Co decagonal approximant

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The anisotropic thermal conductivity κ of Y-Al-Ni-Co decagonal approximant with composition $\text{Al}_{76}\text{Co}_{22}\text{Ni}_2$ [1] has been measured along three orthogonal directions a^* , b and c of the Y-Al-Ni-Co unit cell, where (a,c) monoclinic atomic planes are stacked along the perpendicular b direction. The phononic contribution $\kappa_{\text{ph}} = \kappa - \kappa_{\text{el}}$ was estimated by subtracting the electronic contribution κ_{el} from the total conductivity using the Wiedemann-Franz (WF) law, $\kappa_{\text{el}} = L(T) \cdot \sigma(T) \cdot T$ ($L(T)$ – temperature dependent Lorentz number) and the measured electrical conductivity data $\sigma(T)$ on the same specimens [2]. Though the use of the WF law is a rough approximation, in this way determined κ_{ph} gives an indication of the anisotropy of the phononic spectrum. At room temperature (RT), we get the anisotropy: $\kappa^{a^*} = 12.5$ W/mK, $\kappa_{\text{el}}^{a^*} = 9.1$ W/mK with their ratio $(\kappa_{\text{el}}^{a^*}/\kappa^{a^*})_{\text{RT}} = 0.73$, $\kappa^b = 46.3$ W/mK, $\kappa_{\text{el}}^b = 29.2$ W/mK with $(\kappa_{\text{el}}^b/\kappa^b)_{\text{RT}} = 0.63$ and $\kappa^c = 17.4$ W/mK, $\kappa_{\text{el}}^c = 12.2$ W/mK with $(\kappa_{\text{el}}^c/\kappa^c)_{\text{RT}} = 0.70$. Electrons are thus majority heat carriers for all three directions. The anisotropic thermal conductivities appear in the order $\kappa^b > \kappa^c > \kappa^{a^*}$ and similarly $\kappa_{\text{el}}^b > \kappa_{\text{el}}^c > \kappa_{\text{el}}^{a^*}$, which is identical to the order in which the anisotropic electrical conductivities appear $\sigma^b > \sigma^c > \sigma^{a^*}$. The anisotropic κ_{ph} 's appear in the same order, $\kappa_{\text{ph}}^b > \kappa_{\text{ph}}^c > \kappa_{\text{ph}}^{a^*}$, so that the phononic conductivity is the highest along the b direction perpendicular to the (a,c) atomic layers, whereas the two in-plane conductivities are lower and show smaller anisotropy. For all directions, κ_{ph} 's show a typical phonon umklapp maximum at about 40 K. While it is expected that the anisotropic electronic thermal conductivities κ_{el} should appear in the same order as the anisotropic electrical conductivities (both are related to the electronic density of states), it is not a priori obvious that the anisotropic phononic thermal conductivities should also appear in this order, as κ_{ph} is related to the vibrational density of states. Striking anisotropy in thermal conductivity of the Y-Al-Ni-Co is due to the anisotropy of the structural symmetry.

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Keywords: thermal conductivity, decagonal approximants, Y-Al-Ni-Co

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Hall coefficient of the Y-Al-Ni-Co decagonal approximant

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We have investigated Hall coefficient of the Y-Al-Ni-Co decagonal approximant with the composition $\text{Al}_{76}\text{Co}_{22}\text{Ni}_2$ [1]. The crystalline-direction-dependent measurements were performed along three orthogonal directions a^* , b and c of the Y-Al-Ni-Co unit cell. For all combinations of directions, the R_H values are typical metallic in the range $10^{-3}\text{m}^3\text{C}^{-1}$ showing weak temperature dependence, which disappears at higher temperatures. The Hall coefficient exhibits pronounced anisotropy, where the magnetic field in a given direction yields the same Hall coefficient for the two measured directions of the current in the perpendicular plane. The observed anisotropy is analyzed in terms of the anisotropic structure of the Y-Al-Ni-Co phase [2] and compared to the anisotropy of the Hall coefficient of the d -Al-Ni-Co decagonal quasicrystals [3]. For d -QCs, universality of the Hall-effect anisotropy was reported for the d -Al-Ni-Co, d -Al-Cu-Co and d -Al-Si-Cu-Co [3] where $R_H > 0$ for the field lying in the quasiperiodic plane (corresponding to the in-plane coefficients $R_H^{a^*}$, $R_H^c > 0$ of Y-Al-Ni-Co), whereas R_H changes sign to negative for the field along the periodic direction (corresponding to $R_H^b \approx 0$ of Y-Al-Ni-Co). The above d -QCs also exhibit similar weak temperature dependence of R_H as Y-Al-Ni-Co, so that there is a good analogy between d -QCs and their approximant Y-Al-Ni-Co.

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Keywords: Hall coefficient, decagonal approximants, Y-Al-Ni-Co phase

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**Orientation-dependent NMR study of the giant-unit-cell intermetallics β -Al₃Mg₂,
Bergman-phase Mg₃₂(Al,Zn)₄₉, and ξ' -Al₇₄Pd₂₂Mn₄**

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We present a ²⁷Al NMR study of three giant-unit-cell complex metallic compounds, β -Al₃Mg₂, the “Bergman-phase” Mg₃₂(Al,Zn)₄₉, and ξ' -Al-Pd-Mn, which contain some hundreds up to more than a thousand atoms in the unit cell. The NMR spectra of monocrystalline samples are strongly inhomogeneously broadened by the electric quadrupole interaction and the line shapes are featureless and powderlike, but still exhibit significant orientation-dependent variation of the intensity on the satellite part of the spectrum in the magnetic field. Measuring orientation-dependent satellite intensity in appropriate frequency windows yields rotation patterns that can be related to the structure and symmetry of the giant unit cells. For a theoretical reproduction of the rotation patterns, we derived a distribution of the electric-field-gradient (EFG) tensors for each of the investigated compounds from existing structural models using point-charge and *ab initio* calculations. The EFG distribution yields important structural information on the manifold of different local atomic environments in the unit cell and distinguishes crystallographically inequivalent lattice sites from the equivalent ones.

Microstructure Selection during Solidification of Al-Mn-Be-Cu Alloys

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For a materials scientist a correlation between microstructure and properties plays the most important role in the process of the alloy development. Nowadays, the materials are growing more complex since they contain increasing number of the alloying elements. According to the Gibbs phase rule the maximum number of phases F taking part in the equilibrium ($p = \text{const}$) amounts $F = K + 1$; with K indicating the number of components. As a result, even during equilibrium solidification of multicomponent alloys many phases and many reactions can take place, leading to variety of microstructural constituents. (A term "microstructural constituent" denotes homogeneous or heterogeneous part of microstructure, formed during particular reaction upon solidification or solid state transformation.) Furthermore, by increasing the cooling rate (or undercooling below the equilibrium transition temperature) additional metastable phases may appear, and ultimately even a glass phase might form.

In such complicated situations, it would be desirable to predict the microstructure and properties by relatively simple diagrams; e. g. as a function of the cooling rate or undercooling. Such convenient diagrams useful for multicomponent metallic alloys (e. g. steels) have been used for long; for example, TTT-diagrams (Time – Temperature – Transformation) and CCT-diagrams (Continuous Cooling – Transformation).

For solidification of complex aluminium alloys a CCS (Continuous Cooling – Solidification) diagram is proposed. The qualitative presentations of the order of appearance and type of microstructural constituents and their respective volume fractions are shown on the example of an Al-Mn-Be-Cu alloy. In the selected $\text{Al}_{94}\text{Mn}_2\text{Be}_2\text{Cu}_2$ alloy several phases were present: Al-rich solid solution, intermetallic phase Al_xMn_y (probably $\text{Al}_{10}\text{Mn}_3$), as well as icosahedral quasicrystalline phase; this could be a part of different microstructural constituents. In order to construct the TTS diagram the alloy was solidified using very different cooling rates ranging from 20 K/min (Differential Scanning Calorimetry) and up to $\sim 10^5$ – 10^6 K/s (melt-spinning). Afterwards the samples were characterized using different metallographic techniques.

Keywords: Al-alloy, quasicrystal, microstructure selection, solidification

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