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BOOK OF ABSTRACTS

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Honorary Doctorate Lecture

D-01

The Discovery of Quasi-Periodic Crystals and its consequences

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Crystallography has been one of the mature sciences. Over the years, the modern science of crystallography that started by experimenting with x-ray diffraction from crystals in 1912, has developed a major paradigm – that all crystals are ordered and periodic. Indeed, this was the basis for the definition of “crystal” in textbooks of crystallography and x-ray diffraction. Based upon a vast number of experimental data, constantly improving research tools, and deepening theoretical understanding of the structure of crystalline materials no revolution was anticipated in our understanding the atomic order of solids.

However, such revolution did happen with the discovery of the Icosahedral phase, the first quasi-periodic crystal (QC) in 1982, and its announcement in 1984 [1,2]. QCs are ordered materials, but their atomic order is quasiperiodic rather than periodic, enabling formation of crystal symmetries, such as icosahedral symmetry, which cannot exist in periodic materials. The discovery created deep cracks in this paradigm, but the acceptance by the crystallographers' community of the new class of ordered crystals did not happen in one day. In fact it took almost a decade for QC order to be accepted by most crystallographers. The official stamp of approval came in a form of a new definition of “Crystal” by the International Union of Crystallographers. The paradigm that all crystals are periodic has thus been changed. It is clear now that although most crystals are ordered and periodic, a good number of them are ordered and quasi-periodic.

While believers and nonbelievers were debating, a large volume of experimental and theoretical studies was published, a result of a relentless effort of many groups around the world. Quasi-periodic materials have developed into an exciting interdisciplinary science.

This talk will outline the discovery of QCs and describe the important role of electron microscopy as an enabling discovery tool.

1. D. Shechtman, I. Blech, Met. Trans. **16A** (1985), p. 1005-1012.
2. D. Shechtman, I. Blech, D. Gratias, J. W. Cahn, Phys. Rev. Lett. **53** (1984), p. 1951-1953.

Tutorial lectures

T-01 – T-06

Aperiodic order in equilibrium systems

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We discuss the nature of aperiodically ordered systems, in terms of their dynamical spectrum and their diffraction spectrum, and compare those descriptions.

We discuss how aperiodic order can arise in ground states and Gibbs states of lattice models. Moreover we discuss how aperiodically ordered systems can provide examples of types of order expected in disordered systems, such as (spin) glasses.

Fusion: a general framework for hierarchical tilings

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One well studied way to construct quasicrystalline tilings is via inflate-and-subdivide (a.k.a. substitution) rules. These produce self-similar tilings, of which the Penrose, octagonal, and pinwheel tilings are famous examples. We present a different model for generating hierarchical tilings we call "fusion rules". Inflate-and-subdivide rules are a special case of fusion rules, but general fusion rules allow the composition rules to change from level to level. Spectral, dynamical, and topological results will be discussed that parallel those known for self-similar tilings.

Recent Progress in Mathematical Diffraction

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Keywords: diffraction, order, model sets

Diffraction methods continue to provide the main tool for the structure analysis of solids. The corresponding inverse problem of determining a structure from its diffraction pattern is difficult and, in general, does not define a structure uniquely.

Kinematic diffraction, which is an approximation that is reasonable for X-ray diffraction where multiple scattering effects can be neglected, is well suited for a mathematical approach via measures. Measures provide a natural mathematical concept to quantify the distribution of matter in space as well as the distribution of scattering intensity. This approach has substantially been developed since the discovery of quasicrystals required an extension of the methods used to compute the diffraction of periodic crystals.

The need for further insight emerged from the question of which distributions of matter, beyond perfectly periodic crystals, lead to pure point diffraction patterns, hence to diffraction patterns comprising sharp Bragg peaks only. More recently, it has become apparent that one also has to study continuous diffraction in more detail, with a careful analysis of the different types of diffuse scattering involved.

In this tutorial review, we summarise key results, putting particular emphasis on the analysis of non-periodic structures. Following the presentation in our recent review articles [1,2], general results are introduced and discussed on the basis of various characteristic examples, with minimal use of formal arguments or proofs. A systematic, and more rigorous, development of the theory (including lots of references) can be found in [3].

1. M. Baake and U. Grimm, “Mathematical diffraction of aperiodic structures”, Chem. Soc. Rev. **41** (2012) p. 6821 – 6843; arXiv:1205.3633.
2. M. Baake and U. Grimm, “Kinematic diffraction from a mathematical viewpoint”, Z. Kristallogr. **226** (2011) p. 711 – 725; arXiv:1105.0095.
3. M. Baake and U. Grimm, “Aperiodic Order: A Mathematical Invitation” (Cambridge University Press, Cambridge), in press.

Symmetry, excitations, and defects in quasicrystals

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Keywords: long-range order, indistinguishability, symmetry, point groups, dislocations, phasons

The discovery of quasicrystals has changed our view of some of the most basic notions related to the condensed state of matter, leading to a new underlying paradigm for the notion of a crystal as a solid with long-range positional order [1]. This paradigm shift brought about a new fundamental understanding of the basic characteristics of a crystal – its symmetry, its elementary excitations, and its typical defects [2]. Before we knew about quasicrystals, it was believed that crystals break the continuous translation and rotation symmetries of the liquid-phase into a discrete lattice of translations, and a finite point group of rotations. Quasicrystals, on the other hand, possess no such symmetries – there are no translations, nor, in general, are there any rotations, leaving them invariant. Does this imply that no symmetry is left, or that the meaning of symmetry should be revised? Without an underlying lattice, can we describe the elementary excitations? Can we even talk about dislocations without a lattice? If so, what are they like? How can we characterize them?

In this tutorial I shall review these and other notions, related to the symmetry-breaking transition from a liquid to a crystal, using the notion of *indistinguishability*, which was introduced many years ago by Rokhsar, Wright, and Mermin [3,4]. This will allow me to provide some physical and geometric intuition, while avoiding the formal use of abstract high-dimensional spaces.

The author acknowledges support from the Israel Science Foundation through Grant No. 556/10.

1. R. Lifshitz, *What is a crystal?* Z. Kristallogr. **222** (2007), p. 313.
2. R. Lifshitz, *Symmetry breaking and order in the age of quasicrystals*, Isr. J. Chem. **51** (2011), p. 1156.
3. D. S. Rokhsar, N. D. Mermin, D. C. Wright, Phys. Rev. B **35** (1987), p. 5487.
4. D. S. Rokhsar, D. C. Wright, N. D. Mermin, Acta Crystallogr. A **44** (1988), p. 197.

Valence Electrons and Bonding in Quasicrystals

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Keywords: electronic structure, covalent bond, Zintl compound

Quasicrystals (QCs) are long-range ordered materials with rotational symmetry incompatible with translational one. Natural questions arising from such aperiodic ordered systems are those concerning motion of quantum particles, such as electrons. Electronic structures of QCs have drawn much attention from the very beginning and been studied from two different points of view. First, quantum-mechanical motion of particles in a quasiperiodic potential is of special interest. Numerical and analytical studies have been done on wave functions and eigenvalue spectra for tight-binding models on Penrose lattice and others. The second point of view concerns the electronic structures of real materials [1]. Questions to be answered are why alloy phases with such complicated structures are stabilized, what novel physical properties are expected in such non-periodic systems, and so on. We shall review current understandings on electronic structures and stabilization mechanism, based on the *ab initio* calculation of electronic structures of QC-related compounds.

The Hume-Rothery (HR) idea, as the unique general theory predicting phase stability of intermetallic compounds, has been applied widely to various systems, in particular, to compounds with structural complexity including QCs. In the HR mechanism, the Brillouin-zone and Fermi-sphere interaction, which was based on a nearly-free electron picture, plays a vital role. Meanwhile, it turned out that the covalent nature of electronic states, which seems more nicely described in a tight-binding picture, is more essential in some intermetallic compounds. Recently, we reported for Al-Li compound, which is related to so-called Bergmann-type QCs, that a combination of Al and Li leads to a potential landscape for electrons favoring covalent bonding between Al's and hence the electronic stabilization [2]. A similar bond formation in Bergman Al-Li compound is realized in so-called Zintl compound, which is a compound of elements with very different electro-negativities. In this lecture, we try to emphasize how chemistry of constituent elements leads to phase stability of QC-related compounds. After a brief introduction of traditional idea on the stabilization mechanism based on the HR concept, we shall discuss chemical bonding and hybridization effects in QC-related compounds. Similarity with the Zintl phases will be emphasized for some QC-related compounds.

1. Y. Ishii and T. Fujiwara, in “Quasicrystals”, ed. T. Fujiwara and Y. Ishii (Elsevier, Amesterdam) (2008), p.171-208.
2. K. Nozawa and Y. Ishii, Phys. Rev. Lett. **104** (2010), p. 226406.

Chemical bonding in intermetallic compounds

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Keywords: intermetallic compound, chemical bonding, Zintl concept, electron localizability

Intermetallic compounds in general and complex metallic phases in particular show physical properties often interesting for applications and serve frequently as important components for materials design. An attempt to find a direct causal link between the crystal structure and the chemical bonding for this group of inorganic substances visualizes a lack of reliable information especially on the atomic interactions [1].

Chemical bonding in intermetallic compounds and its relation to the crystal structure is a rather open question. In rare cases, in a system possesses enough electrons, all the necessary bonds can be realized as two-centre-two-electron (2c-2e) bonds: for crystal structures in which all atoms are tetrahedrally coordinated, one needs four electrons per atom to form all the existing bonds. Reducing the number of electrons makes it impossible to form all bonds as 2c-2e interactions.

The way to 'save' electrons in such cases is described by the Zintl-Klemm concept [2,3] – the most efficient model characterizing the interplay between chemical composition and crystal structure of intermetallic compounds. Keeping the system of 2e-2c bonds as a starting point, further reduced number of electrons requires multi-centre bonding or softening of the 2e requirement for an optimal description. Following the considerations above, further depletion of the electronic system consequently leads to the formation of multicentre bonds with more than three centres per bond as discussed in the Wade-Mingos model. In terms of the electronic band structure, one speaks here about the formation and filling of the bands. The stabilization of the structural motif is attributed to the Hume-Rothery mechanism via interaction of the Fermi surface with the Brillouine zone [4,5]. This model yields electron numbers which are sufficient for the stabilization of some structural patterns based on the close or closest packing of spheres.

Electron localizability approach (ELI/ED) opens access to the bond definition in real space, gives a possibility of Zintl-like electron counting for large group of intermetallic phases and allows revealing of the – on first glance unexpected - relation between organometallic and intermetallic compounds [6,7].

1. Yu. Grin in "Comprehensive Inorganic Chemistry II", Elsevier (in print).
2. W. Klemm, E. Bussman, Z. Anorg. Allg. Chem. **319** (1963) p. 297.
3. H. Schäfer, B. Eisenmann, W. Muller, Angew. Chem. **85** (1973), p. 742.
4. W. Hume-Rothery in "Materials Science and Engineering", McGraw Hill, NY (1967).
5. U. Mizutani, "Hume-Rothery Rules for Complex Metallic Alloys", T&F, London (2010).
6. F. R. Wagner *et al.* Chem. Eur. J. **108** (2007), p. 5724.
7. M. V. Butovski *et al.*, Nature Chem. **2** (2010), p. 741.

Invited Talks

I-01 – I-24

In-situ HRTEM observations of growth process of decagonal quasicrystals

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Keywords: growth, high-resolution transmission electron microscopy, decagonal quasicrystals, Al-Ni-Co

Quasicrystals possess quasiperiodicity, where the structure cannot be described simply by the repetition of a unit cell like conventional crystals. This fact raises the question of how quasicrystals grow, i.e., what physical mechanism makes the growth of quasicrystals possible. While crystals can grow by copying a unit cell via local atomic interactions, nonlocal structural information seems to be required in the growth of quasicrystals. This problem has attracted much attention ever since the first discovery of a quasicrystal in 1984, and several theoretical growth models [1-3] have been proposed. However, no experimental studies have so far been reported, and it is still unclear whether these theoretical growth models apply to the real quasicrystals. In the present study, we have conducted in-situ high-temperature electron microscopic (HRTEM) observations of the growth process of decagonal quasicrystals to elucidate the growth mechanism.

The growth process of a decagonal quasicrystal of $Al_{70.8}Ni_{19.7}Co_{9.5}$ was observed by HRTEM in the temperature range 1073-1173K. Tiling patterns with the edge length of about 2nm were constructed from a series of the HRTEM images. They were analysed in the framework of the projection method. Here, we followed the procedures in our previous work [4]. These observations and analyses showed the followings. Newly attached tiles were not necessarily consistent with the tiles that had already been constructed. After a few tens of seconds, the newly attached tiles repaired themselves to become consistent with the already-constructed tiles by a series of phason flips.

1. G. Y. Onoda, P. J. Steinhardt, D.P. DiVincenzo and J. E. S. Socolar, Phys. Rev. Lett. **60** (1988), p. 2653.
2. A. S. Keys and S. C. Glotzer, Phys. Rev. Lett. **99** (2007), p. 235503.
3. H-C. Jeong, Phys. Rev. Lett. **98** (2007), p. 135501.
4. K. Edagawa, K. Suzuki and S. Takeuchi, Phys. Rev. Lett. **85** (2000), p. 1674.

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Discovery of quasicrystalline thin film formation from perovskites

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Keywords: 2D quasicrystal, $BaTiO_3$, thin film, dodecagonal, perovskites

Perovskite oxides with their cubic or pseudo-cubic crystal structure are a fascinating class of materials which contains insulators, metals, semiconductors, and superconductors with nearly identical lattice parameters. Some are magnetically ordered in various structures and many are catalytically active. The properties of individual perovskites can be altered in a controlled fashion by substitution of ions, by application of strain, or incorporation of defects. In addition, due to the structural equivalence perovskites with different properties can be combined in multilayer systems to produce functional materials with unique properties [1].

However here we report on an interface-driven quasicrystal (QC) thin film formation from the classical perovskite oxide $BaTiO_3$ on a Pt(111) substrate. $BaTiO_3$ is the most studied ferroelectric perovskite oxide which has an easily accessible ferroelectric to paraelectric phase transition at 400 K. Due to matching lattice conditions it can be grown epitaxially on selected metal substrates. On Pt(001) and on Pt(111) periodic thin films of either $BaTiO_3(100)$ or $BaTiO_3(111)$ have been grown depending on substrate orientation and preparation conditions [2-4]. As we demonstrate here, alternatively an aperiodic quasicrystalline structure can be formed by annealing an initially 1.4 nm thick $BaTiO_3$ film on Pt(111). Upon annealing at 1250 K in UHV the material restructures in a 2D quasicrystalline wetting layer in between a few thicker $BaTiO_3(111)$ islands.

Surface sensitive electron diffraction (LEED) shows a bright and sharp pattern with dodecagonal symmetry. High-resolution scanning tunneling microscopy (STM) images reveal that the surface structure is composed by an arrangement of quadratic and triangular building blocks as they are the typical elements of a 2D quasicrystalline lattice with dodecagonal symmetry. The Fourier transform of the high-resolution STM data is in excellent agreement with the measured LEED data. Our analysis is strengthened by by the powerful combination of both techniques. The FFT is used as the key for correlating the local structural information of STM with the global structural information as derived from LEED.

1. I. Vrejoiu, M. Alexe, D. Hesse, and U. Gösele, Adv. Funct. Mater. **18** (2008), p. 3892.
2. S. Förster and W. Widdra, Surface Science **604** (2010), p. 2163.
3. S. Förster, M. Huth, K.-M. Schindler, and W. Widdra, J. Chem. Phys. **135** (2011), p. 104701.
4. S. Förster, K. Meinel, K.-M. Schindler, and W. Widdra, Surf. & Interf. Anal. **44** (2012), p. 628.

Quasicrystal and its periodic approximant – do they fit to each other?
Epitaxial crystal growth experiments in the Al-Co-Ni system

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Keywords: Al-Co-Ni, Czochralski, epitaxy

As soon as large enough quasicrystals became available, the deposition of thin layers of various elements that usually crystallize in periodic structures was investigated on crystallographically well-defined quasicrystalline substrates. The main focus of these studies has been the question whether or not it is possible to force monolayers or even multiple layers of periodic phases into a quasiperiodic structure [1].

In general, epitaxy is defined as the oriented growth of one crystal onto another and a lattice mismatch of less then 5 % is regarded as a prerequisite. If the unit cells of the crystals do not fit to each other, no epitaxial growth is possible and the appropriate phases will be considered as incommensurable. Since quasicrystals are aperiodic and therefore no unit cell can be defined in the direct space, according to the classical definition of epitaxy an epitaxial intergrowth between a periodic phase and a quasicrystal should not be possible.

A more general definition of epitaxy has been proposed by Franke et al. [2] based on the concept of locking into registry at the interface. Accordingly, the essence of epitaxy is not the existence of a common interface unit cell, but whether the interface energy reaches a local minimum concerning lateral shifts of the crystals with respect to each other [3]. This can be achieved, if the interface of the two half-crystals has at least two projected non-collinear reciprocal lattice vectors in common [2]. This definition can be applied to all crystals including quasicrystals.

Using the Czochralski method we investigate if it is possible to grow a (bulk) quasicrystal onto a periodic seed (approximant) – or the other way around. For these experiments the system Al-Co-Ni has been chosen because the decagonal quasicrystal and its monoclinic approximant Y-$Al_{13}(Co,Ni)_4$ can be grown from Al-rich melts of only slightly changed composition. First experiments will be presented and discussed.

1. V. Fournée, J. Ledieu, M. Shimoda, M. Krajčí, H.-R. Sharma, R. McGrath, Isr. J. Chem. **51** (2011), p. 1314 – 1325.
2. K. J. Franke, P. Gille, K.-H. Rieder, W. Theis, Physical Review Letters **99** (2007), p. 036103.
3. A. Zangwill in “Physics at Surfaces”, (Cambridge University Press, Cambridge) (1990).

Soft quasicrystals with 12- and 18-fold rotational symmetry

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Keywords: soft quasicrystals, neutron scattering, X-ray scattering, polymers

Over the past decade quasicrystalline order has been reported in many soft-matter systems. We have found quasicrystals with 12- and 18-fold rotational symmetry (Q12, Q18) in aqueous solutions of polymer micelles, which are particularly soft systems. [1] Transitions from an FCC phase to Q12 and subsequently to Q18 upon cooling could be followed by time-resolved small-angle X-ray and neutron scattering. Recent investigations using cryo-scanning electron microscopy indicate that the micelles are arranged in the form of mosaic two-length scale quasicrystals, which have recently been identified by Dotera *et al.* using Monte-Carlo simulations of particles with square-shoulder repulsion. The results indicate that these soft systems are special types of quasicrystals having a direct relation to the hexatic phase observed in smectic liquid crystals.

1. S. Fischer, A. Exner, K. Zielske, J. Perlich, P. Lindner, S. Deloudi, W. Steurer and S. Förster, Proc. Natl. Acad. Sci. **108** (2011), p. 1810.

Beyond metallic quasicrystals: The colloidal road in experiments and simulations

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Keywords: quasicrystals, colloids, computer simulations

Despite many efforts in recent years no metallic quasicrystals have been discovered with symmetries other than icosahedral, decagonal and dodecagonal.

Colloids on the other hand provide toy systems which can be modified in many different ways: their repulsive interaction can be varied by adding charges and salt; the interference of laser beams can lead to an external optical potential that mimics the influence of a quasiperiodic surface with more symmetries realizable than enumerated above.

Experimental studies have revealed new quasiperiodic stripe phases formed in decagonal and tetradecagonal quasicrystals as a function of density and strength of the laser field. Recently, kinks and antikinks formation has been observed in friction studies on quasicrystalline surfaces. Unfortunately, experimental studies are restricted in parameter space and do not allow to study arbitrary symmetries due to the large number of laser beam phases that must be controlled.

Simulation studies, however, have been able to confirm the experimental structures and extend the results to a much larger parameter space and to further symmetries. Thus it was shown that stripe phases occur in all cases and why they are energetically advantageous.

Dynamical simulation studies deal with phason flips and diffusion in the stripe and quasicrystal phases. Phason flips in the stripe phases could be studied by applying continuous drifts and gradients to the laser field. They stabilize the structures and reduce the number of defects.

With the help of brownian dynamics the behavior of colloids moving in quasiperiodic fields has been analyzed numerically in detail. Flips of particle rows have been observed if the particles are non-interacting. Depending on the direction and velocity of the changing laser field single particles are found moving in phase or in antiphase direction. A classification of the different regimes will be presented. In the case of repellant particles a consecutive decay of the structure is observed for an increasing laser potential shift since the particles can no longer follow the potential minima. This leads to phason drift-induced melting.

Finally the results are summarized and related to the non-metallic quasicrystals, for example phononic systems or soft-matter quasicrystals.

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Al-based F-type icosahedral alloys
~ a novel view from X-ray crystallography ~

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Keywords: F-type icosahedral quasicrystals, approximants, canonical cell tilings

Amongst the unsolved challenges in quasicrystal research remains the determination of atomic arrangements in Al-based F-type icosahedral quasicrystals, e.g., i-$Al_{70}Pd_{20}Mn_{10}$ [1] and i-$Al_{65}Cu_{20}Fe_{15}$ [2]. These quasicrystals were discovered the earliest of all the families of thermodynamically stable quasicrystals and have so far been the subject of a number of publications, aiming at their structures, properties and applications. Still, the current state of understanding of their atomic arrangements is largely speculative, leaving almost no consensus among the researchers.

Generally speaking, a common strategy to solve the structure of an icosahedral quasicrystal rests on two steps: Step 1 is a crystal structure analysis, which usually uses single-crystal X-ray diffraction, of an approximant crystal to clarify the fundamental building units (or clusters) and the rules for their local packing. Step 2 is a geometrical modelling of the arrangement of the clusters to determine the long-range quasiperiodic ordering of the structure. Although the success of this strategy in solving the structure of the binary icosahedral quasicrystal, i-$Cd_{5.7}Yb$ [3], is still fresh in memory, in the case of the Al-based quasicrystals the lack of highly ordered approximants has long prevented us (at Step 1) from dispelling uncertainties about their local building units.

Now a revival of this old puzzle is seen after our discovery of a new Al-Pd-Cr-Fe compound which is a cubic approximant (lattice constant ~ 40 Å) to i-$Al_{70}Pd_{20}Mn_{10}$ [4]. The quality of our sample allowed a fine structure analysis using single-crystal X-ray diffraction, whereby a full description of the crystal structure was attained. The crystal has two kinds of interpenetrating clusters, called pseudo-Mackay and mini-Bergman clusters, whose centres define the vertices of a canonical cell tiling. Generalizing these results gives a universal framework for describing a wide range of complex crystal structures. A recent survey of the alloy system Al-Pd-Mo-Fe has culminated in the discovery of yet another approximant crystal with an even larger unit cell. This new crystal could provide further evidence that the present framework is applicable to a broad class of complex structures including the quasicrystals.

1. A. P. Tsai, A. Inoue, Y. Yokoyama and T. Masumoto, Mater. Trans. JIM **31** (1990), p. 98.
2. A. P. Tsai, A. Inoue and T. Masumoto, Jpn. J. Appl. Phys. **26** (1987), p. L1505.
3. H. Takakura, C. P. Gomez, A. Yamamoto, M. de Boissieu & A. P. Tsai, Nat. Mater. **6** (2007), p. 58.
4. N. Fujita, H. Takano, A. Yamamoto and A. P. Tsai, Acta Cryst. A **69** (2013), p. 322.

Gold's Impact on the Occurrence of Fivefold and Pseudo-fivefold Symmetry in Polar Intermetallics

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Recent exploratory syntheses of polar intermetallic compounds containing gold have established this element's extraordinary ability to stabilize complex networks of icosahedra, dodecahedra, pentagonal bipyramids, as well as first sodium-containing, Bergman-type, icosahedral quasicrystal. Gold's behavior in this metal-rich chemistry arises from its high electronegativity among metals, the significant relativistic effects on its valence orbitals, its low valence *s*, *p* electron count, as well as its filled 5*d* orbitals. This presentation will summarize our group's recent systematic exploration of ternary alkali or alkaline earth metal–Au–Ga systems, and a discussion of a new quasicrystal in the Na–Au–Ga system.

Thermal rectification in icosahedral quasicrystals

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Keywords: thermal diode, electron thermal conductivity, pseudogap, aperiodic structure

Thermal rectification, which means the direction dependent heat flow, is observable in bulk composites consisting of two materials possessing different temperature dependence of thermal conductivity. [1,2] The thermal conductivity of one of the constituent materials in such composites increases with increasing temperature while that of the other decreases. Although the mechanism of bulk thermal rectifier is very simple, it is fairly difficult to find materials possessing thermal conductivity drastically increasing with increasing temperature at high temperatures above 300 K because lattice thermal conductivity moderately decreases with temperature and electron thermal conductivity generally has less obvious temperature dependence at high temperatures.

We realized that the thermal conductivity unusually increases with increasing temperature even above 300K, provided that the material is characterized by the narrow energy gap or pseudogap of a few hundred meV in width together with aperiodic structure. These conditions lead to a very small lattice thermal conductivity and the unusual electron thermal conductivity, the magnitude of which is much larger than the value expected from the Wiedemann-Franz law. We also realized that the Al-based icosahedral quasicrystal is one of the best materials satisfying the required conditions.

By carefully considering the mechanism leading to the large evolution of electron thermal conductivity at high temperatures, we selected Al-Cu-Fe icosahedral quasicrystal as the best component of thermal rectifier. We succeed in finding the composition where the thermal conductivity at 1000 K exceeds 9 times larger value of room temperature thermal conductivity. [3] The prepared Al-Cu-Fe icosahedral quasicrystal was directly connected with the materials possessing a thermal conductivity decreasing with increasing temperature: (a) a insulator of a high Debye temperature, (b) a material characterized by non-harmonic oscillation of atoms, or (c) a material possessing an order-disorder phase transition. As a result, a large thermal rectification ratio $TRR = j_{q1} / j_{q2} > 1.6$ was observed for all cases at high temperatures above 300 K. We calculate *TRR* for some different conditions, and found that the calculated values showed good consistency with the experimental ones. The calculation let us also realize that we may observe much large *TRR* exceeding 2.4 to be used in practical applications.

1. M. Peyrard, Europhys Letters **76** (2006), p. 49.
2. N. A. Roberts, D. G. Walker, International Journal of Thermal Sciences **50** (2011), p. 648.
3. T. Takeuchi, Hiroki Goto, R. Nakayama, Y. Terazawa, K. Ogawa, A. Yamamoto, T. Itoh, M. Mikami, Journal of Applied Physics **111** (2012), p. 093517.

Tiling space of Taylor-Socolar tilings

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Keyword: Taylor-Socolar tiling, quasicrystals, parity tiling

Taylor-Socolar tiling has been introduced as an aperiodic mono-tile tiling. We give a model set description for this tiling and get the property of quasicrystal structure.

Identifying all the rotated versions of tiles in the Taylor-Socolar tiling with white hexagonal tiles and all the reflected versions of tiles with gray hexagonal tiles, we can make a parity tiling from the Taylor-Socolar tiling. It turns out that Taylor-Socolar tiling is mutually locally derivable from this parity tiling, which forgets all the decorations on the tiles.

We also look at a tiling space each tiling of which is locally indistinguishable from the Taylor-Socolar tiling and study the structure of this space through well-known p-adic space.

Topological Bragg peaks and how they characterise tilings

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A substantial part of the study of tilings is based on the study of their associated dynamical system. For instance, Bragg peaks in the diffraction show up as eigenvalues of the dynamical system. But more can be said if we concentrate on the topology. We will discuss how the class of repetitive Meyer tilings and the class of cut & project tilings can be characterised, up to conjugacy, by the topological spectrum of the dynamical system.

Quasicrystals and crystals tiled with pentagons in water and silicon

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Bulk water is known to form a wealth of ice polymorphs and two distinct amorphous phases. Less is known of the structures that confined and interfacial water can adopt, and whether there is a correspondence between the structures and phase diagrams of water in bulk and in confinement. In this talk I will discuss the results of our studies of the phase behavior of a water bilayer confined between two non-hydrogen bonding walls and show that a water bilayer also presents rich polymorphism, including an ice crystal fully tiled by pentagons and a quasicrystal, the first ever reported for water. The water quasicrystal and the ice polymorph tiled with pentagons are not templated by the confining surfaces. This demonstrates that these novel phases are intrinsically favored in bilayer water and suggests that these structures could be relevant not only for confined water but also for the wetting and properties of water at interfaces. I will also discuss the relationship between the water and silicon phase diagrams, in bulk and in confinement, and our prediction of a marginally stable silicon bilayer quasicrystal.

Phase transitions in organic aperiodic composites

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Keywords: phase transitions, critical phenomena, sliding modes

Aperiodic crystals have the property to possess long range order without translational symmetry. These crystals are described within the formalism of superspace crystallography. In this talk, we will focus on symmetry breakings which take place in such crystallographic superspace groups, considering the prototype family of *n*-alkane/urea. Studies performed by diffraction using neutron and synchrotron sources reveal multiple structural solutions implying or not changes of the dimension of the superspace [1,2]. Once the characterization of the order parameter and of the symmetry breaking is done, we will present the critical pretransitionnal phenomena associated to phase transitions of group/subgroup types [3]. Coherent neutron scattering and inelastic X-ray scattering allow a dynamical analysis of different kind of excitations in these materials (phonons, phasons) [4]. The inclusion compounds with short guest molecules (alkane C_nH_{2n+2}, n varying from 7 to 13) show at room temperature unidimensional "liquid-like" phases. The dynamical disorder along the incommensurate direction of these materials generates new structural solutions at low temperature (intermodulated monoclinic composite, commensurate lock-in) [5].

1. B. Toudic, P. Garcia, C. Odin, et al., Science **319** (2008), p. 69.
2. B. Toudic, P. Rabiller, L. Bourgeois, et al., Europhys. Lett. **93** (2011), p. 16003.
3. C. Mariette, L. Guérin, P. Rabiller, et al., Phys. Rev. **B87** (2013), p. 104101.
4. B. Toudic, R. Lefort, C. Ecolivet, et al., Phys. Rev. Lett. **107** (2011), p. 205502.
5. C. Mariette, M. Huard, P. Rabiller, et al., J. Chem. Phys. **136** (2012), p. 104507

Intermetallic structures: Constituents, Compositions, and Complexity

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Keywords: intermetallic phases; crystal structure statistics; complex intermetallics

The structures of intermetallics are generally regarded as being simple and belonging to a few easily-understood structure types. However, throughout the different intermetallic and crystal systems, numerous complex structures can be found that contain hundreds or thousands of atoms in one unit cell, amounting up to the record structure in the Al–Cu–Ta-system with more than 23 000 atoms in one unit cell [1]. Among the most complex structures, mainly highly symmetric compounds of very diverse intermetallic constitutions can be found [2].

With respect to translational and point-symmetry, the occurrence of complex intermetallics resembles that of all intermetallic phases [3]. Now we are examining the distribution of different intermetallic compounds over the compositional space. For this we extract all structural data on intermetallics contained in a database for analysis [4]. The fact that preferred compositions occur at ratios of small integer numbers is broadly accepted and closely resembles the constitution of molecules. But what is the mechanism behind more intricate compositions: are the respective "metallic molecules" simply larger? Is it actually possible to identify the respective building units within the metal structure? How do coordination polyhedra and clusters in general evolve over a compositional range?

Always bearing in mind the characteristics of complex intermetallics, we will try to approach these questions and uncover systematics within the realm of the structure formation of intermetallic compounds. Ultimately, nothing less than the ability to purposefully search for desired structures containing specific elements could be the aim of such a knowledge basis, i.e. "materials design" in the form of an anticipation of functional structures and – ideally – their subsequent synthesis.

1. T. Weber, J. Dshemuchadse, M. Kobas, M. Conrad, B. Harbrecht, W. Steurer, Acta Cryst. B **65** (2009), p. 308-317.
2. J. Dshemuchadse, D. Y. Jung, W. Steurer, Acta Cryst. B **67** (2011), p. 269-292.
3. J. Dshemuchadse, W. Steurer, *MRS Proceedings* **1517** (2012).
4. P. Villars, K. Cenzual, *Pearson's Crystal Data*, Release 2012/13.

Oxidation and Passive oxide layers characterization on Al-Cr-Fe Complex Metallic Alloys

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Al-Cr-Fe Complex Metallic Alloys (CMA) are Al- based intermetallic crystalline approximants of quasicrystalline phases that are characterised by large unit cells and very complex structures (hundreds atoms/unit cell). These materials exhibit high corrosion resistance for pHs ranging from 0 to 14[1,2]. This remarkable corrosion behaviour can be combined with their additional low adhesion, low friction coefficient and low reflectivity and exploited in resistant "multifunctional" coatings. However, the influence of ageing (in air or in electrolyte) of the nm-thick surface oxide in relation with the surface properties of Al-Cr-Fe CMA still needs to be fundamentally understood. Recently, single phase large grain single- or poly-crystals of the orthorhombic $Al_{80}Cr_{15}Fe_5$ (unit cell dimensions a = 12.5006 Å, b = 12.6172 Å and c = 30.6518 Å and 306 atoms) were prepared and their electrochemical behaviour characterised.

During this talk, the oxidation mechanisms of the alloy in different environments (UHV, air) will be reported[3]. Electrochemical and photoelectrochemical characterisations of these alloys will be presented and discussed. Moreover, results on Hard X- Ray Photoelectron Spectroscopy (HAXPES) characterization of the nm- thick passivation oxi-hydroxide produced during electrochemical treatment (potentiostatic anodic polarisation) will be introduced. HAXPES is a *non-destructive* synchrotron based technique which is particularly suited to study buried interfaces.

The HAXPES technique allowed the study of the in-depth composition gradients of the protecting passive oxide layer (6 to10 nm –thick) together with its metal/oxide interface difficult to be assessed by conventional XPS. Higher excitation energies from 3 to 10 keV (experiments at ID32 beamline of ESRF) allowed investigating the alloy composition under the oxide to formulate the oxidation mechanisms.

Molecular films with long-range quasiperiodic structures.

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Keywords: quasicrystalline surfaces, thin films, molecules.

When prepared in ultrahigh vacuum conditions, quasicrystal surfaces present specific planes of the bulk structure as surface terminations [1]. These surface planes show a highly complex potential energy landscape for adsorbates and it was expected that such surface planes might be used as templates to grow novel quasiperiodic structures. This has been realized for a few systems, mainly soft metals (Pb, Bi or Sb) and rare gases (Xe) [2]. In all these systems, only the first wetting layer is quasiperiodic. At larger coverages, the adsorbates tend to recover their crystalline structures.

Other attempts have focused on the possibility to enforce a quasiperiodic structure in molecular films deposited on the same surfaces. Molecules are bigger entities than metal adatoms and they could potentially self-assemble into a quasiperiodic structure if only a subset of quasilattice sites act as trap sites. This hypothesis has been tested using mainly C_{60} fullerene molecules and more recently using pentacene $C_{22}H_{14}$ [3-4]. However it has been found that both molecules strongly bond to the surface which leads to a disordered structure, except at very low coverages where indications of preferred adsorption sites were reported [3].

In this presentation, we will show that beautiful molecular films with long-range quasiperiodic order can actually be formed on different quasicrystalline surfaces, including the 10-fold surfaces of AlCuCo and AlNiCo decagonal phases and the 5-fold surfaces of AlPdMn and AlCuFe icosahedral phases. The growth and the structure of these films are investigated by scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). The diffraction patterns are drastically improved after the formation of the molecular films compared to the clean surfaces, especially at low electron beam energy. The structure of the completed films can be understood by molecular decoration of the tilings used to describe the clean surfaces. We will also report on the electronic structure of the films by photoemission and scanning tunneling spectroscopies.

1. P. A. Thiel, Ann. Rev. Phys. Chem. **59** (2008) p. 129.
2. V. Fournée, J. Ledieu, M. Shimoda, M. Krajčí, H. R. Sharma, R. McGrath, Isr. J. of Chem. **51** (2011) p. 1326.
3. J. Ledieu, C. A. Muryn, G. Thornton, R. D. Diehl, T.A. Lograsso, D. W. Delaney, R. McGrath, Surf. Sci. **472** (2001) p. 89.
4. K. M. Young, J. A. Smerdon, H. R. Sharma, M. Lahti, K. Pussi, R. McGrath, Phys. Rev. B **87** (2013) p. 085407.

Calculating electronic structure of complex disordered alloys to study their magnetic and transport behaviours

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Keywords: electronic structure, disorder, thermoelectricity, crystal stability

Electronic structure calculations of some complex intermetallic alloys are performed to enlighten their electronic, magnetic and transport properties, which are strongly governed by chemical disorder. The Green function multiply scattering formalism in the Korringa-Kohn-Rostoker (KKR) method [1,2] with new developments [3] was implemented to determine accurately and unambiguously electron dispersion curves in complex periodic systems, even with large unit cell. This methodology combined with the coherent potential approximation (CPA), which allows to account for chemical disorder in multi-atom alloys, is then applied to investigate various classes of materials.

We present the results of electron transport properties calculations based on the complex energy Fermi surface analysis and Boltzmann transport theory in thermoelectric materials [4], where the influence of doping and alloying is discussed in details. We emphasize that *ab initio* modelling reasonably predicts temperature and carrier concentration range to optimize their thermoelectric energy conversion.

Furthermore, an interplay among crystal stability, electronic and magnetic properties is investigated in Fe-based σ-phases, which are regarded as good approximants of quasicrystals, due to their complex crystallographic structure and high coordination numbers. We show the electronic structure and formation energy calculations appear really helpful to interpret hyperfine interactions studied by Mossbauer spectroscopy [5].

Finally, results of the fully charge and spin selfconsistent KKR-CPA calculations of exemplary high entropy alloys are discussed. Despite the fact that these alloys consist of more than five different elements, they surprisingly crystallize in simple bcc or fcc structures with random distribution of atoms on the same crystallographic site. The relative crystal stability in relation to the evolution of their electronic and magnetic properties is theoretically studied.

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1. A. Bansil, S. Kaprzyk, P. E. Mijnarends and J. Tobola, Phys. Rev. B **60** (1999), 13396.
2. T. Stopa, S. Kaprzyk and J. Tobola, J. Phys.: Condens. Matter **16** (2004), 4921
3. S. Kaprzyk, Comp. Phys. Comm. **183** (2012), 347.
4. K. Kutorasinski, J. Tobola and S. Kaprzyk Phys. Rev. B **81** (2010), 174203.
5. J. Cieslak, J. Tobola and S. Dubiel, Phys. Rev. B **87** (2013), 195205.

Intrinsic anisotropic magnetic, electrical and thermal transport properties of *d*-Al-Co-Ni decagonal quasicrystals

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Keywords: decagonal quasicrystals, anisotropy, magnetism, physical properties

To address the questions on the anisotropy of bulk physical properties of decagonal quasicrystals and the intrinsic physical properties of the *d*-Al-Co-Ni phase, the anisotropic magnetic susceptibility, the electrical resistivity, the thermoelectric power, the Hall coefficient, and the thermal conductivity of a *d*-Al-Co-Ni single-grain sample of exceptional structural quality were investigated [1]. Superior structural order on the local scale of atomic clusters was confirmed by ^{27}Al NMR spectroscopy. The measurements were performed along the 10-fold periodic direction of the structure and along three specific crystallographic directions within the quasiperiodic plane, corresponding to the 2 and 2' twofold symmetry directions and their bisector. The specific heat, being a scalar quantity, was determined as well. The measurements of the second-rank bulk tensorial properties confirm the theoretical prediction that a solid of decagonal point group symmetry should exhibit isotropic physical properties within the quasiperiodic plane and anisotropy between the in-plane and the 10-fold directions. The *d*-Al-Co-Ni exhibits anisotropic diamagnetism with stronger diamagnetism for the magnetic field along the 10-fold direction. Electrical and thermal transport is metallic in the 10-fold direction but largely suppressed within the quasiperiodic plane, the main reason being the lack of translational periodicity that hinders the propagation of electrons and phonons in a nonperiodic structure. The third-rank Hall-coefficient tensor shows sign-reversal anisotropy related to the direction of the magnetic field when applied in the 10-fold direction or within the quasiperiodic plane. The observed anisotropy is not a peculiarity of quasicrystals but should be a general feature of solids with broken translational periodicity in two dimensions.

1. M. Bobnar, P. Jeglič, M. Klanjšek, Z. Jagličić, M. Wencka, P. Popčević, J. Ivkov, D. Stanić, A. Smontara, P. Gille and J. Dolinšek, Phys. Rev. B **85** (2012), p. 024205.

Tetrahedron dynamics in Tsai-type quasicrystals and their approximants

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Keywords: lattice dynamics, neutron scattering, simulation

The icosahedral quasicrystals (QC) i-AgZnSc and i-MgZnSc and the Zn_6Sc 1/1 approximant are built up from triacontahedral clusters, arranged on a non-periodic and a bcc lattice, respectively. These clusters evidence icosahedral symmetry, except for the innermost shell, which is a symmetry-breaking tetrahedron [1]. In the Sc_6Zn 1/1 approximant these tetrahedral shells are at the origin of the observed order-disorder phase transition during which they orient anti-parallel along the [110] direction of the cubic high temperature phase [2]. In the QC, on the other hand, no such transition is evidenced.

We present a combined experimental and simulation study of the tetrahedron disorder in the Zn_6Sc 1/1 approximant and the quasicrystalline phases i-AgZnSc and i-MgZnSc. For these systems neutron scattering experiments strongly indicate a dynamic tetrahedron disorder with tetrahedra "jumping" between different orientations. These experimental findings are interpreted by molecular dynamics simulations, using oscillating pair potentials, indeed evidencing that the tetrahedra are exposed to constant reorientations on a picosecond timescale [3].

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1. M. de Boissieu *et al.*, Nature Materials, **6** (2007), p. 977.
2. T. Ishimasa *et al.*, Phil. Mag., **87 (**2008), p. 2887.
3. H. Euchner *et al.*, Journal Phys. Cond. Mat. **24** (2012), p. 415403.

Orientational interaction and ordering transitions of tetrahedra in the Cd_6Ca approximant

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Keywords: Cluster interaction, Structural transition, Simulation

The simplest (1/1 approximant) of *i*-CaCd is Cd_6Ca. At low temperature, the important degrees of freedom are the orientations of the tetrahedral Cd_4 inner shells of the Tsai clusters which sit on a bcc lattice and are known experimentally to have various ordering transitions. By constrained relaxations of neighboring clusters in a fixed environment of other clusters, we fitted the orientational pair interaction of first and second nearest neighbor cluster [1]. The interactions tend to be frustrated, giving multiple predicted phase transitions as a function of pressure and temperature. We characterize the (p,T) phase diagram and the nature of the ordering transitions.

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1. W. Choi, C. L. Henley, and M. Mihalkovic, preprint (http://arxiv.org/abs/1212.5583).

Localization, nonlinearity and topological phases in quasiperiodic photonic lattices

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Keywords: photonic quasicrystals, transport

The propagation of photons in photonic waveguide lattices is described by the same equations used to describe the propagation of electrons in atomic crystals. In a recent set of experiment we have studied the propagation of light in lattices with quasi-periodic modulations of various lattice parameters, creating a versatile playground for the study of the transport properties of quasiperiodic systems under various conditions.

In a first set of experiments we have observed the signature of a localization phase transition [1], predicted to occur already in one-dimension in golden-ratio incommensurate lattices (the Aubry-Andre model). In this case, all the photonic states of the system are transformed from being extended to being tightly localize at a singular value of the quasiperiodic modulation amplitude. As a result the transport properties of the lattice change, which we probe via wave-packet expansion measurements. In addition, our experimental setup enables us to introduce nonlinear interactions between the propagating waves, thus allowing us to compare experimentally the effect of nonlinear interactions before and after the localization transition.

In a different set of experiments combined with a theoretical study, we described and probed the topological properties of quasicrystals [2,3]. We observed topologically protected edge-states in quasi-periodic systems, measure a topological phase transition at the interface between two topologically in-equivalent quasi-periodic systems, and used the topological protection of the edge states to realize an adiabatic pump. We found an analytical connection between two families of quasi-periodic models – the incommensurate (Aubry-Andre) and the Fibonacci lattices [4], which we use to study the connection between the topological and the transport properties of these different quasi-periodic models.

1. Y. Lahini, R. Pugatch, F. Pozzi, M. Sorel, R. Morandotti, N. Davidson, Y. Silberberg, Phys. Rev. Lett. **103** (2009), 13901.
2. Y.E. Kraus, Y. Lahini, Z. Ringel, M. Verbin, O. Zilberberg, Phys. Rev. Lett. **109** (2012), 106402.
3. Y.E. Kraus, O. Zilberberg, Phys. Rev. Lett. **109** (2012), 116404.
4. M. Verbin, O. Zilberberg, Y.E. Kraus, Y. Lahini, Y. Silberberg, Phys. Rev. Lett. **110** (2013), 076403.

Quantum criticality in a magnetic Au-Al-Yb quasicrystal

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Keywords: Quantum Criticality, Magnetic Quasicrystal, Critical State

Quasicrystals are metallic alloys that possess long-range, aperiodic structures with diffraction symmetries forbidden to conventional crystals. Since the discovery of quasicrystals by Schechtman *et al.* at 1984, there has been considerable progress in resolving their geometric structure. For example, it is well known that the golden ratio of mathematics and art occurs over and over again in their crystal structure. Due to this quasi-periodicity, an unusual electronic state that is neither extended nor localized is expected; neither they are extended as in periodic crystals nor localized as in amorphous materials. However, such an unusual state has not yet been observed. The quasicrystal that we study here is a gold-aluminum-ytterbium alloy described as $Au_{51}Al_{34}Yb_{15}$ [1]. In the present study, we report the first observation of quantum ($T = 0$) critical phenomena of the Au-Al-Yb quasicrystal − the magnetic susceptibility and the electronic specific heat coefficient arising from strongly correlated $4f$ electrons of the Yb atoms diverge as $T \rightarrow 0$. Furthermore, we observe that this quantum critical phenomenon is robust against hydrostatic pressure. By contrast, there is no such divergence in a crystalline approximant $Au_{51}Al_{35}Yb_{14}$, a phase whose composition is close to that of the quasicrystal and whose unit cell has atomic decorations (i.e., icosahedral clusters of atoms) that look like the quasicrystal. We propose a peculiar quantum critical behaviour of the Au-Al-Yb quasicrystal to reflect this unusual state expected for quasicrystals. These results indicate that the quantum criticality is associated with the unique electronic state of quasicrystal, i.e., a spatially confined critical state [2].

1. T. Ishimasa, Y. Tanaka and S. Kashimoto, Phil. Mag. **91** (2011), p. 4218.
2. K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura and T. Ishimasa, Nature Materials **11** (2012), p. 1013.

Phason modes in the Sc-Zn icosahedral quasicrystal

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Keywords: Phason, Diffuse scattering, Tsai-type quasicrystals

Using high resolution x-ray diffraction and absolute scale diffuse scattering measurement we have studied the structural quality and quasicrystalline perfection of the recently discovered binary icosahedral quasicrystal $Sc_{12}Zn_{88}$ [1]. We show that the Bragg peaks are systematically shifted from their ideal quasicrystalline position under a uniform phason strain. The Bragg peaks also display a significant broadening scaling with Q_{perp} and interpreted as a uniform phason strain distribution. A large amount of diffuse scattering is observed around the Bragg peak, with maxima along directions parallel to three-fold axis. This diffuse scattering can be fully interpreted within the hydrodynamic theory of quasicrystals and is resulting from quenched in long wavelength phason fluctuations. We find that the ratio of the phason elastic constant K2/K1 is equal -0.53 i.e. it is close to a three-fold instability. When compared to the ternary icosahedral phase i-ZnMgSc we find that the amount of diffuse scattering is much larger and is accompanied by a drastic diminution of the high Q_{perp} reflection intensities, with the maximum Q_{perp} value observed equal to 3 to be compared to 7 [2, 3]. This is in agreement with a much larger perpendicular Debye-Waller in the $Sc_{12}Zn_{88}$ binary icosahedral phase. All those results indicate that the binary $Sc_{12}Zn_{88}$ phase is close to a structural instability, probably quenched in for kinetic reasons.

1. P. C. Canfield, et. al., Phys. Rev. B **81** (2010), p. 020201
2. M. de Boissieu, et. al., Phys. Rev. Lett. **95** (2005), p. 105503.
3. T. Janssen, et. al., Aperiodic Crystals, Oxford University Press, Aachen (2007).

Inverse Hall-Petch like mechanical behaviour in nanophase Al-Cu-Fe quasicrystals: A new phenomena

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Keywords: Nanoquasicrystal, Mechanical milling, Inverse Hall-Petch behaviour

The structural and mechanical stability of quasicrystals (QC) are important issues for their applications at high temperatures and stresses. These materials are brittle due to the immobility of dislocations at room temperature. Thus, the current efforts are directed to improve the ductility of these materials through grain refinement down to nanoscale level by different advanced processing techniques. High-energy ball milling is one of the processes to produce nano-quasicrystalline (n-QC) materials and nano-composite from these alloys. In the case of Al-Fe-Cu alloys, it has been reported that after prolonged milling at high intensity, the QC phase transformed to the disordered B2 (i.e., BCC) phase. However, in the present investigation, we have synthesized the nano-structured QC (n-QC) phase without any type of phase transformation occurring by milling the powder at lower intensities.

The aim of the present work is to report the detailed investigation and the analysis of our results on the Hall-Petch (HP) and Inverse Hall-Petch (IHP) behaviour of n-QC $Al_{62.5}Cu_{25}Fe_{12.5}$ alloys. It is found that the hardness increases with decreasing grain size down up to 40 nm, exhibiting the HP relationship, whereas for grains smaller than 40 nm, IHP behaviour is identified. This is attributed to the complexities of the structure and deformation mechanisms in quasicrystalline alloys. The IHP behaviour in the nano-quasicrystalline phase could be attributed to shearing of atoms in the grain boundaries, leading to grain boundary sliding mechanisms in nano-scale microstructures quasicrystalline grain boundaries. These results are analyzed based on the dislocation pile-up model as well as the grain boundary shear models applicable to nanomaterials.

(3+2) Dimensional Incommensurate Modulation in melilites Electrolytes

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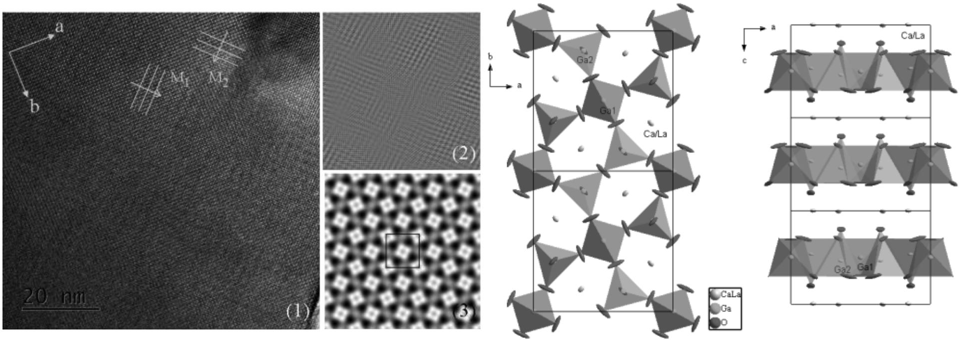
Gallate melilites $[RE_{(1-x)}Ln_{(1+x)}]_2[Ga]_2[Ga_2O_{7+x/2}]_2$ (RE=Ca, Sr; *Ln* = Nd, La, $0 \leq x \leq 0.5$) are efficient oxide ion conductors at intermediate temperatures (~750°C) with non-rational crystallographic modulations presumed to play a key role in significantly enhancing oxygen mobility. In melilites, modulation waves can be imaged by high angle annular dark field and bright field scanning transmission electron microscopy with contrast quantified through electron scattering simulation. Single crystals grown using an optical floating zone furnace have been investigated using transmission electron microscopy, powder and single crystal X-ray diffraction [1-3].



(a) (b)

Figure 1. (a) Nano-scale modulation waves. (b) Crystal structure $[CaLa]_2[Ga]_2[Ga_2O_7]_2$

Oxide ion conductivity in melilites is interstitially mediated, and a crystallographic prerequisite for these SOFC electrolytes to function is a flexible framework that relaxes to allow the passage of interstitial oxygen. Moreover, by increasing the average charge of the interlayer cations [RE*Ln*], up to 0.32 excess oxygen per structural formula unit (*sfu*) can be introduced to the tetrahedral layers [4]. Interstitial oxygen is located near the apical position of the GaO_4 tetrahedra and intralayer ‘diffusion’ is accompanied by cooperative flexing of the tetrahedral layers. In contrast, interlayer oxygen mobility along *c* is not favoured. Relaxation of the tetrahedral network is essential for oxygen migration, and the incommensurate nature of melilite arises from layer flexing, induced by changes in the interlayer cation composition, that cooperatively stabilises nano-scale volumes containing superstoichiometric oxygen.

1. F. Wei, Tim Williams, Tao An, T. Baikie, C. Kloc, Jun Wei, T. White, Journal of Solid State Chem., Accepted 2013.
2. F. Wei, T. Baikie, T. An, C. Kloc, J. Wei, and T. White, Inorganic Chemistry **51** (2012), p. 5941-5949.
3. F. Wei, T. Baikie, T. An, M. Schreyer, C. Kloc, T White, J. Am. Chem. Soc. **133** (2011), p. 15200-15211.
4. M.-R. Li, X. Kuang, S.Y. Chong, Z. Xu, C. I. Thomas, H. Niu, J. B. Claridge, M. J. Rosseinsky, Angew. Chem. Int. Ed. **49 (**2010), p. 2362 -2366.

Contributed Talks

O-01 – O-32

Formation of quasicrystals and other exotic crystal structures in a soft-core fluid: a tale of two length scales

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Keywords: soft matter, quasicrystal growth, structure formation

A two-dimensional system of soft particles interacting via a two-length-scale potential is studied. This pair potential is chosen so as to model the effective interaction between polymeric macromolecules with a hydrophobic core and a hydrophilic fringe. Density functional theory reveals the existence of a fluid phase and two crystalline phases with different lattice spacing. Of these the larger lattice spacing crystalline phase takes the form of a ‘crystal liquid’ state with a small fraction of mobile particles. Near the transition between this phase and the smaller lattice spacing crystalline phase, quasicrystalline structures may be created in a quench from the uniform liquid by a competition between linear instability at one scale and nonlinear selection of the other crystal structure. The results are confirmed using Brownian dynamics simulations.

Theoretical foundations of the Hume-Rothery electron concentration rule for structurally complex alloys

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Keywords: FLAPW-Fourier method, Hume-Rothery stabilization mechanism, Hume-Rothery electron concentration rule

The Full-potential Linearized Augmented Plane Wave (FLAPW)-Fourier method has been shown to be very well suited to extract both the Fermi diameter $(2k_F)^2$ and the square of the *critical* reciprocal lattice vector $|\mathbf{G}|_c^2$ associated with lattice planes interfering with electrons at the Fermi level [1, 2]. This allows us to interpret the origin of a pseudogap at the Fermi level in terms of the Fermi surface-Brillouin zone (FsBz) interactions and to elucidate the physics behind the Hume-Rothery electron concentration rule.

We have revealed that the interference condition $(2k_F)^2 = |\mathbf{G}|_c^2$ is well satisfied in a number of structurally complex metallic alloys (CMAs) characterized by a pseudogap at the Fermi level. The number of electrons per unit cell, **e/uc**, given by the product of electrons per atom ratio **e/a** and the number of atoms per unit cell N, is directly derived from $(2k_F)^2$ while the structure information is reflected in *critical* $|\mathbf{G}|_c^2$. The physics behind the Hume-Rothery electron concentration rule is established by constructing **e/uc** versus $|\mathbf{G}|_c^2$ diagram by performing the FLAPW-Fourier analysis for a large number of CMAs. Included are the Samson compound β-Al_3Mg_2, 2/1-2/1-2/1 approximants, 1/1-1/1-1/1 approximants covering Al-Mn and Al-Cu-Fe in the MI-type family, Al-Mg-Zn and Al-Li-Cu in RT-type one and Cd_6Ca and Zn_6Sc in Tsai-type one. We revealed that all the data points fall on a straight line with a slope of 3/2 on log-log scale, indicating the fulfillment of the interference condition $(2k_F)^2 = |\mathbf{G}|_c^2$. This is taken as evidence that the Hume-Rothery stabilization mechanism holds for all CMAs studied, regardless of whether the transition metal elements are involved or not.

1. U. Mizutani, "Hume-Rothery Rules for Structurally Complex Alloy Phases", (CRC Press, Taylor & Francis Group, Boca Raton) (2010).
2. U. Mizutani, M. Inukai, H. Sato and E.S. Zijlstra, Chem.Soc.Rev. **41** (2012), p. 6799.

Configurational entropy of atomistic quasicrystals in 2D

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Keywords: Structure, stability, entropy

The random tiling hypothesis of Henley and Elser states that the configurational entropy due to the phason flips stabilizes a quasicrystal at elevated temperatures. When its influence decreases at low temperatures, a transition to a periodic crystal occurs.

In a recent publication [1] we confirmed the random tiling hypothesis for a monatomic two-dimensional decagonal model quasicrystal. When the atoms interact by a double-well Lennard-Jones-Gauss potential, a random Tübingen triangle tiling is forming. We calculated the free energy and phason elastic constants over a wide range of temperatures and found that, indeed, the configurational entropy term, favouring a quasicrystal, at high temperatures overcomes the internal energy, favouring periodicity. Thus, quasicrystals are high temperature phases.

The phason contributions to entropy and free energy were taken into account using an approximation of uncorrelated phason flips. In this approach we applied an Ising-type Hamiltonian for flipable vertices. It is exact for low temperatures, where few flips are excited, but may become invalid at high temperatures.

Here we study the temperature range for which the approximation of uncorrelated phason flips is valid, in more detail. We employ the method of thermodynamic integration. For the reference state, which we had taken previously as Einstein quasicrystal, we now take the triangle tiling at the melting point, as done for patchy particles in [2].

1. A. Kiselev, M. Engel, H.-R. Trebin, Phys. Rev. Lett. **109** (2012), p. 225502.
2. A. Reinhardt, F. Romano and J.P.K. Doye, ArXiv:**1302.2592** (2013).

Quasicrystals as Catalysts for the Steam Reforming of Methanol: A Study of the Leached Surfaces of Single Grain Quasicrystals

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Keywords: Leached Quasicrystal Surfaces, Faceted Microstructure, Catalysis

Steam Reforming of Methanol had previously been performed over several quasicrystalline alloys to find promising levels of activity and selectivity while remaining stable at high temperatures [1,2]. Our experiments have investigated the structural effects on single grain *i*-AlCuFe and *d*-AlNiCo quasicrystals, which have been leached at varying times in NaOH using scanning electron microscopy (SEM). Other investigations have taken place over powdered samples that have provided little detail regarding the role of the underlying quasicrystal. The fivefold surface of the *i*-AlCuFe was investigated along with the tenfold and two surfaces of the *d*-AlNiCo. Orientated pentagonal cavities and partially revealed dodecahedral cavities were observed and analysed in leached *i*-AlCuFe [3]. Both materials produced nanoparticular precipitate. The precipitate contains a mix of Cu and Fe in *i*-AlCuFe and in *d*-AlNiCo, Ni and Co which have been observed through AFM, EDX, XPS and UPS. Understanding the properties of these nanoparticles is important to investigate the optimisation of the leaching technique for facilitating catalytic activity.

1. A. P. Tsai. and M. Yoshimura, Applied Catalysis A: General, **214**(2) (2001), p. 237-241.
2. B. P. Ngoc *et al.*, Catalysis Letters **131,** (2009), p. 59–69.
3. T. P. Yadav *et al.*, Aperiodic Crystals, Springer (2013), p. 275-282.

Ultrathin quasicrystal films deposited on silicon for controlling friction and adhesion

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Keywords: ultrathin quasicrystal films, friction, adhesion

Quasicrystal materials are interesting in many applications when both good mechanical and tribological (friction, wear resistance) and adhesive properties are required in the same time. It relates in particular to Micro/Nano Electro Mechanical Systems (MEMS/NEMS) and nanofabrication processes where tool is in permanent sliding contact with the formed material e.g. in nanoimprinting [1,2]. In such applications ultrathin films are used to control frictional and adhesive interactions at sliding interfaces. The substrate (structural) material used to fabricate functional components (e.g. a mold in imprinting process) is usually silicon wafer. The thickness of the deposited film should be very low and usually is below one micrometer sometimes going down to only several nanometers (e.g. to protect magnetic layer in computer hard disks).

We have performed intensive studies towards the optimization of Physical Vapour Deposition (PVD) technique to deposit Al-Cu-Fe quasicrystal ultrathin films on silicon and we tested them to identify their mechanical properties (nanohardness, Young`s modulus), nanoscale wear resistance as well as frictional and adhesive behaviors. The aim of the studies was to find best films possessing in the same time best frictional and adhesive properties.

The complex set of methods of characterization during tests has been applied: nanoindentation (nanohardness, Young`s modulus) , Atomic Force Microscopy (AFM) (friction, pull-off force (adhesion), nanowear tests) and wettability studies to identify surface free energy (with identification of polar and dispersion components). The results of these intensive studies towards minimization of friction and adhesive properties as a function of PVD process parameters will be presented and discussed together with the consideration of special problems appearing during deposition of quasicrystal ultrathin films on silicon substrate.

The partial support from appliCMA and 3SMVIB projects is kindly acknowledged.

1. M. Madou, Fundamentals of Microfabrication and Nanotechnology, Vols 1-3, 3rd ed., CRC Press, Boca Raton (2012).
2. S. Landis (ed), Nano-Lithography, ISTE - J. Wiley, London-Hoboken (2011).

Simulation study of two-lengthscale quasicrystals

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Keywords: soft matter, quasicrystal, simulation

Over the past decade quasicrystalline order was reported in many soft-matter systems including dendrimers, star terpolymers, and diblock copolymer micelles, establishing soft quasicrystals (QCs) as an integral part of the field [1,2]. The existence of QCs in solutions of fuzzy macromolecular micelles suggests that they must be induced by a generic mechanism rather by specific chemistry. The most evident common feature of micelles stemming from their open architecture is deformability but so far no direct link to quasicrystallinity has been established. We explore a simple model which captures many aspects of the soft interaction between the micelles [3], showing that it leads to a hierarchy of novel random QCs. Using numerical simulations, we study two-dimensional hard disks decorated with square-shoulder repulsion to find a coherent sequence of QCs with 10-, 12-, 18-, and 24-fold orientational symmetry [4]. These QCs originate from mosaics of tiles based on local arrangements of the particles, which can be regarded as generalizations of the hexagonal lattice. Our results emphasize the importance of packing constraints in the formation of quasicrystals, and they could be used for targeted design of certain classes of these materials.

1. T. Dotera, Israel J. Chem. **51** (2011), p. 1197.
2. T. Dotera, J. Polym. Sci. Pol. Phys. **50** (2012), p. 155.
3. F M. A. Glaser, G. M. Grason, R. D. Kamien, A. Košmrlj, C. D. Santangelo, and P. Ziherl, EPL **78** (2007), p. 46004.
4. T. Dotera, T. Oshiro and P. Ziherl, in preparation.

Stability of quasicrystals in colloid-polymer mixtures

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Keywords: quasicrystal, colloid, colloid-polymer mixture

In order to obtain interesting new metamaterials, soft quasicrystals built out of colloids or polymer micelles are in the focus of recent research. A big advantage of studying colloidal quasicrystals is that individual particle positions are directly observable, e.g., by using video-microscopy. However, a theoretical explanation of the stability or a prediction of the self-assembly process of colloidal quasicrystals remain a challenging task to date.

We investigate the ground state (T=0) stability of colloid-polymer mixtures. In our model, the colloidal interactions are dictated by a repulsive screened Coulomb potential, whereas the presence of polymers yield an attractive depletion force between them. Hence, we obtain an isotropic two-length scale pair interaction potential that we use to support the two incommensurate length scales of the quasicrystal that we want to obtain. By minimizing the corresponding lattice sums, we search for parameter sets where the system prefers quasicrystalline ordering rather than any other crystalline structure. We determine the phase diagram in order to characterize the appropriate parameter ranges where quasicrystals occur, i.e., we explain what polymer concentration, what depletion length, and what density are needed to grow quasicrystals with a given symmetry. Therefore, our calculations explain how in experiments colloidal building blocks have to be designed in order to achieve self-assembly of intrinsic colloidal quasicrystals.

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Decagonal quasicrystals - some new aspects

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Keywords: quasicrystals, decagonal phase, structure

Why are some intermetallic phases quasiperiodic although they could be (and are in many cases) periodic for a slightly different stoichiometry? And what governs the growth of quasicrystals? Phenomenologically, there are a couple of crucial factors contributing to the phase stability known such as the valence-electron concentration, the Hume-Rothery mechanism, the contribution of entropy etc., however, the processes occuring on atomic scale during crystal growth are still unresolved.

Decagonal quasicrystals (DQC) have in common that they can be described as cluster coverings [1]. The underlying tilings for both Al- and Zn-Mg-based DQC are all closely related to rhomb or pentagon Penrose tilings or to Masakova tilings [2]. It has been shown that the quasiperiodic packing of columnar clusters results quite naturally from the contraint that the local chemical composition of the clusters has to be as close as possible to the global one [3]. It has also been demonstrated that the flat or slightly puckered atomic layers in DQC can play an important role for guiding their growth by coupling the fivefold local symmetry of the clusters to the quasiperiodic long-range order [4].

Here we will present this model in greater detail and show that the outer columnar cluster shells, which form the flat atomic layers, can be seen as slightly distorted hexagonal close packed layers. We illustrate these findings by experimental observations.

1. W. Steurer, Chem. Soc. Rev. **41 (**2012), p. 6719.
2. S. Deloudi, F. Fleischer and W. Steurer, Acta Crystallogr. B **67** (2011), p. 1
3. W. Steurer and S. Deloudi, Struct. Chem. **23 (**2012), p. 1115.
4. W. Steurer, Z. Anorg. Allg. Chem **637** (2011), p. 1943.

High temperature structures of decagonal Al-Cu-Rh and Al-Cu-Ir quasicrystals

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Keywords: decagonal quasicrystal, high-temperature structure,

The in-situ high-temperature measurements of d(ecagonal)-Al-Cu-Rh and d-Al-Cu-Ir quasicrystals were performed at temperatures up to ~1000 °C (air-blowing furnace) at the Swiss-Norwegian beamline at ESRF in Grenoble, France with the PILATUS 2M pixel detector. The RT structures of both decagonal phases were recently published [1].

The Al-Cu-Rh sample was measured at RT, 950 °C, 880 °C, 810 °C and 740 °C (in this order). No phase transition occurred in the investigated range of temperatures. A careful investigation of the integrated datasets revealed, as expected, a clear increase of the physical space ADPs with temperature. The plots of $F_{\mathrm{RT}}/F_{\mathrm{HT}}$ versus $k_{\|}$ show an increasing trend. This is related to an obvious increase of the amplitude of the thermal motion of atoms with temperature. No clear trend for the increase of the perpendicular space ADPs could be observed. The plots of $F_{\mathrm{RT}}/F_{\mathrm{HT}}$ versus $k_{\perp}$ do not show any significant trend. This means, that there is no indication for the increase of the phasonic disorder with temperature, which would be a proof for a kind of entropy stabilization [2]. The structures at all five temperatures were subsequently refined to *R-values* below 0.07. Their atomic structures are essentially very similar at all temperatures, except for some minor changes. The ADPs increase as expected. The refined value of the overall phasonic ADP is the same at all temperatures. The results contradict the concept of a special entropy stabilization mechanism for decagonal quasicrystals.

The d-Al-Cu-Ir sample undergoes a phase transition at ~750 °C. At RT (sample quenched form 950 °C) and at temperatures above 750 °C the structure is ~4 Å ($P10_5$/mmc space group) with two atomic layers per period and no detectable diffuse scattering [1]. Below 800 °C the diffuse scattering occurs, both in the diffraction pattern layers related to the ~4 Å structure and in the inter-layers related to the ~8 Å superstructure. Below 750 °C the inter-layer maxima of diffuse scattering become Bragg reflections, which proves the formation of an ~8 Å superstructure. The diffuse scattering is still present in all layers of the diffraction pattern. The space group of the superstructure is *P*5/m2c. A model of the superstructure based on the two-colour Penrose tiling has been derived.

1. P. Kuczera, J. Wolny, W. Steurer, Acta Crystallogr. B, 68 (2012), p. 578.
2. W. Steurer, Z. Anorg. Allg. Chem., 637 (2011), p. 1943.

A new family of binary magnetic icosahedral quasicrystals based on rare earths and cadmium

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Keywords: quasicrystals, magnetism, flux growth

The formation and stability of quasicrystalline phases, as well as the ways in which aperiodicity modifies electronic, vibrational and magnetic properties, have been intense topics of research over the past thirty years. Stable binary quasicrystalline phases are valuable for studying stabilization mechanisms and the thermodynamics in binary phase diagrams. Moreover, the discovery of a family of local-moment bearing binary quasicrystals provides the compositionally simplest system for the study of magnetic interactions in aperiodic compounds. Here we report the discovery of a family of at least seven rare earth icosahedral binary quasicrystals, i-R-Cd (R = Gd - Tm, Y), six of which bear localized magnetic moments [1].

In support of our discovery of i-R-Cd we have experimentally re-evaluated the Cd-rich regions of the binary R-Cd phase diagrams and have determined the compositions of the deeply peritectic i-R-Cd phases. We further show that these magnetic quasicrystals contain the same basic structural elements, namely Tsai-type rhombic triacontahedral (RT) clusters of atoms, as found in the non-moment-bearing i-YbCd5.7 icosahedral phase [2, 3] and RCd6 periodic approximants despite differences in composition. Finally, we present data that strongly suggests that the new quasicrystal phases enter into a low-temperature spin-glass (SG) state rather than manifest antiferromagnetic order as found for the RCd6 approximants [4-6].

1. A. I. Goldman, T. Kong, A. Kreyssig, A. Jesche, M. Ramazanoglu, K. W. Dennis, S. L. Bud'ko and Paul C. Canfield, Nature Materials (accepted for publication).
2. A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura and T. J. Sato, Nature **408** (2000), p. 537.
3. H. Takakura, C. Pay Gómez, A. Yamamoto, M. de Boissieu and A. P. Tsai, Nature Materials **6** (2007), p. 58.
4. R. Tamura, Y. Muro, T. Hiroto, K. Nishimoto and T. Takabatake, Phys. Rev. B **82** (2010), p. 220201(R).
5. M. G. Kim, G. Beutier, A. Kreyssig, T. Hiroto, T. Yamada, J. W. Kim, M. de Boissieu, R. Tamura, and A I. Goldman, Phys. Rev. B **85** (2012), p. 134442.
6. A. Mori, H. Ota, S. Yoshiuchi, K. Iwakawa, Y. Taga, Y. Hirose, T. Takeuchi, E. Yamamoto, Y. Haga, F. Honda, R. Settai and Y. Ōnuki, J. Phys. Soc. Jpn. **81** (2012), p. 024720.

Quasicrystal–polymer composites for additive manufacturing technology

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Keywords: Quasicrystal, Composite, Selective laser sintering

Rapid manufacturing technologies are evolving extremely rapidly with innovative processing methods and emerging new markets. The Selective Laser Sintering (SLS) process is one of the main methods for rapid prototyping through additive manufacturing. It allows for building freeform parts based on 3D computer-aided design. The most frequently used materials are polyamide-based composites, either filled with ceramic or metallic particles. The range of composites compatible with the process is actually quite limited and material innovations in this field are rather scarce. For example, aluminium particles are currently added in a polyamide matrix to obtain SLS parts with a metallic appearance, good finishing properties and high stiffness. But there is no material solution for tribological applications of parts fabricated by this process. Furthermore, because quite some porosity is remaining after processing those parts, they are not leak-tight, which forbids their use in many fluidic applications without post-impregnation of a resin.

Toy model (left) and intake manifold of a car engine (right), both made by SLS [1].

A real improvement in additive manufacturing technology can be realized by resorting to unconventional materials like quasicrystals. The talk will show that when Al-based quasicrystalline particles are used as filler particles in a polymer matrix, processed parts show reduced friction and improved wear resistance compared to all other composites used today in SLS technology. In addition, the parts contain almost no porosity and are leak-tight, thus allowing their direct use in fluidic applications. Our new light-weight composite extends the materials choice compatible with the SLS process and offers improved functional performance. It is commercialized since 2011 under the trend mark ‘PAQc’ and enters the fabrication of parts for customers applications.

1. S. Kenzari, D. Bonina, J.M. Dubois and V. Fournée, Materials & Design **35** (2012), p. 691.

Theoretical hardness of Al-based quasicrystals evaluated by the cluster-resonance model

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Keywords: Quasicrystals; cluster-resonance model; hardness model

Although hardness has been widely accepted as an essential parameter of materials, the dependence of hardness on microstructure remains an open issue. Based on the idea that the hardness of quasicrystals (QCs) is intrinsic and equivalent to the rupture of the weakest bonds per unit volume, a novel atomic-level hardness model for QCs is established within the framework of the cluster-resonance model [1-3]. A good agreement between calculated and measured hardness values is obtained.

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1. G. Han, J. B. Qiang, Q. Wang, Y. M. Wang, C. L. Zhu, S. G. Quan, C. Dong, P. Häussler, Philos. Mag. **91** (2011), p. 2404.
2. G. Han, J. B. Qiang, F. W. Li, L. Yuan, S. G. Quan, Q. Wang, Y. M. Wang, C. Dong, P. Häussler, Acta Mater. **59** (2011), p. 5917.
3. C. Dong, Q. Wang, J. B. Qiang, Y. M. Wang, N. Jiang, G. Han, Y. H. Li, J. Wu, J. H. Xia, J. Phys. D: Appl. Phys. **40** (2007), p. R273.

Decorated silver-mean chain with mixed spectrum

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Keywords: tilings, diffraction, mixed spectrum

We present a decorated version of the silver-mean chain (SMC), which has a mixed diffraction spectrum with a pure point and a singular continuous component. This decorated SMC is generated by a primitive substitution rule. Geometrically, the tiles are the same as for the usual SMC, but tiles come now in two colours each. If tiles of opposite colour are decorated with weights of opposite sign, a structure is obtained which has singular continuous diffraction spectrum. Conversely, if tiles of opposite colour are decorated the same way, the usual SMC is recovered, which has pure point spectrum. A generic decoration thus leads to a structure with mixed spectrum.

Examples of this kind can actually be constructed in a systematic way, also in higher dimensions. Starting with a substitution tiling known to be pure-point diffractive, we can split each tile into two subtypes, a barred and an unbarred variant. The two variants are then coupled by a suitable twist in the substitution rule, so that the twisted rule commutes with the bar operation. Under certain conditions, which we shall discuss and which are frequently met, a substitution tiling with mixed spectrum is then obtained.

Hyperbolic icosahedral tiling of Buckyballs

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Keywords: hyperbolic icosahedral tiling, Buckyballs, colour symmetry

Icosahedral polyhedra composed of 20 regular hexagons and 12 regular pentagons are shortly termed Buckyballs, they have the same structure as C_{60} molecules termed fullerene; the vertices of Buckyballs are occupied by carbon atoms. Both, Buckyball and fullerene, are called after the famous architect Buckminster Fuller. A Buckyball consists of 120 fundamental areas, the geometry of the fundamental area should be discussed. A dense packing of Buckyballs – or of fundamental areas – is not possible in Euclidean space. However, one may it imagine in hyperbolic space. For visualisation the Poincaré disc should be extended to a Poincaré ball.

Sharing of four Buckyballs at a vertex will be considered. Four edges and six facets – two pentagons and four hexagons – are sharing a vertex. Therefore, the symmetry of a vertex point is $\bar{4}2\mathrm{m}$ ($\bar{4}$ stands for a fourfold axis with inversion) which is lower than tetrahedral $\bar{4}3\mathrm{m}$ due to the lack of threefold axes at vertex points. The hexagons of the Buckyballs are no mirror planes in the three-dimensional tiling considered presently whereas the pentagons are.

Colour symmetry of this tiling will be considered similar as formerly in planar hyperbolic tilings [1,2]. Colour symmetry with two colours is allowed. The colour symmetry of the vertices can be described as $\underline{\bar{4}2}\mathrm{m}$ (underlining symbolizes change of colour). Colour changes at hexagons. Therefore, the two colours form via pentagons continuous areas which interpenetrate each other. The according superstructure is formed by extending Buckyballs of the first colour with enlarged facets of pentagons which build larger rotated pentagons. These pentagons form dodecahedra with vertices at Buckyball centres of the second colour, 20 dodecahedra are sharing a vertex. In this way a regular 3D hyperbolic tiling is formed.

Buckyball tilings with eight Buckyballs sharing a vertex require distortion of hexagons preserving threefold symmetry. Their colour symmetry as well as that of its dual tiling (equivalent with colouring vertices) will be discussed and visualised by coloured intersections.

1. D. Frettlöh, Z. Kristallogr. **223** (2008) p. 773.
2. R. Lück, and D. Frettlöh, Z. Kristallogr. **223** (2008) p. 782.

Multidimensional paperfolding structures

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Keywords: substitution systems, multidimensional "paperfolding", "paperfolding" tilings

The paperfolding sequence is one of the standard, paradigmatic substitution systems [1,2,3]. We have solved the longstanding problem of generalizing the paperfolding sequence to higher dimensions.

For physical applications, such as templates for fabrication of photonic, phononic and plasmonic nanostructures it is important to construct two- and three-dimensional analogs of substitution sequences. Recently we have constructed a two-dimensional paperfolding structure by a recursive algorithm which, however, made the structure extremely fractal and hence inconvenient for physical applications [4].

We present a general recursive scheme for constructing genuine regular paperfolding structures in any dimension. Here we explicitly construct the two-dimensional version, compute its symbolic complexity referred to rectangles and show its Fourier transform. We also show the first generations of the three- and four-dimensional versions. Moreover, we derive from the structures novel tilings. Finally we discuss possible multidimensional generalizations of the dragon curve.

1. M. Dekking, M. Mendès-France and A.J. van der Poorten, Math. Intelligencer **4** (1982), p. 130-138; 173-181; 190-195.
2. J.-P. Allouche and J. Shallit, “Automatic sequences: theory, applications, generalizations” (Cambridge University Press, Cambridge) (2003).
3. S.I. Ben-Abraham, D. Shapira and A. Quandt, Acta Cryst. A **69** (2013), p. 123-130.
4. S.I. Ben-Abraham and A. Quandt, Phil. Mag. **91** (2011), p. 2718 - 2727.

Tight-binding model for an optical quasilattice with cold atoms

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Keywords: electronic properties, optical lattice, quasicrystals

Cold atoms in optical lattices provide a way to realize electron tight-binding models which were previously considered purely theoretical artifacts. In periodic systems, tight-binding Hamiltonians for nearest neighbor hopping have been realized on a variety of lattices, such as the honeycomb and graphene-like structures that have lately received a lot of attention due to their novel electronic properties. It has been shown that it is also possible to realize the Hubbard model for interacting electrons using cold atoms. There have also been a few studies of incommensurate and quasiperiodic structures . In the one dimensional case, one can obtain an incommensurate potential along one spatial direction using laser beams of different wavelengths. A delocalization transition in such a so-called bichromatic 1d potential was recently reported to have been observed in this type of system [1]. In two and three dimensions, several groups have attempted to create quasiperiodic structures of five-fold symmetry and to study the properties of the resulting Bose-condensate [2]. However, very little is known about the electronic properties and in particular the single electron wavefunctions in these two dimensional systems.

We will present some results obtained by numerical diagonalization for tight-binding Hamiltonians defined on two dimensional models for the five-fold and eight-fold symmetric case. We will present results for the expected wave functions in various regimes of filling factor and other parameters, and compare these with the results known for the octagonal and Penrose tilings.

1. B. Deissler, M. Zaccanti, G. Roati, C. D'Errico, M. Fattori, M. Modugno, G. Modugno, M. Inguscio, Nature Phy. **6** (2010), p. 354.
2. L. Guidoni, C. Triche, P. Verkerk, G. Grinberg, Phys. Rev. Lett. **79** (1997), p. 3363
3. L. Sanchez-Palencia, L. Santos, Phys. Rev. A **72** (2005), p. 053607.

Magnetic Currents in Aperiodic Tilings

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Keywords: octagonal tiling, magnetic structure, magnetricity

The dipolar spin ice have attracted much attention because of their intriguing ground state ordering and non-equilibrium, elementary excitations known as emerging magnetic monopoles.

Until now the spin-ice properties of periodic, infinite lattices have been investigated [2]. We present a theoretical study of magnetic dipolar spin ice on aperiodic lattices of finite dimensions. We consider an octagonal tiling as well as a new type of frustrated spin network with pentagonal loops and long-range quasiperiodic structural order [3]. Especial attention is paid to the evolution and the distribution of excitations with magnetic charges as a function of magnetic field and magnetic potential.

It is demonstrated that depending on the micromagnetic reversal mechanism in individual particles charge ordered states or accumulation of magnetic charges can be observed.

1. A. Schumann, P. Szary, E. Y. Vedmedenko, and H. Zabel, New J. Phys. **14** (2012), p. 035015.
2. A. Jaganatthan, B. Motz, and E. Y. Vedmedenko, Phil. Mag. **93** (2010), p. 2765.

Plastic deformation of refractory metal high-entropy alloys

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Keywords: High-entropy alloys, plastic deformation, dislocations

High-entropy alloys (HEAs) are substitutional solid solutions formed in multicomponent metallic systems [1]. Their components, usually five or more, are present in approximately equiatomic proportion. True HEAs solidify as single phase of simple average crystal structure with bcc or fcc lattice. The constituting atoms are randomly distributed on the crystal lattice, making these materials a crystalline counterpart of metallic glasses.

We have characterized the plastic-deformation behaviour of HEAs, containing the refractory metals Zr, Nb, Ti, Ta, and Hf in the temperature range from room temperature up to 300 °C. Samples grown by the zone-melting technique were uniaxially deformed in compression. Stress-strain curves were recorded and incremental tests such as stress relaxations and temperature cycles were conducted to determine the thermodynamic activation parameters of the plastic deformation process. Deformed samples were investigated by transmission electron microscopy to characterize the microstructure after deformation, the dislocation densities, and the Burgers vectors of the dislocations.

The yield stress is temperature dependent and ranges between about 600 and 900 MPa. Activation parameters can be determined up to about 100 °C. We find activation volumes of the order of 1 nm^3 and an activation enthalpy of about 1 eV. At higher temperatures, recovery processes taking place during the deformation impede the determination of activation parameters. The dislocations possess [1 1 1] Burgers vectors as expected for bcc structures.

1. J.W. Yeh et al., Adv. Eng. Mater 6 (2004), p. 299.

The complex metallic alloy $Al_{13}Co_4$: Metadislocation core structure and atomic model for metadislocation motion

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Keywords: Complex metallic alloys, plastic deformation, metadislocations

We have analysed metadislocations in the complex alloy $Al_{13}Co_4$. The core structure is studied using aberration-corrected high-resolution scanning transmission electron microscopy. Different types of metadislocations with Burgers vectors of $\vec{b} = \pm\tau^{-n} b(0 \quad 1 \quad 0)$ (n = 3, 4) are found which are associated to four and six planar defects, respectively. They are escorted by phason defects and move, in contrast to metadislocations in most other complex alloys, by pure glide. We present a first model of metadislocation motion which involves coordinated jumps of atoms along various crystallographic directions.

Ag-Based Quasicrystals and Approximants as a Template to Grow Metallic Thin Films

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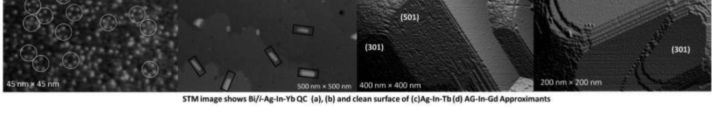
Keywords: Quasicrystals, Crystalline Approximants, Surfaces, Thin Film

Quasicrystals are metallic alloys which show long-range order with lack of periodicity and translational symmetry and posses classically forbidden rotational symmetry such as fivefold and tenfold symmetry. Quasicrystal approximants are also metallic alloys whose chemical composition and atomic structure are close to their parent quasicrystals. [1] However, they are periodic with large unit cells. [2] Approximants play a crucial role in understanding structure of quasicrystals because of their similarity with quasicrystals and the fact that their structure can be well-defined using conventional structure analyses techniques. [3]

During the past decade, the surface of quasicrystals have been studied intensively and they have been chosen as an intriguing substrate for thin film formation due to existence of large range of adsorption sites in comparison with conventional crystals.[4]

In this study, scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) have been employed to characterize Ag-In-RE (RE=Yb, Gd and TB) 1/1 approximant clean surfaces and thin film formation on both. *i*-Ag-In-Yb quasicrystal and Ag-In-RE 1/1 approximant surfaces. Quasicrystalline multilayer of Bi was observed on *i*-Ag-In-Yb quasicrystal surface. The purpose of using approximants as templates is to compare thin film formation with their parent quasicrystals.



STM image shows Bi/*i*-Ag-In-Yb QC (a), (b) and clean surface of (c)Ag-In-Tb (d) AG-In-Gd Approximants

1. A. I. Goldman and R. F. Kelton, Reviews of modern physics **65** (1993), p. 213.
2. H. R. Sharma, M. Shimoda, and A. P. Tsai, Advances in Physics **56 (3)** (2007), p. 403.
3. C. Cui and A. P. Tsai, Journal of Alloys and Compounds (2012).
4. R. McGrath *et al*. J. Phys. Condense. Matter **22** (2010), p. 084022.

STM Studies on the Surface of Ag-In-Yb 1/1 approximant

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Keywords: surface, STM, approximants

We present STM studies on the (100) surface of Ag-In-Yb 1/1 approximant. The surface exhibits a periodic step-terrace structure with a periodicity of a half of the lattice constant (***a***), in accordance with the crystalline structure. Terraces observed are classified into two types depending on the size and the character of the STM images.

The larger terraces (***L***) appear periodically at every ***a***/2 along the [100] direction. High resolution images of the ***L***-terrace show bright spots (protrusions) forming a square lattice with a lattice size of ***a***. The smaller ones (***S***-terraces) are very narrow and appear both upper and lower sides of the ***L***-terraces. The STM images of ***S***-terrace show rather elongated patterns. These ***L-*** and ***S-*** terraces form a periodic sequence, ***LSSLSSL***…. These features are discussed on the basis of the cluster structure.

Temperature Dependence of Ag Film Roughness and Interlayer Spacing During Deposition on Complex Al-Pd-Mn Surfaces: Comparison with Periodic Substrates

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The morphology of thin metal films deposited on metal substrates is often dominated by kinetic rather than thermodynamic factors. These factors can assessed by studying film characteristics as a function of deposition temperature. In this study, we report a comparison of the roughness of thin Ag films deposited on surfaces of a quasicrystal (five-fold icosahedral Al-Pd-Mn), an approximant of this quasicrystal, and low-index Ag surfaces, at temperatures below and up to ambient. Kinetic effects lead to an increase in roughness with increasing temperature for the Al-Pd-Mn substrates, but a decrease in roughness over the same range on Ag(111) and Ag(100). The nature of these effects is discussed. In addition, we observe that interlayer spacings in the film depend upon layer height, for the Al-Pd-Mn substrates. A useful refined definition of roughness for a system with variable interlayer spacing is presented.

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Molecular orbital picture extracted from the band structure of a realistic approximant crystal with semimetallic or semiconducting bandgap

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Keywords: Quasicrystalline approximant, pseudo-Mackay cluster, Molecular orbital

Discovery of semiconducting quasicrystal or its approximant crystal is desired by reasons of genuine curiosity whether solid state physics permits it or not, and of more immediate interest to possibility as a highly efficient thermoelectric material. Although bandgap formation is theoretically predicted for some hypothetical approximant crystals [1], such ones have not synthesized experimentally. Recently we found truly semimetallic band structure in a model of a cubic approximant crystal, $Al_{39}Cu_8Ir_{15}$, and also semiconducting ones in partially substituted models. Present study focuses on revealing the mechanism of bandgap formation in these models. We selected the semimetallic $Al_{39}Cu_8Ir_{15}$ model as the primal target because we can construct an idealized model without chemical and structural disorders, and furthermore, its composition and optimized structural parameters are in good agreement with experiments [2, 3], in other words, it is realistic.

Because most of approximant crystals have characteristic clusters in their structures, their band structures should be understood on the basis of the molecular orbitals of the clusters. For that purpose, we have developed a method for extracting convenient molecular orbitals from the calculated band structure. The method utilizes the Hoffmann's crystal orbital overlap population (COOP) [4], which represents the degree of hybridization (between a pair of orbitals). The central idea is that COOP between *already hybridized* orbitals should be small, *i.e.* COOPs (between possible pairs) should be minimized by optimizing the molecular orbitals, or hybridization coefficients, to extract the hybridized molecular orbitals, which may understandable. We chose pseudo-Mackay cluster with formula $Al_{38}Ir_{13}$ as a main building block and extracted its molecular orbitals by using the above method. In the presentation, we will show the detailed results and discuss about them, especially about the relation between the molecular orbitals and the mechanism of bandgap formation.

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1. M. Krajčí and J. Hafner, *Phys. Rev.* B **68** (2003), p. 165202.
2. D. Kapush, B. Grushko and T.Ya. Velicanova, *J. Alloys Compd.* **493** (2010), p. 99.
3. J. Dshemuchadse, P. Kuczera and W. Steurer, *Intermetallics* **32** (2013), p. 337.
4. R. Hoffmann, "*Solids and Surfaces: A Chemist's View of Bonding in Extended Structures*", (WILEY-VCH, New York) (1988), p. 43.

Sub-diffusive electronic states in Penrose and octagonal tilings

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Keywords: Quantum diffusion, Penrose tiling, octagonal tiling, electronic transport

The understanding of the remarkable transport properties of quasicrystals is a long standing question that still does not have a definite answer. It has been shown that medium range quasiperiodic order in AlMn, AlCuFe and AlCuCo quasicrystals leads to an “insulator like” behavior (see Refs. [1-3] and Refs therein). In one dimensional quasiperiodic tilings, critical states have been found showing a new type of electron localization. A major question is whether these states persist in higher dimension. Up to now very few quantum transport calculations have been performed for two- and three-dimensional quasiperiodic tilings (see in particular [4-8]). A non-ballistic regime has been shown in generalized Rauzy tilings [5,6], but with metallic conduction.

Here we report on our recent numerical results on quantum diffusion in two dimensional Penrose tiling and octagonal tilling. We show that long range quasiperiodic order induces a sub-diffusive regime at some energies. Therefore, a small shift of the Fermi energy can cause a quasiperiodic system without defects to undergo a Metal-Insulator transition. Finally the sub-diffusive behaviour is destroyed by a static disorder in agreement with the fact that conductivity increases when disorder increases in some quasiperiodic systems.

1. T. Grenet, in “Quasicrystals: Current Topics”, ed. E. Belin-Ferré, C. Berger, M. Quiquandon and A. Sadoc, (World Scientific, Singapor) (2000) p. 455.
2. T. Fujiwara, T. Mitsui, and S. Yamamoto, Phys. Rev. B **53** (1996), p. 2910(R).
3. G. Trambly de Laissardière, J. P. Julien and D. Mayou, Phys. Rev. Lett. **97** (2006), p. 026601.
4. B. Passaro, C. Sire, V. G. Benza, Phys. Rev. B **46**, (1992) p. 13751.
5. F. Piéchon and A. Jagannathan, Phys. Rev. B **51** (1995), p. 179.
6. A. Jagannathan, Phys. Rev. B 61 (2000), p. 834(R).
7. S. Roche and D. Mayou, Phys. Rev. Let. **79** (1997), p. 2518.
8. F. Triozon, J. Vidal, R. Mosseri and D. Mayou, Phys. Rev. B **65** (2002), p. 220202(R).

Orientation interactions of pseudo-Mackay clusters in $Al_{11}Ir_4$ and approximants of *i*-AlPdMn

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Keywords: icosahedral Al-Mn-Pd simulation pseudo-Mackay cluster-interaction

We develop a real-space based decoration framework to describe *i*-AlPdMn, and particularly its 1/1 and 2/1 cubic approximants, in which pseudo-Mackay Icosahedron (pMI) clusters are placed on the even vertices of a “canonical cell” tiling using linkages shorter by a factor 1/t compared to the *i*-AlMnSi model, while $Al_{12}Pd$ icosahedra are placed on the odd vertices. The pMI inner shells are $Al_{10}Mn$ [and Al_9Mn?] clusters which can take on various orientations relative to their icosahedrally symmetric cages. Our AlPdMn structure is consistent with thermodynamic stability if and only if the relative orientations of the clusters are optimized. By relaxing (under empirical potentials) a large number of trial configurations with random orientation patterns, we fit a set of cluster-cluster interactions for the purpose of determining the ordering pattern. Such interactions could conceivably play the role of matching rules, promoting an ordering tendency of the cluster network itself. The same kinds of clusters and cluster linkages occur in $Al_{11}Ir_4$, which can be considered as the 1/1 approximant of a hypothetical quasicrystal closely related to *i*-AlPdMn; in that material, the diffraction refinement of Grin et al [1] agrees perfectly with a structure consisting of a disordered mix of cluster orientations.

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1. Y. Grin, K. Peters, U. Burkhardt, K. Gotzmann and M. Ellner, Z. Krist. **212** (1997), p. 439.

Metadislocation core structure in the ε-Al-Pd-Mn phases

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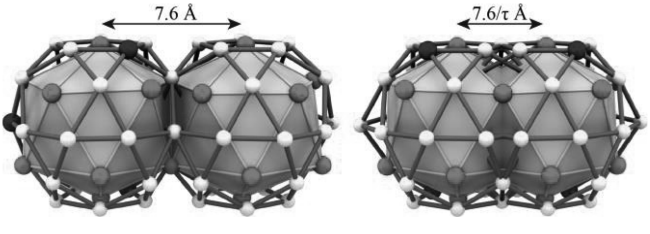
Keywords: Al-Pd-Mn, metadislocations, decagonal quasicrystal, ε-phases, pseudo-Mackay cluster

In the past we have energy optimized the bulk structures of ε-phases of Al-Pd-Mn using quantum mechanical *ab initio* calculations and molecular dynamics [1]. All phases consist of columns of pseudo-Mackay icosahedra (PMI) whose projections form tilings of hexagons, pentagons and nonagons. The gaps in between the PMI columns are filled with glue atoms in the form of large bicapped pentagonal prisms (LBPP). The 16 Å decagonal phase of Al-Pd-Mn comprises further tiles. We have constructed several fictitious approximants containing such tiles, have decorated them with PMI and LBPP clusters and have energy optimized the component clusters. It turned out that, while the PMI clusters can be kept essentially unchanged, the LBPPs must be adjusted in the occupancy with Al atoms depending on their positions in the various tiles. In this way we obtain cluster decorations for all tiles found in the ε- and decagonal phases.

The metadislocation cores of the ε-phases can be partially decorated using the same cluster decoration rules as for the decagonal phase. For the remaining part of the cores this description fails. Recent microscopy images [2, 3] indicate that these remaining parts contain PMI-PMI next neighbors with a $1/\tau$ shorter distance than usually (see figure below). We generated an approximant containing such interpenetrating PMI cluster columns. Preliminary results of the decoration rules for this defect are presented.

All structures were optimized by molecular dynamics annealing with specially developed EAM potentials, followed by further relaxation with *ab initio* calculations. The quality of a structure is judged by its position within the convex hull of stable, experimentally known phases of the Al-Pd-Mn phase diagram.



1. B. Frigan, A. Santana, M. Engel, D. Schopf, H.-R. Trebin, M. Mihalkovic, Phys. Rev. B **84** (2011), p. 184203.
2. M. Feuerbacher, L. Houben, M. Heggen, in EMC 2008, Vol. 2: Materials Science, p. 645.
M. Heggen, M. Feuerbacher, Acta Mat (2013), in press, http://dx.doi.org/10.1016/j.actamat.2013.03.023

Re-entrant spin glass in a Tsai-type approximant

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Keywords: magnetism, re-entrant spin-glass, approximant

Recently, a long-range antiferromagnetic order was observed in a series of Cd_6R(R=rare earth) approximants and much attention has been paid to their magnetic structures. In this paper, we will report re-entrant spin-glass (RSG) behaviour in a Au-based 1/1 cubic approximant which is composed of Tsai-type icosahedral clusters. Both the magnetic susceptibility and specific heat show that a paramagnetic phase at ambient temperature first becomes ferromagnetic and then transforms into a spin-glass state with decreasing temperature. This is the *first* observation of a RSG in quasicrystal-related materials. The origin of the spin-glass behaviour will be discussed and explained based on the detailed crystalline structure obtained from the recent single crystal structural analysis.

Ferro- and ferri-magnetic ordering in ternary Tsai-type magnetic icosahedral quasicrystalline approximants

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Since the discovery of icosahedral quasicrystal (*i*-QC) by D. Schechtman et al. [1], much attention has been paid to their complex atomic structure as well as to peculiar physical properties which originate from the quasiperiodic order. Up to date, localized spin systems of the *i*-QCs and its approximants (APs) has been investigated, however, there are no reports on the occurrence of ferromagnetic ordering in magnetic QCs and APs [2].

Here, we report the *first* observation of ferro- and ferri-magnetic transitions in ternary intermetallic compounds, Au-(Si,Ge)-R (R= rare-earth) APs, which are composed of Tsai-type icosahedral cluster [3]. For example, Au-Si-Gd AP exhibit clear ferromagnetic transition at T_c = 22.5 K in both magnetic susceptibility and specific heat. The detail of magnetic properties in others Au-based systems will be discussed in the presentation.

1. D. Shechtman *et al.*, Phys. Rev. Lett. **53** (1984), p. 1951.
2. For a review, see T. J. Sato, Acta Crystallogr. **61** (2005), p. 39.
3. G. H. Gebresenbut *et al.*, J. Phys.: Condens. Matter **25** (2013), p. 135402.

Triangle-square tiling in Mn-Cr-Si alloys

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Keywords: Triangle-square tiling, dodecagonal, Mn-Cr-Si

A dodecagonal quasicrystal is characterized by 12-fold diffraction symmetry. The framework of the quasicrystal structure is understood, in the ideal case, as a quasiperiodic tiling of two kinds of tiles: an equilateral triangle and a square with the same edge length. This quasiperiodic tiling satisfies the inflation rule governed by the factor $2+\sqrt{3}$. Actually dodecagonal quasicrystals have been observed in a variety of materials from metals to organic substances. However, in the case of transition metal alloys, our knowledge on this type of quasicrystal is limited. The purpose of the present work is to elucidate structural details of triangle-square tiling appearing in Mn-Cr-Si alloys in order to reach a dodecagonal quasicrystal with higher quality.

Near the composition of $Mn_{70}Cr_{10}Si_{20}$ two stable intermetallic compounds are formed. One is high-temperature σ-phase ($P4_2/mnm$, a = 8.793 Å, c = 4.616 Å) and the other hexagonal phase ($P6/mmm$, a = 16.985 Å, c = 4.625 Å) stable below approximately 940 ºC. The latter is $Mn_{70}V_{10}Si_{20}$ type [1, 2]. Both are layered structures along the *c*-axes, and can be interpreted as periodic triangle-square tiling with the edge length approximately 4.55 Å in the *c*-plane. A unit cell of the σ-phase includes 4 triangles and 2 squares, and the hexagonal phase 14 triangles and 6 squares. Then, the number ratios between triangles and squares are 2.00 and 2.33, respectively. The number ratio $4/\sqrt{3} \approx 2.31$ for the quasiperiodic tiling is in between them. In other words, these two phases are approximants to a dodecagonal quasicrystal. This is the reason why this alloy system is attractive. (A half of the unit cell of the hexagonal phase corresponds to the second generation triangle inflated by $2+\sqrt{3}$.)

We have studied a transient state, or intermediate state, in the $Mn_{76}Cr_6Si_{18}$ and $Mn_{70}Cr_{10}Si_{20}$ alloys annealed at 650~700 ºC for 150-1500 h. Under such annealing condition, the quenched σ-phase was slowly transformed to the low-temperature hexagonal phase. X-ray powder diffraction experiments indicated apparent coexistence of the two phases. However, electron microscopy has revealed the following complex triangle-square tiling appearing partly in these specimens; (1) a region exhibiting almost 12-fold symmetric diffraction pattern, (2) domains of a orthorhombic crystal consisting of 10 triangles and 5 squares, and (3) non-periodic arrangement of dodecagons consisting of 12 triangles and 6 squares. In this arrangement, the centre of each dodecagon is positioned at a periodic square lattice with an edge length 17 Å. There are two orientations for dodecagons, and they are randomly selected. This is the first observation of the second generation square in the transition metal alloys.

1. H. Iga, M. Mihalkovic and T. Ishimasa, Phil. Mag. **91** (2011) p. 2624.
2. S. Kashimoto *et al*., Phys. Rev. **B84** (2011) 224201.

Stability of the acute rhombohedron in Cd-based quasicrystals

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Keywords: first-principles calculation, quasicrystals formation mechanism

The discovery of the stable binary quasicrystals (QCs) Cd-Yb/Ca [1] offered the samples without the chemical disorder, which is a source of the structural ambiguities of QCs. Therefore the binary QCs have contributed greatly to understanding QCs, and another second element forming QCs with Cd have been tried to find. However, although more than 10 kinds of Cd-based binary approximants (APs) and ternary QCs have been found, no other binary Cd-based QCs, except the isostructural Zn-Sc [3], has been reported so far. The binary AP can form with various rare-earth (RE) elements like Yb, Ca, Y, Gd, Tb and so on, but QCs can form with only Yb or Ca. The aim of this study is to find the reason why Cd-based QCs form with only Yb and Ca.

The structural building unit of the Cd-based QCs is the five-layered rhombic triacontahedral (RTH) cluster [2], and the RE element occupy the icosahedral third shell. In 1/1 AP phases, all atoms are involved in the RTH cluster and the unit cell is composed of interpenetrating two RTH clusters at room temperature. In QC phases, 94% of the component atoms are involved in the RTH cluster, and an acute rhombohedron (AR) containing four Cd atoms and two RE atoms are filling the gap between RTH clusters. The main structural difference between the APs and QCs is the AR. Therefore stability of the AR seems to relate to that of the QC phase, and there may be a reason that the AR can be stabilized with only Yb and Ca. So, we calculate the cohesive energy of rhombohedral Cd_4RE_2, whose unit cell is the AR, with several kinds of RE including Yb and Ca by the first-principles calculations. The AR is composed of four Cd atoms being on the edges and vertices, and two RE atoms sitting on a diagonal line of the AR. Among the RE elements, Yb and Lu have the atomic radius as large as Ca (1.97Å), but atomic radii of other RE elements are about 1.8Å. The ratio of the atomic radii of Cd and Yb/Ca is about 1.3, but it decreases to about 1.2 for other RE elements. We shall calculate the equilibrium lattice parameters and cohesive energy of the rhombohedral Cd_4RE_2 for several RE elements in order to examine the effect of the atomic size and investigate cohesive mechanisms in the electronic structure of the AR.

1. A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura and T. J. Sato, Nature **408** (2000), p. 537.
2. H. Takakura, C. P. Gómez, A. Yamamoto, M. de Boissieu and A. P. Tsai, Nature Matter. **6** (2006), p. 58.
3. P. C. Canfield, M. L. Caudle, C.-S. Ho, A. Kreyssig, S. Nandi, M. G. Kim, X. Lin, A. Kracher, K.W. Dennis, R. W. McCallum, and A. I. Goldman, Phys. Rev. B., **81** (2010), p. 020201(R).

Electronic Properties and Complexity of Al-based Complex Metallic Alloys (CMAs)

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Keywords: density of states, formation, stability

Many compounds based on aluminium alloyed with transition elements or simple metals contain a large number of atoms in their crystal unit cell. As a consequence of the resulting structure complexity, their physical properties depart significantly from the ones of the elemental constituents. This is especially true for electron-related properties like heat transport or the Al3p partial density of states at the Fermi energy, which scale as simple power laws of the number of atoms in the primitive unit cell. Furthermore, presence of localised, d-like states below the Fermi level is systematically observed, even in the absence of any transition metal constituting element, like e.g. in the β-Al_3Mg_2 Samson phase. The relative intensity of this contribution to the total density of states correlates also with the structural complexity of the compound. Thus, complexity plays a key role, via Hume-Rothery and hybridization effects, in the selection, formation and stability of Al-based CMAs.

The results will be interpreted in terms of self-organized criticality [1]. In order to promote discussion about the essence of the quasicrystalline state ("why are the atoms where they are?"), a preliminary model will be suggested.

1. P. Bak, *How Nature works: the science of self-organized criticality* (Copernicus Press, New York, 1996).

Formation and bonding of bare and hydrogenated B- and Al-icosahedral or planar clusters

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Keywords: icosahedral cluster, ion trap, chemical bonding

We have constructed a unified picture for B- and Al-based icosahedral cluster solids [1,2]. And, we have proposed the new concepts of "metallic-covalent bonding conversion" [3,4] and "self-compensation" [5] in the both solids. We have also investigated pure and hydrogenated B- and Al-clusters [1,4,6]. In this paper, we will report the formation and structure of bare and hydrogenated B- and Al-12 or 13 atoms-clusters. Then, we will discuss about the stability and bonding nature of these clusters, and compare between isolated clusters and those in solids.

We report the formation of icosahedral $B_{12}H_8^+$ through ion-molecule reactions of the decaborane ion ($B_{10}H_x^+$ (x= 6-14)) with diborane (B_2H_6) molecules in an external quadrupole static attraction ion trap. The hydrogen content n of $B_{12}H_n^+$ is determined by the analysis of the mass spectrum. The result reveals that $B_{12}H_8^+$ is the main product. Ab initio calculations indicate that $B_{12}H_8^+$ preferentially forms an icosahedral structure rather than a quasi-planar structure. The calculations of the relative energies show that clusters with fewer hydrogen atoms preferentially form planar structures, whereas those with more hydrogen atoms preferentially form icosahedral structures. This is considered to be "π-σ bonding conversion" by adding or removing hydrogen atoms to or from the $B_{12}H_n^+$ cluster.

On the other hand, metallic bonding icosahedral Al_{13}^- cluster is well known to be very stable and covalent bonding icosahedral $Al_{12}H_{12}^{2-}$ cluster is stable similar to $B_{12}H_{12}^{2-}$ one. This is "metallic-covalent bonding conversion" with or without an atom at the centre of icosahedron, which occurs in the approximant crystals, 1/0-Al_{12}Re and 1/1-AlReSi [3]. However, n dependence of the structure and bonding nature for $Al_{12}H_n^+$ cluster is complicated and not clear.

1. K. Kimura, M. Takeda, M. Fujimori *et al.*, J. Solid State Chem. **133** (1997), p. 302.
2. K. Kimura, J. T. Okada, H. Kim *et al.*, Mater. Res. Soc. Sym. Proc. **886** (2006), p. F06-10.
3. K. Kirihara, T. Nagata, K. Kimura *et al.*, Phys. Rev. B **68** (2003), p. 014205.
4. M. Yamaguchi, Y. Ohishi, S. Hosoi *et al.*, J.Phys. :Conf. Ser. **176** (2009), p. 012027.
5. H. Hyodo, A. Nezu, K. Soga, and K. Kimura, Solid State Science **14** (2012), p. 1578.
6. Y. Ohishi, K. Kimura, M. Yamaguchi *et al.*, J. Chem. Phys. **128** (2008), p. 124304.
7. Y. Ohishi, K. Kimura, M. Yamaguchi *et al.*, J. Chem. Phys. **133** (2010), p. 074305.

Poster Presentations

P-01 – P-84

Investigation of the growth of quasicrystals by using a Phase Field Crystal Model

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Keywords: growth, phase-field-crystal-model, defect-trapping, fluid-liquid interface

We employ a dynamical phase field crystal model to simulate the growth of quasicrystals from supercooled fluids. This technique represents a simplified classical functional density theory [1], where a free energy functional is minimized with respect to density fields. Because the model retains some information on atomic lengths scale it naturally incorporates elastic deformations, misfit strains, and the formation of defects. Since the dynamics on diffusive times scale is included, this model is an ideal tool for studying colloidal and self-assembly nanoparticles systems. While the original formulation contains only one length scale and allows only triangular phases, it is relatively simple to adapt this method to qusicrystalline system by incorporating additional lengths scale [2,3] which are incommensurate with each other. The eight, ten, and twelve fold symmetries are easily obtained with two length scales, while a seven fold structure requires three incommensurate length scales.

We study the phase behavior predicted by the phase field crystal model and investigate the growth of quasicrystals for parameter sets that are either close or far away from the critical temperature. While close to the critical temperature we observe that quasicrystals grow perfectly without any defects, the growth far away from the critical temperature is strongly anisotropic and leads to the trapping of a lot of defects. We analyze the positions of the defects by decomposing the density field in its individual Fourier components as described in Ref. [4].

The phase field crystal model with two or more incommensurate length scales can provide new and deeper insights into the growth mechanism of quasicrystalline structures.

1. K. R. Elder, N. Provatas, J. Berry, P. Stefanovic, and M. Grant, Phys. Rev. B **75** (2007), p. 064107 .
2. J. Rottler, M. Greenwood, and B. Ziebarth, J. Phys.: Condens. Matter **24** (2012), p. 135002.
3. R. Lifshitz and D. M. Petrich, Phys. Rev. Lett. **79** (1997), p. 1261.
4. L. Korkidi, K. Barkan, R. Lifshitz in “Aperiodic crystals”, ed. Springer Netherlands, (2013), p. 117.

Investigation of quasicrystalline approximant in Al-Pd system

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Keywords: Al-Pd system, ε-phase, phase diagram, DTA, XRD, SEM

Up to date many complex metallic alloys were studied regarding to occurrence of quasicrystalline phases. Although the ternary systems based on Al-Pd-TM (TM = Co, Fe, Cr, Mn) were investigated [1, 2], the phase diagram and thermodynamic description of Al-Pd system was not refined with regard to the new experimental results. This work deals with investigation of decagonal quasicrystalline approximants of ε-family phases in Al-Pd binary system. The samples with compositions $Al_{74}Pd_{26}$ and $Al_{73}Pd_{27}$ were analysed using scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), X-ray diffraction analysis (XRD), differential thermal analysis (DTA) and differential scanning calorimetry (DSC). The comparison between experimentally determined thermodynamic quantities and computed quantities derived from existing thermodynamic model [3] shows that this model should be corrected according to experimental results. At present Gruschko [4] refined the phase diagram of Al-Pd system based on experimental results. We summarized the experimental results and we attempted to modify the thermodynamic model of ε_6 phase by defining this phase as non-stoichiometric. To optimize the thermodynamic database of Al-Pd system, the thermochemical data related to forming enthalpies of ε_6 and ε_{28} phases are needed.

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1. A. Smontara, I. Smiljanić, A. Bilušić, B. Grushko, S. Balanetskyy, Z. Jagličić, S. Vrtnik, J. Dolinšek, Journal of Alloys and Coumpounds **450** (2006), p. 92.
2. I. Černičková, R. Čička, P. Švec, D. Janičkovič, P. Priputen, J. Janovec in “Aperiodic crystals”, eds. S. Schmid et al., (Springer, Dordrecht) (2013), p. 133.
3. M. Li, Ch. Li, F. Wang, W. Zhang, Intermetalics **14** (2006), p. 39.
4. B Grushko, Journal of Alloys and Coumpounds **557** (2013), p. 102.

Characterization of rapidly solidified $Al_{65}Cu_{20}Fe_{15}$ alloy in form of powder or ribbon

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Keywords: Al-Cu-Fe, quasicrystal, rapid solidification

Al-Cu-Fe quasicrystalline alloys exhibit unique combination of physical, thermal and mechanical properties. Due to their thermodynamic stability, non-toxicity, and low production cost they have potential for practical applications. [1,2]. Formation of icosahedral phase depends on chemical composition of the alloy and solidification rates [3-5]. Although there have been many investigations concerning the alloys solidified with different cooling rates, the microstructure of rapidly solidified alloys is not well understood.

The $Al_{65}Cu_{20}Fe_{15}$ alloy has been prepared by conventional casting and melt spinning or atomisation techniques. It was found that the icosahedral I-phase was the main phase in all investigated alloys. In the conventionally cast alloy the following phases have been identified additionally: λ-$Al_{13}Fe_4$, β-AlCu(Fe) and Θ-Al_2Cu. In the melt-spun alloy the formation of Θ-Al_2Cu phase is avoided, while in the atomised powder the I-phase coexists with small amount of copper rich β-AlCu(Fe) phase. The melt-spun flakes consists of I-phase dendrites and λ-$Al_{13}Fe_4$ or β-AlCu(Fe) located in interdendritic spaces and the grains of the I-phase at the areas close to the wheel side. Similar cellular-dendritic microstructure was observed in the atomised powder. The amount of β-AlCu(Fe) was reduced with the decrease of the size of powder particles.

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1. E. Huttunen-Saaivirta, J Alloys Comp. **363** (2004), p. 150.
2. J.M. Dubois, Chem. Soc. Rev. **41** (2012), p. 6760.
3. F. Faudot, A. Quivy, Y. Calvayrac, D. Gratias and M. Harmelin, Mater. Sci. Eng. **A133** (1991), p. 383.
4. S. M. Lee, H.J. Jeon, B. H. Kim, W. T. Kim and D. H. Kim, Mater. Sci. Eng. **A304-306** (2001), p. 871.
5. E. Huttunen-Saarivita and J. Vuorinen, Intermetallic **13** (2005), p. 885.

Colloidal assemblies on incommensurate and quasicrystalline substrates

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Keywords: Epitaxy, Colloids, Self-Assemblies

By using Brownian dynamics simulations, we investigate the deposition of colloidal particles on quasicrystalline and incommensurate triangular substrates. The particles interact via screened-Coulomb interactions and an attractive part that arises from depletion forces mediated by polymers.

In case of stretched triangular substrates, we observe the formation and growth of colloidal structures such as pyramids or rims. We determine how the shape and height of the evolving structures depend on the substrate geometry and strain. This is of crucial importance for the production of tailored meta materials, e.g., of photonic crystals.

Finally we study the growth dynamics of the pyramids, rims, and quasicrystalline structures. We also analyze the rearrangements that occur if for readily grown structures the lattice geometry is further changed.

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Fermi surface-Brillouin zone interactions in 2/1-2/1-2/1 Bergman-type approximant $Na_{27}Au_{24}Ga_{34}$

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Keywords: 2/1-2/1-2/1 approximant, FLAPW-Fourier method, Hume-Rothery stabilization mechanism

Recently, Smetana et al. identified the $Na_{26}Au_{25}Ga_{29}$ alloy as a 2/1-2/1-2/1 Bergman-type approximant with space group $Pa\overline{3}$ containing 680 atoms in the a=23.446 A unit cell [1]. The aim of the present work is to discuss the origin of the pseudogap at the Fermi level in terms of the interference condition or Fermi surface-Brillouin zone (FsBz) interactions by performing the Full-potential Linearized Augmented Plane Wave (FLAPW) electronic structure calculations with subsequent FLAPW-Fourier analysis. A model structure free from chemical disorder was constructed with the minimum sacrifice from the experimentally determined structure. The FLAPW band calculations were performed for the model structure with the composition $Na_{27}Au_{24}Ga_{34}$ while keeping the experimental atom positions unchanged and that after the structure relaxation.

A shallow pseudogap is found at the Fermi level in the total density of states in both cases. The Fermi diameter $(2k_F)^2$ is deduced to be 105.0±1.0 in units of $(2\square/a)^2$ and the electrons per atom ratio **e/a** to be 1.66. This is slightly higher than the nominal **e/a**=1.53 obtained under the assumption that $(\mathbf{e/a})_{Na}=1.0$, $(\mathbf{e/a})_{Au}=1.0$ and $(\mathbf{e/a})_{Ga}=3.0$. The square of the *critical* reciprocal lattice vector $|\mathbf{G}|_c^2$ is found to be 104 from the FLAPW-Fourier spectra [2]. The fulfilment of the interference condition $(2k_F)^2=|\mathbf{G}|_c^2$ led us to conclude that the pseudogap originates from FsBz interactions. The number of electrons per unit cell **e/uc** turns out to be 1129. The **e/uc** versus $|\mathbf{G}|_c^2$ dataset is found to fall on the already established 3/2-power law line on a log-log diagram. This means that the present approximant obeys the Hume-Rothery stabilization mechanism.

1. V. Smetana, Q. Lin, D. K. Pratt, A. Kreyssig, M. Ramazanoglu, J. D. Corbett, A. I. Goldman and G. J. Miller, Angewandte Chemie International Edition **51** (2012), p. 12898.
2. U. Mizutani, M. Inukai, H. Sato and E. S. Zijlstra, Chem.Soc.Rev. **41** (2012), p. 6799–6820.

Search for a icosahedral quasicrystal and approximant in Zn-TM systems

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Keywords: quasicrystal, approximants

The icosahedral(i) Zn-Sc quasicrystal(QC) was discovered by P.C.Canfield in 2010 [1]. However, other i-QC has never been found in Zn-based binary systems.

In this work, we searched for a new Zn based binary quasicrystal as well as approximant crystals in a Zn-rich point of Zn-TM systems.

Samples were prepared using a self-flux method. Pure elements of Zn(6N) and TM with initial compositions of $Zn_{100-X}TM_X$ with X in the range between 0.1 and 1.0 were placed in an alumina crucible, sealed inside a quartz tube under argon atmosphere. The elements were melted at 700°C for 10h, and slowly cooled to 430°C. Then, single grains were separated from the melt using a centrifuge. The characterization of the samples was performed by powder X-ray diffraction.

The results of the phase obtained will be presented in the poster.

1. P. C. Canfield *et al.*, Phys. Rev. B **81** (2010), p. 20201

Synthesis of Ni-bearing crystalline approximants

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Keywords: approximant, transition metal, rare-earth

In this work, alloys in the M-Ni-Rare-earth (RE) systems were investigated in order to elucidate the possibility of the formation of a Ni bearing approximant phase. Mother ingots in the M-Ni-RE systems with various metals (M) were prepared in an arc furnace and then they were melt-spun onto a Cu wheel. The obtained phases before and after melt-spinning were examined by X-ray diffraction. As a result, we have obtained 1/1 approximant (AP) in the Ga-Ni-Yb system. The phase stability and magnetic property of the Ga-Ni-Yb 1/1 AP will be presented at the poster session with the results on the other M-Ni-RE systems.

Defect lines in colloidal structures grown on quasicrystalline substrates

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Keywords: Quasicrystal, Colloids, Defects

We study a colloidal model system in order to investigate the properties of defect lines in colloidal quasicrystalline structures that grow on substrates.

Colloidal suspensions, dispersions of micro-sized particles in a fluid, are a well known model system in statistical physics. The behaviour of such particles on substrates is important for a lot of applications like photonic crystals, colloidal nanofilms or novel materials with special rheological or frictional properties.

We design our substrates with quasicrystalline symmetry from aperiodic tilings or patterns of interfering laser beams [1,2]. In addition, by spatial varying phononic and phasonic displacement fields [3], a point defect can be incorporated into the system with a well-defined Burgers vector.

The growth process is studied by using Monte-Carlo simulations. For appropriate substrate patterns, we observe the formation of colloidal layers with distinct quasicrystalline symmetry.

In order to investigate the influence of the defects on the growth process, we decompose the average colloidal positions for each layer into their individual density modes (cf. [4]). Such an analysis reveals the positions of the defects in each layer and their topology. We find that the direction in which a defect line turns in a growing quasicrystalline structure depends on the Burgers vector.

We kindly acknowledge the Deutsche Forschungsgemeinschaft for financial support (Schm 2657/2).

1. J. Mikhael, G. Gera, T. Bohlein, and C. Bechinger, Soft Matter **7** (2011), p. 1352.
2. M. Schmiedeberg and H. Stark, Phys. Rev. Lett. **101** (2008), p. 218302.
3. P. De and R. A. Pelcovits, Phys. Rev. B **35** (1987), p. 8609.
4. L. Korkidi, K. Barkan, and R. Lifshitz, arXiv:1211.3446 (2012).

Formation of the icosahedral Al-Cu-Fe phase by solid state reaction

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Keywords: quasicrystals, solid-state reaction

In the context of industrial applications, quasicrystal powders show great potential as composite materials fillers, especially for metal matrix and polymer composite [1, 2]. Several methods such as mechanical alloying, gas-atomisation [3, 4] are used now to produce the quasicrystal powders. Furthermore, the use of this method on an industrial scale appears difficult because of the high cost and complexity of the process – less expensive and more efficient synthesis techniques are therefore needed. A possible candidate technique is the conventional solid-state synthesis, a very simple and low cost method of fabricating quasicrystalline powders in large quantities.

In this study we investigated the formation of the Al-Cu-Fe icosahedral phase in the solid-state synthesis, depending on the initial composition and annealing conditions. Pellets with nominal compositions of $Al_{63}Cu_{24}Fe_{13}$, $Al_{62}Cu_{25.5}Fe_{12.5}$ and $Al_{65}Cu_{20}Fe_{15}$ have been annealed at 550, 650 and 750 °C between 2 and 20 hours and subsequently rapid cooled. At the initial stages of annealing, body-centered cubic β-AlFe(Cu) and monoclinic λ-$Al_{13}Fe_4$ phases as well as icosahedral phase are formed. Evolution of the icosahedral phase during annealing is due to dissolution of the β and λ phases. The concentration of the icosahedral phase in all the samples studied increased with increasing annealing temperature from 550 to 650 °C and reached its maximum value after annealing for 20 hours at 650 °C. The maximum concentration of icosahedral phase was close to 100 per cent in $Al_{63}Cu_{24}Fe_{13}$. The obtained result allows to state that the solid-state synthesis is promising method for producing of large amounts of quasicrystalline powder for industrial applications.

1. Y. H. Qi, Z. P. Zhang, Z. K. Hei, C. Dong, J. Alloys Comp. **285** (1999), p. 221-228.
2. P. D. Bloom, K. G. Baikerikar, J. U. Otaigbe, V. V. Sheares, Mater. Sci. Eng. **294** (2000), p. 156-159.
3. S. M. Lee, J. H. Jung, E. Fleury, W. T . Kim, D. H. Kim, Mater. Sci. Eng. A **294–296** (2000), p. 99-103.
4. P. Barua, V. Srinivas, B. S. Murty, Phil. Mag. A **80** (2000), p. 1207-1217.

Quasicrystalline phase in Al-Mn-Fe-X melt spun ribbons – structure and stability

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Keywords: quasicrystals, melt-spinning, stability

Aluminium alloys strengthened with quasicrystalline particles exhibit interesting mechanical properties, especially high strength [1, 2]. Structure responsible for these properties consisting of small quasicrystalline particles embedded in an aluminium matrix can be formed in various processes including rapid quenching [3].

In this work, alloys with nominal compositions $Al_{91}Mn_6Fe_2X_1$ (X=Cr, V, Ti, Mo, W) were prepared by the melt-spinning method. The aim of the study was to investigate the effects of subsequent alloying elements on the structure, morphology, and stability of quasicrystalline phase present in the sample.

Substitution of manganese by other elements, especially characterized by low diffusion coefficient in aluminium, improves thermal stability of quasicrystalline phase confirmed by the DSC measurements.

The studies of the structure, morphology and composition of the quasicrystals were performed by X-ray diffraction and TEM techniques including electron diffraction, EDS microanalysis and high resolution imaging. It was found that all of investigated alloys contained mainly two phases α-Al and quasicrystalline phase of icosahedral type.

Transformation of quasicrystalline phase into stable crystalline phase during heating was studied for all the alloys revealing formation of different phases depending on alloying element used.

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1. A. Inoue, M. Watanabe, M. H. Kimura, F. Takahashi, A. Nagata and T. Masumoto, Materials Transactions JIM **33** (1992), p. 723.
2. M. Galano, F. Audebert, A. G. Escorial, I. C. Stone and B. Cantor, Journal of Alloys and Compounds **495** (2010), p. 372.
3. A. Inoue, H. Kimura, and S. Yamamura, Metals and Materials International **9** (2003), p. 527.

Formation and evolution of quasicrystals in amorphous Zr-Cu-Ni-Al-Ag alloys

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Keywords: Zr-Cu-Ni-Al-Ag, amorphous alloy, quasicrystallization, thermal analysis, electron microscopy

Thermal dynamic properties and structural changes related to the quasicrystallization process in melt-spun $Zr_{65}Al_{7.5}Ni_{10}Cu_{17.5-x}Ag_x$ amorphous alloys (x=0, 5, 10, 17.5 at%) have been studied by means of differential scanning calorimetry (DSC) analysis, transmission electron microscopy (TEM) and X-ray diffraction (XRD) techniques. The results show that substituting of Cu with Ag has a remarkable influence on many aspects of the Zr-Al-Ni-Cu amorphous alloy system, including microstructural features, thermal stabilities, crystallization behaviors, hardness, quasicrystal-forming and glass-forming abilities, and so on. The melt-spun $Zr_{65}Al_{7.5}Ni_{10}Cu_{17.5}$ amorphous alloy, which is free of Ag, has the best glass-forming ability. A proper amount of addition of Ag by replacing part of Cu can improve the quasicrystal-forming ability greatly. However, a negative effect will dominate if the Ag-content is over about 5 at%. For the Zr-Al-Ni-Cu-Ag alloys in melt-spun and glass transition states, the existence of quasicrystal-like ordering in local regions with diameters of 3-4 nm has been confirmed by high-resolution electron microscopy observations. We have found that, unlike the two-stage crystallization process in the Zr-Al-Ni-Cu-Ag system reported previously, the crystallization process in the $Zr_{65}Cu_{12.5}Ni_{10}Al_{7.5}Ag_5$ amorphous alloy can be divided into three stages. At the initial stage, the icosahedral quasicrystal (I-phase) was formed as primary phase from the amorphous matrix without apparent compositional variation. In comparison with the amorphous matrix, the I-phase was formed with a composition slightly rich in Zr,Ag,Ni and poor in Cu, Al. I-phase was formed with high nucleation and growth rates by consuming the amorphous matrix, and this leaded to a structure with closely packed grains at the first stage of crystallization. However, the residual amorphous phase still exists at this stage. Stable crystalline phases with sandwich-like morphology were found to form in the final stage.

Nanoquasicrystalline phase in mechanically alloyed and heat-treated $Al_{73}Cu_{11}Cr_{16}$

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Keywords: mechanical alloying, nanoquasicrystalline phase, decagonal phase

As it was shown in previous work [1], long-term mechanical alloying of powder with nominal composition of $Al_{73}Cu_{11}Cr_{16}$ followed by annealing at 700 C during 1 hour gives rise to the formation of pure decagonal quasicrystal. In the current work transmission electron microscopy (TEM), thermal analysis with heating above the melting temperature and measurement of chemical composition were carried out to determine structure, thermal stability and exact chemical composition of the decagonal quasicrystal.

According to the TEM investigation the average grain size of quasicrystalline phase is about 60 nm and its periodicity along the 10-fold axis shown to be 1.26 nm.

Chemical composition was determined by both the inductively coupled plasma atomic emission spectroscopy (ICP-AES) and energy-dispersive spectroscopy (EDS). The composition of as-annealed quasicrystalline phase was found to be $Al_{71.5}Cu_{11.5}Cr_{16.5}Fe_{0.5}$ (EDS) whereas as-milled powder had slightly different composition – $Al_{72.7}Cu_{11.1}Cr_{15.7}Fe_{0.5}$ (ICP-AES) and $Al_{72.2}Cu_{11.1}Cr_{16.2}Fe_{0.5}$ (EDS). Small amount of iron appears in the powder due to wear of milling tools.

Differential thermal analysis revealed that the decagonal phase is stable up to about 800 C. Above this temperature it undergoes the two-stage melting which ends at about 1150 C. The melted and then slowly cooled (20 K/min) sample remains the pure decagonal quasicrystal.

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1. A. P. Shevchukov, T. A. Sviridova, S. D. Kaloshkin, V. V. Tcherdyntsev, M. V. Gorshenkov, M. N. Churyukanova, D. Zhang, Z. Li, Journal of Alloys and Compounds http://dx.doi.org/10.1016/j.jallcom.2013.02.043.

Tsai-type quasicrystal and its approximant in Au-Al-Tm alloys

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Keywords: quasicrystal, approximant, Tsai-type, Au-based alloy, Rietveld refinement

In Au-based alloys, only five quasicrystals, Au-(Ga, In, Sn)-Ca, Au-(Al, In)-Yb [1], are known. It may be important to add new member of Au-based quasicrystal containing lanthanoids in order to understand unusual properties of intermediate valance state of Yb and the related quantum critical phenomena recently reported in Au-Al-Yb. Here we present experimental results on stable icosahedral quasicrystal and its cubic 1/1 approximant in Au-Al-Tm system.

Alloy ingots of $Au_xAl_{100-x-y}Tm_y$ were synthesized in narrow compositions of $48 \leq x \leq 49.6$ and $14.6 \leq y \leq 17.5$. Specimens were prepared by arc-melting under an atmosphere of Ar on water-cooled hearth. They were annealed at 800~910℃ for 50~100 hours. In order to study the phase stability, some specimens were melted at 1020℃ and slowly cooled to 820℃. Powder X-ray diffraction experiments were carried out with CuKα radiation. The crystal structure of the approximant was analyzed by Rietveld method using the Au-Al-Yb model (space group $Im\bar{3}$) as a starting model.

A P-type icosahedral quasicrystal was formed almost exclusively at $Au_{49}Al_{34}Tm_{17}$ in both as-cast and annealed specimens. The quasicrystal was also formed in the melted specimen successively annealed at 820℃ for 8.5 hours with the 1/1 approximant. Thus the quasicrystal is regarded as a stable phase in this alloy system. Six-dimensional parameter of this quasicrystal was determined to be $a_{6D} = 7.412(2)$ Å.

A 1/1 approximant was formed around $Au_{49}Al_{36}Tm_{15}$ in both as-cast and annealed specimens. In particular, the approximant was formed exclusively at $Au_{49.0}Al_{36.2}Tm_{14.8}$. The Rietveld analysis successfully converged with $\mathcal{R}_{wp} = 5.85$ % with the lattice parameter $a = 14.158(1)$ Å. This model includes 87.8 Au, 64.2 Al, and 24.0 Tm atoms, and then 176.0 atoms in total. The corresponding composition is $Au_{49.9}Al_{36.4}Tm_{13.6}$ that agrees with both the nominal composition and the analyzed composition $Au_{49}Al_{36}Tm_{15}$ by EPMA. With respect to the chemical ordering, the Au-Al-Tm approximant is similar to the Au-Al-Yb, but with 100% occupation of M8 site (see Ref. [1] for the site classification). Details of the model will be presented.

In conclusion, we have observed two new stable phases in Au-Al-Tm alloys; one is $Au_{49}Al_{34}Tm_{17}$ quasicrystal and the other $Au_{49}Al_{36}Tm_{15}$ 1/1 approximant. In both phases Tm with fixed valence, namely trivalent Tm, is expected, and then they may be valuable as a standard substance to understand the unique properties of Au-Al-Yb phases.

1. T. Ishimasa, Y. Tanaka and S. Kashimoto, Phil. Mag. **91** (2011), p. 4218-4299

Structure of Al-Fe-Ni decagonal quasicrystal studied by Cs-corrected STEM

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Keywords: decagonal quasicrystal, Al-Fe-Ni, Cs-corrected STEM

Structure of Al-Fe-Ni decagonal quasicrystal in an $Al_{72}Ni_{24}Fe_4$ alloy consists of two quasiperiodic planes along the periodic axis. We characterized the atomic arrangements in the two planes with high-angle annular dark-field (HAADF) and annular bright-field (ABF) images obtained by a spherical aberration corrected (Cs-corrected) scanning transmission electron microscopy (STEM).

In observed HAADF-STEM images taken with the incident beam parallel to the periodic axis, sites for transition-metal (TM) atomic columns and mixed sites (MS) for the columns of Al and TM atoms appear as separated bright dots with different contrasts. From an arrangement of bright dots in the HAADF-STEM images, we can directly determine the arrangements of TM atoms and MS on the two quasiperiodic planes. From the STEM HAADF, the sites for TM atoms on the two quasiperiodic planes are determined to be located at lattice points in a Penrose lattice of an edge-length of 0.25 nm, and they are also determined to be arranged with pentagonal tiling of an edge-length of 0.76 nm. Furthermore, we also can characterize the atomic arrangements of TM atoms and MS on the structure including glue regions between the large clusters by a bond-orientational ordered (BOO) arrangements of TM atoms and MSs.

In observed ABF-STEM images, all atomic columns including those of Al atoms appear as dark dots, and the separated dots are located in a lattice of 0.13 nm. Thus, with HAADF and ABF-STEM images, the arrangements of all atoms in the large cluster, including an arrangement of Al atoms, were determined.

The obtained structure of the Al-Ni-Fe decagonal quasicrystal is concluded to be similar to the Al-Co-Ni decagonal quasicrystal referred as to Ni-rich basic structure in an $Al_{72}Co_8Ni_{20}$ alloy [1]. In addition, we will discuss about the occupation domains of the arrangements of TM atoms with BOO in an ideal pentagonal lattice of an edge-length of 3.2 nm.

1. K. Hiraga and A. Yasuhara: Mater. Trans. **54** (2013), pp. 720-724

Preparation of nanocrystalline Pd-TM alloy catalysts from Al-Pd-TM quasicrystals and approximants

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Keywords: nanocrystalline, Pd-TM alloy, catalyst

Most Al-based quasicrystals (QCs) contain catalytically active metals such as Pd, Ni or Cu. Therefore, the catalytic properties of some QCs have been examined so far and results are found to be promising [1-4]. For example Al-Cu-Fe QC powder leached in NaOH aqueous solution shows a higher reactivity and thermal stability than conventional copper catalysts in steam reforming of methanol (SRM) [1,4]. The quasiperiodic structure of the Al-Cu-Fe QC plays an important role in the formation of a homogeneous leached layer that is responsible for the high activity and stability for SRM [4]. However, there are few studies with respect to preparation of alloy catalysts focused on complexity or quasiperiodicity for QCs and approximants. Recently, we found that nanocrytalline Pd-TM alloys can be prepared by the selective leaching of Al from Al-Pd-TM (TM=Ni, Co) QCs. Alloying between Pd and TM occurred in a self-assembled manner during leaching process. The advantage of this method is that there is no restriction of reduction properties of the constituent metals because neither metal complexes nor metal salts were used in the process, and hence instead of core-shell structure, a homogeneous solid solution would be formed in nanoparticles.

We will show here the leaching behaviors, the properties of catalysis and hydrogen absorption of nanocrystalline Pd-TM alloys obtained from Al-Pd-TM (M=Ni, Co) QCs and approximants.

1. A. P. Tsai and M. Yoshimura, Appl. Catal. A **214** (2001), p. 237-241.
2. B. P. Ngoc, C. Geantet, J. A. Dalmon, M. Aouine, G. Bergeret, P. Delichere, S. Raffy, S. Marlin, Catal. Lett. **131** (2009), p. 59-69.
3. J. Highfield, T.Liu, Y. S. Loo, B. Grushko, A. Borgna, Phys. Chem. Chem. Phys. **11** (2009), p. 1196-1208.
4. T. Tanabe, S. Kameoka, A. P. Tsai, Appl. Catal. A **384** (2010), p. 241-251.

Evolution of the β phase flux dissolution during quasicrystal formation

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Keywords: quasicrystals, peritectic reaction, flux dissolution

The quasicrystalline as well as periodic phases were obtained during directional crystallization of an Al–Cu–Fe alloy for a chemical composition close to the compositional triangle in which the quasicrystalline phase occurs [1].

During crystallization of single quasicrystalline ψ phase Al_6Cu_2Fe, the flux dissolution of the β phase apparently plays an essential role in a peritectic reaction leading to the quasicrystalline ψ phase formation.

The main result of this investigation is related to the experimental visualization of evolution of the flux dissolution of the high temperature β phase, which apparently provides necessary material for peritectic formation of quasicrystalline ψ phase. We assume [1] that solid droplets of the β phase, formed primarily by the surface tension of liquid in a space of a bubble or shrinkage, may have a significant contribution during the flux dissolution to the peritectic reaction $\beta + \lambda + L \rightarrow \psi$ identified, for example, by Lograsso and Delaney [2]. The β phase consumption by dissolution was confirmed during investigations of phase transformations of Al–Cu–Fe alloys performed by Zhang et al. [3]. The attractive flux dissolution morphology of cubic β phase confirmed a high structural perfection of the primary crystallized droplet-like single crystals.

1. M. Surowiec, W. Bogdanowicz, J. Krawczyk, B. Formanek, M. Sozanska, Phil. Mag. **91** (2011), p. 2458.
2. T.A. Lograsso and D.W. Delaney, J. Mater. Res. **11** (1996), p. 2125.
3. L.M. Zhang, J. Schneider and R. Lück, Intermetallics **13** (2005), p.1195.

A search for new quasicrystal approximants in the Al-Pd-Cr-Fe and Al-Pd-Mo-Fe systems

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Keywords: Crystal structure, F-type icosahedral quasicrystal

Recently, it has been reported that a stable approximant for Al-based F-type icosahedral quasicrystals could be obtained in $Al_{70}Pd_{20}Cr_3Fe_7$ alloy by annealing at around 850℃. Single crystal X-ray diffraction has been successfully used to solve the crystal structure, which is described with two kinds of cluster [1]. Still, there has been no other approximant reported on F-type icosahedral quasicrystal with comparable stability. Our present aim is to search for new approximants by seeking suitable conditions such as temperature, component and composition.

It turns out that a diffraction pattern similar to that of quasicrystal was observed from an $Al_{70}Pd_{20}Cr_3Fe_7$ sample by annealing at 750℃ for 48h by X-ray diffraction and electron beam diffraction, while several phases were indicated through annealing at 950 ℃ for 48h. However, no identification of new approximants is observed only by changing temperature.

The second attempt to obtain new approximant is done by replacing Cr with Mo. Here, three samples of different compositions, $Al_{70}Pd_{20}Mo_xFe_{(10-x)}$ with x=3,5,7 are synthesised. The sample with x=3 is most likely to have the least amount of impurity, for which slow cooling (cooling rate, 5K/h) from the melting point was attempted to make a single crystal. A X-ray powder diffraction pattern similar to that in $Al_{70}Pd_{20}Cr_3Fe_7$ (cooling rate, 10K/h) by 10K/h is demonstrated as shown in Fig.1. Though the difference between the two patterns is very small, single crystal X-ray diffraction has revealed that new sample includes two different approximants with lattice constants of about 40Å and 60Å. Results of structure analysis with X-ray diffraction will be presented.

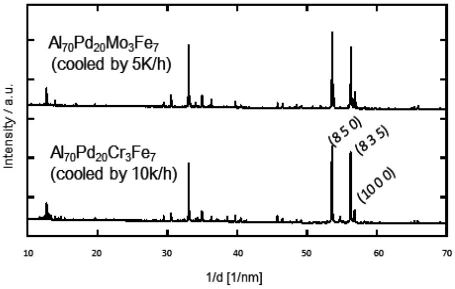

Fig.1. Powder X-ray diffraction pattern (SPring-8, Beam line BL15XU)

1. N. Fujita *et al.*, Acta Cryst. A **69** (2013), p. 322-340.

Finite element method for static problems of cubic quasicrystals

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Keywords: cubic quasicystals, finite element method, crack.

Cubic quasicrystals are an important kind of three-dimensional quasicrystals, whose mechanical behaviors, especially elasticity and defects of quasicrystals, have been investigated extensively by numerous experimental and theoretical researches. Beyond the scope of classical elasticity, apart from classical phonon displacement field, there is phason displacement field in the elastic theory of the quasicrystals, which makes the analytical solution difficult to be obtained.

In this paper, a three-dimensional finite element algorithm for static problems is deduced from the variation of a kind of general potential function of cubic quasicrystals. A quasicrystal column containing a penny-shaped crack is investigated. The comparisons with the analytical stress intensity factors show that the numerical solution's precision and efficiency are satisfactory. Then a cubic quasicrystal three point bending specimen is modeled in this paper. The coupled displacement and stress fields of cubic quasicrystals are simulated, and the differences of those from crystals are analyzed.

The results of the two examples show that the finite element procedure can be used to solve more complicated boundary value problems. These also provide important information for further studying the deformation and fracture of the new solid phase and understanding clearly the interplay of the interaction between the phonon and phason activity.

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Crystal structure refinement of RE-Au-Sn (RE=Yb and Gd) approximants using single crystal x-ray diffraction data

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Key words: quasicrystal approximant, crystal structure refinement

The crystal structures of two quasicrystal approximants, YbAuSn and GdAuSn, have been refined by collecting single crystal x-ray diffraction data. Both materials have shown basic polyhedral cluster units that are similar to those found in Tsai-type icosahedral quasicrystals [1]. The basic polyhedral units can be described as concentric shells of disordered tetrahedron, dodecahedron, icosahedron, icosi-dodecahedron and defect-triacontahedron, listed consecutively from the inside to out. The YbAuSn compound is found to be a 2/1 approximant crystal with well-defined chemical order at the cluster level, similar to that found in ternary 1/1 approximants [2]. The chemical order in the current compounds has been carefully analyzed. Moreover, magnetic measurements confirm that the valence state of Yb in the YbAuSn compound is +2.

1. A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura, and T. J. Sato, Nature (London) **408** (2000), p. 537.
2. Girma Hailu Gebresenbut, Ryuji Tamura, Daniel Eklöf and Cesar Pay Gomez, J. Phys.: Condens. Matter **25** (2013), p. 135402.

Tile Hamiltonian approach to decagonal ZnMgY quasicrystal

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Keywords: Mg-Zn-Y decagonal, simulation, tile Hamiltonian

We model the large-scale order in d-ZnMgY, a stable decagonal quasicrystal alloy of the layered Frank-Kasper type, which consists of a 10-fold-symmetric rectangle-triangle tiling with a deterministic two-layer binary decoration. First, from empirical ZnMg pair potentials fitted to ab-initio data, we extract an effective Hamiltonian in terms of tiling degrees of freedom, which attributes an energy cost to each vertex type[1]. Then we carry out Monte Carlo annealing of the tiling with this effective Hamiltonian, using a nonlocal updating algorithm [2]. We find that, in low energy states, the subset of tiling vertices with fivefold symmetry form a highly constrained supertiling at a larger scale. This is similar (but not identical) to the supertiling seen in high-resolution electron microscope images by E. Abe [3]. We also identify the Mg sites which are favorable for substitution by Yttrium; we show how the addition of a small fraction of Y can make the decagonal phase thermodynamically stable. In fact, d-MgZnY is predicted to be stable only at higher temperatures but the new composition d-MgZnSc should be stable even at T=0.

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1. M. Mihalkovic, C. L. Henley, J. Richmond-Decke, and M. Oxborrow, preprint (http://arxiv.org/abs/1112.3951).
2. M. Oxborrow and C. L. Henley, Phys. Rev. B **48** (1993), p. 6966.
3. E. Abe, T. J. Sato, and A. P. Tsai, Phys. Rev. Lett. **82** (1999) 5269.

A cubic quasicrystal in a rapidly-solidified Mg-Al alloy

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Keywords: structure, STEM, cubic

It is commonly accepted that the definition of quasicrystal should include an rotational symmetry forbidden in periodic crystals. On the other hand, the quasicrystal with a crystallographic point group is possibly argued both theoretically and experimentally [1,2]. In a rapidly-solidified Mg-Al alloy, intriguing electron diffraction patterns (EDPs) were reported, which show a cubic symmetry with aperiodic arrays of Bragg reflections that appears in relation with the irrational number $\sqrt{3}$ [2]. In the present work, we investigate the detailed structure of the rapidly-solidified Mg-Al phase based on direct structure observations using STEM.

In the Mg-Al system there exists β-Mg_2Al_3 phase in the vicinity of the composition Mg-61 at.% Al, which consist of icosahedral and tetrahedral close packing [3]. In a rapidly-solidified Mg-61 at.% Al alloy, 2-fold, 3-fold, and 4-fold EDPs are obtained, which shows that the structure has the cubic point group. However, the relevant diffraction spots are arranged aperiodically. Especially in the 2-fold EDP, a high density of the spots is observed, and the corresponding HADDF-STEM image shows several remarkable features. Two length scales, L and S, can be definitely observed, and they are arranged quasiperiodically along the 3-fold axis. Both the number ratio and length ratio of L and S are estimated to be around 1.38, and their arrangement can be well described by the hyperspace crystallography. Namely, a physical space tilted by the angle θ, where $\tan\theta \approx 1.38$, with respect to the 2-dimensional square lattice successfully generates the observed quasiperiodic pattern. We construct a simple model without detailed atomic decoration, and the simulated EDPs of the model reproduces fairly well the experimental patterns. Further analysis of the images reveals that the present quasiperiodic structure has similar local structure to the β-Mg_2Al_3 phase; two lengths correspond to L and S may be reasonably defined.

The quasicrystal with a cubic symmetry is unambiguously determined for the first time, based on a direct structural observation. The present results strongly suggest that the noncrystallographic rotational symmetry is not an essential factor to form the quasiperiodic structure, raising a very fundamental, universal question on the physical origin of a long-range order of condensed matters.

1. R. Lifshitz, Journal of Alloys and Compounds **342** (2002), p. 186
2. P. Donnadieu, H.L. Su, A. Proult, M. Harmelin, G. Effenberg and F. Aldinger, J.Phys. I France **6** (1996), p. 1153
3. S. Samson, Acta Cryst. **19** (1965), p. 401.

Tetrahedron ordering in the Cd_6Tb and Zn_6Sc 1/1 quasicrystalline approximants: Experiment and Simulation

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Keywords: quasicrystal approximant, phase transition, domain

The discovery of binary quasicrystal $Cd_{5.7}Yb$ and $Cd_{5.7}Ca$ breaks a path to deeply investigate structure and physical properties of quasicrystal [1,2]. For nowadays, the technique determining atomic structure of binary quasicrystal has been developed maturely [3], however, study quasicrystal directly is still a challenging work. As counterparts of icosahedral quasicrystal, Cd_6R (R=rare elements) as well as Zn_6Sc 1/1 approximants, are expected to play a key role to understand different properties of quasicrystal.

Other than quasicrystals, most of the cubic approximants have been evidenced an order-disorder phase transition from space group Im-3 to Cc or C2/c, and the ordering of innermost Cd4/Zn4 tetrahedron in Tsai-type cluster is indicated as the trigger factor [4-5]. According to symmetric operation, 6 domains with different orientations are obtained in the low temperature phase [6].

We will present high-resolution x-ray diffraction and diffuse scattering in situ measurements using synchrotron data. And this will be compared with atomic scale molecular dynamic simulation. The structural phase transition is observed at ~190 K and 159 K for Cd_6Tb and Zn_6Sc respectively. Diffuse scattering with respect of temperature is discussed both experimentally and simulatively to Zn_6Sc. A deep measurement is carried out with some fundamental reflections below Tc, and the 3-D peak splitting contributed by different domains is visualized using a new method.

1. A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura and T. J. Sato, Nature **408** (2000), 537.
2. J.Q. Guo, E. Abe and A.P. Tsai, Phys. Rev. B **62** (2000), R14605.
3. H. Takakura, C. P. Gómez, A. Yamamoto, M. de Boissieu and A. P. Tsai, Nature Materials **6** (2007), 58.
4. R. Tamura, Y. Murao, S. Takeuchi, M. Ichihara, M. Isobe and Y. Ueda, J. J. Appl. Phys. **41** (2002), L524.
5. R. Tamura, K. Edagawa, C. Aoki, S. Takeuchi and K. Suzuki, Phys. Rev. B **68** (2003), 174105.
6. T. Yamada, H. Euchner, C. P. Gómez, H. Takakura, R. Tamura and M. de Boissieu, J. Phys.: Condens. Matter **25** (2013), 205405.

Structure prediction of novel stable metal-boride alloys related to quasicrystals

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Keywords: phase stability, structure prediction, quasicrystals

Ab-initio prediction of new stable alloy structures ("...where are the atoms?") is nowadays feasible only under very limited circumstances, with the number of independent atoms being the main limiting factor due to exponentially growing configurational space. On the other hand, as we demonstrate here, the inverse approach is readily available: take a particular – known or hypothetical structure – and ask which alloy system (i.e. combination of species) is most appropriate for it in terms of stability relative to competing structures. We demonstrate this approach starting from known metal-borides B4CrY and B6ReY2, whose structures can be interpreted as decagonal approximants, and several hypothetical structures, representing generalization or variation of the structural motifs found in the former structures. We then assign Wyckoff positions systematically to species from segments of the periodic table, and compute phase stability within the density-functional theory approximation. As a result, we have evaluated phase stability of our target structures across ~1300 ternary and quaternary systems, finding 142 alloy systems with stable B6ReY2 structure type (as compared to few tens of experimentally known systems). In addition, 14 quaternary systems stabilize one hypothetical structure that we designed as a variation of the B6ReY2 phase. These predictions should be amenable to experimental validation.

In situ observation of “phason flip” in realistic annealing simulation of ε-Al-Pd-Co phases

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Keywords: Al-Co-Pd, decagonal quasicrystal, ε-phases, pseudo-Mackay cluster

Using empirical oscillating pair potentials (EOPP) fitted to *ab-initio* Al-Co-Pd data, and energetically optimized structural models of ε-phases from related Al-Mn-Pd compounds [1], we have set up annealing simulation at and below T=1200K of so called ε_{16}-phase with about 400 atoms in primitive cell. The simulation is capable of overcoming diffusion barriers combining molecular dynamics, and lattice-gas like swaps exchanging Al/TM atoms at randomly picked pairs of sites. Upon evolution of annealing, we observe for the first time in realistic simulation effective “jump” of so called pseudo-Mackay cluster; such rearrangement of atoms can be represented as a “flip” of tiling vertex, where the tiling edges connect centers of the pseudo-Mackay clusters about 7.5A apart. Prolonged annealing at low temperatures utilizing adapted version of so called *j-walking* annealing scheme freezes the structure into variants with or without *overlaps,* corresponding to tau-shorter intercluster linkage. Ab-initio total energies of these competing states are nearly degenerate, just few meV/atom unstable against a mixture of Al_9Co_2, $Al_{21}Pd_8$ and ternary Al_9Co_2Pd phases.

1. B. Frigan, A. Santana, M. Engel, D. Schopf, H.-R. Trebin, M. Mihalkovič, Phys. Rev. B 84, 184203 (2011); see also poster of B. Frigan *et al.*

Canonical-cell tiling and real icosahedral approximants

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Over 20 years ago, the "canonical-cell tiling" (CCT) was introduced [1] as a geometrical framework for conveniently representing quasicrystals (and related structures) built around a network of icosahedral clusters. It has gradually become clear that the CCT is rather successful, in that every large approximant that was solved, turned out to be a CCT. In this contribution, we catalogue and evaluate all developments of CCT-based modeling:

(1) results (or lack thereof) from mathematics (failure to construct a 6D-cut quasiperiodic CCT) and from statistical mechanics (some validation of CCT as a random tiling model with great difficulties of simulation)

(2) the development (by us and collaborators) of structure models, based on atoms decorating the cells of the CCT, as a basis to computationally explore the stability of quasicrystal approximants. One lesson from this work is that the uncertainties are mostly related to the largest ("D") cell; given the icosahedral cluster, one can more or less guess the atom arrangement in the three smaller kinds of cell.

(3) realization of canonical cell packings in particular large-cell approximants, in all the major classes of quasicrystal: GaMgPd (Mackay-icosahedron based), as well as AlGaMgZn (Frank-Kasper type), both solved by G. Kreiner with coworkers [2,3]; MgScZn (Tsai cluster-based), as solved by Lin and Corbett for example [4]; and AlCrFePd (based on small pseudo-Mackay icosahedra), as solved recently by Fujita *et al* [5].

We will also compare the CCT framework to the related approach, due to Takakura *et al* [6], of using the cluster network called the "12-fold packing" to generate 6D cut-project structure models that are locally well-packed.

1. C. L. Henley, Phys. Rev. B **43** (1991), p. 993.
2. G. Kreiner, Y. Moguilnikov, U. Burkhardt, M. Schapers, J. Non-Cryst. Sol. **334&335** (2004), p. 17.
3. G. Kreiner, J. of Alloys and Comp. **338** (2002), p. 261.
4. Q. Lin and J. D. Corbett, J. Am. Chem. Soc. **128** (2006), p. 13268.
5. N. Fujita, H. Takano, A. Yamamoto and A.-P. Tsai, Acta Cryst. A **69** (2013), p. 322.
6. H. Takakura, C. P. Gomez, A. Yamamoto, M. de Boissieu and A. P. Tsai, Nature Materials **6** (2007), p. 58.

Compositions of Al-based ternary quasicrystals interpreted using cluster-resonance model

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Keywords: Quasicrystals; cluster-resonance model; Electron concentration

Compositions of ternary Al-based quasicrystals are interpreted with a unified cluster formula [*icosahedron*](*glue*)$_{0,1}$ using the newly developed cluster-resonance model [1] and $e/u = 24$ formalism for ideal metallic glasses, with e/u being the total number of valence electrons accommodated in the unit cluster formula [2]. The icosahedra are derived from the corresponding approximants by the dense packing and cluster isolation criteria [3]. It is found that ternary QCs are always be expressed by third element substitutions on the basic binary cluster formulas [4]. The 24 valence electrons rule implies that the cluster formulas are both chemical and electronic structural units, which are analogous to the molecular formulas for chemical substances.

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1. G. Han, J. B. Qiang, Q. Wang, Y. M. Wang, C. L. Zhu, S. G. Quan, C. Dong, P. Häussler, Philos. Mag. **91** (2011), p. 2404.
2. G. Han, J. B. Qiang, F. W. Li, L. Yuan, S. G. Quan, Q. Wang, Y. M. Wang, C. Dong, P. Häussler, Acta Mater. **59** (2011), p. 5917.
3. J. X. Chen, Q. Wang, Y. M. Wang, J. B. Qiang, C. Dong, Philos. Mag. Lett. **90** (2010), p. 683.
4. H. Chen, J. B. Qiang, Q. Wang, Y. M. Wang, and C. Dong, Isr. J. Chem. **51** (2011), p. 1226.

An Icosahedral Quasicrystal as a Packing of Regular Tetrahedra

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Keywords: quasicrystal, tetrahedron, icosahedral symmetry, 600-cell, 3D Penrose tiling, decoration

We present the construction of a dense, quasicrystalline packing of regular tetrahedra possessing icosahedral symmetry. The tetrahedra of this quasicrystal may be classified into five types of clusters, the convex hulls of which are: the pentakis icosidodecahedron, the dodecahedron, a truncation of the icosahedron, and an irregular tetrahedron. This quasicrystal is obtained by the insertion of eight primitive types of tetrahedra into the icosidodecahedral, dodecahedral, and truncated icosahedral cells occurring in a 3D slice of the Elser-Sloane 4D quasicrystal [1] at the equator of a central 600-cell [2]. The placement of these tetrahedra is determined in correspondence with the arrangement of (irregular) tetrahedra within the vertex-first projection of the 600-cell to 3D, and its substructures. Additionally, it is shown that this quasicrystal can be equivalently produced through a decoration of the prolate and oblate rhombohedra in a three-dimensional Penrose tiling. The presented quasicrystal has a total of 10 "plane classes," defined as the total number of distinct orientations of the planes in which the faces of the tetrahedra are contained. The small number of plane classes was achieved by a special rotation of the tetrahedra discussed in [3].

1. V. Elser and N.J.A. Sloane, J. Phys. A.: Math. Gen. **20** (1987), pp. 6161–6168.
2. J.F. Sadoc and R. Mosseri, J. Phys. A.: Math. Gen. **26** (1993), pp. 1789–1809.
3. F. Fang, K. Irwin, J. Kovacs, and G. Sadler, arXiv:1304.1771 (2013).

Hyperspace analysis of a so-called 1D-quasicrystal in $Al_{71}Ni_{10}Co_{19}$

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Keywords: 1-dimensional quasicrystal, phason, STEM

Ritsch et al. investigated complicated quasicrystalline phases in Al-Ni-Co alloys, and systematically categorized them into representative 9 variant structures, among which the 1-dimensinal quasicrystal (1D-QC) was found around $Al_{71}Ni_{10}Co_{19}$ [1]. This is the only example of the experimentally identified 1D-QC phase so far, and its structure is shown to be reasonably generated by introducing linear phason strains into an ideal decagonal QC structure [1]. The occurrence of 1D-QC implies that the noncrystallographic rotation symmetry is not an essential factor to form quasioperiodic structure. Therefore, it is a very critical issue whether or not the true 1D-QC exists, to understand the origin of a unique aperiodic order. In the resent work, we revisit the 1D-QC in $Al_{71}Ni_{10}Co_{19}$ to investigate further details of the structure, based on electron diffraction and high-resolution STEM imaging. In particular, we attempt to look carefully the true distributions of the lattice points in the hyperspace, and find out that the structure is not a 1D-QC but a large approximant crystal.

The $Al_{71}Ni_{10}Co_{19}$ alloy was synthesized by melting pure elements in an arc furnace under reduced Ar pressure. Pieces of as-cast ingots were annealed at 1100℃ for 11 hours, followed by quenching into water.

The real-space lattice point distributions observed for the so-called 1D-QC structure are indexed with 4 coordinates to lift them up into a hyperspace. Given $\boldsymbol{D}$ as the phason strain matrix, phason strained perpendicular coordinates $\boldsymbol{r}$ reads:

$$\boldsymbol{r} = \boldsymbol{r}^{\boldsymbol{perp}} - \boldsymbol{D} \cdot \boldsymbol{r}^{\boldsymbol{para}}$$

By minimizing the dispersion of $\boldsymbol{r}$, we are able to determine the relevant $\boldsymbol{D}$, by which the true order of the lattice points in the perpendicular space can be derived. According to this *dispersion-minimization* criterion, we have successfully identified a large approximant crystal whose unit cell dimension is 8.4Å×61Å×85Å; this approximant model provides significantly better fits both with the electron diffraction and the STEM image than the previous 1D-QC model does. Disappearances of weak reflections along the certain direction, as due to the phason-related disordering, may easily cause misleading that the structure could be quasiperiodic.

1. S. Ritsch, O. Radulescu, C. Beeli, D. H. Warrington, R. Lück and K. Hiraga, Phil. Mag. Lett. **80** (2000), p. 107.

Structure model of decagonal ZnMgDy

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Keywords: decagonal phase, structure analysis, Frank-Kasper

Herein we report the structure analysis of the decagonal ZnMgDy (d-ZnMgDy) in the family of Frank-Kasper decagonal quasicrystals based on X-ray single crystal diffraction data. Crystals are grown in alloys having the overall composition $Zn_{57.6}Mg_{40.8}Dy_{1.6}$. The alloy is annealed at 375°C for 10 months and quenched to room temperature. X-ray diffraction experiments are 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 (CCD and Pilatus detectors λ=0.6980 Å and λ=0.6631 Å respectively).

The diffraction pattern is indexed by five direct space quasilattice parameters [1] with $a_{1\text{-}4}$ = 3.183(7) Å and a_5 = 5.214(5) Å. The SUPERFLIP program package [2] (based on charge flipping and low density elimination algorithms) is used for structure solution.

The model that leads to the best structure refinement results belongs to the space group of P10/mmm and consists of three large occupation domains located at (0,0,0,0,0), (1/5,1/5,1/5,1/5,1/4) and (2/5,2/5,2/5,2/5,1/4), and one small occupation domain at (0,1/2,1/2,0,1/2). This model was derived from the higher dimensional model discussed earlier for $Al_{65}Cu_{20}Co_{15}$ [3].

A second model obtained by the covering of one type of cluster (24 Å in diameter) with cluster centers obeying a Delone tiling (DT4) reported by Masakova et al. [4], is also investigated.

In addition to these results, the effect of the temperature on the ordering principles of the mentioned phase is a subject of current study. Two high temperature datasets are collected (at 325°C and 375°C) with the previously mentioned SNBL Beamline equipment. Initial results suggest that the phase does not undergo a phase transition or a major structural change.

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1. A. Yamamoto, Science and Technology of Advanced Materials **9** (2008), p. 1.
2. L. Palatinus and G. Chapuis, Journal of Applied Crystallography **40** (2007), p. 786.
3. A. Yamamoto, Scientific Reports RITU **A42** (1996), p. 207
4. Z. Masakova, J. Patera and J. Zich, Journal of Physics a-Mathematical and General **38** (2005), p. 1947.

Low-temperature superstructures of binary $RECd_6$ (RE = Rare Earth) approximants

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Keywords: approximants, superstructure, tetrahedron

The low-temperatures phase of several $RECd_6$ (RE=Rare Earth) approximants of the i-$Cd_{5.7}Yb$ quasicrystal have been determined by single crystal X-ray diffraction using high quality samples. The existence of Cd_4 tetrahedra at the centres of the icosahedral clusters is for the first time unambiguously observed in these phases and the Cd_4 tetrahedra are found to be orientationally ordered below T_c leading to the formation of superstructures with the cell parameters $a' = a\sqrt{2}$, $b' = a$ and $c' = a\sqrt{2}$, where a is the cell parameter of the basic cubic cell above T_c. The superstructures were solved in the monoclinic space group C2/c, with β angles close to 90°. This observation directly verifies that the phase transitions are due to an orientational order-disorder transition of the central Cd_4 tetrahedra. Owing to the absence of disorder in the low-temperature structures, the local distortions of the icosahedral shells surrounding the central tetrahedra are clearly seen. These findings allow us to understand the mechanisms behind the propagation of superlattice ordering and also to better understand the local distortions of the cluster shells of the icosahedral $Cd_{5.7}Yb$ quasicrystal. Finally these results also shed light on the final missing piece of the quasicrystalline $Cd_{5.7}Yb$ structure: the ordering of the Cd_4 tetrahedron [1,2].

1. H. Takakura, C. Pay Gómez, A. Yamamoto, M. de Boissieu, A. P. Tsai, Nat. Mater. **6** (2007), p.58.
2. T. Yamada, H. Euchner, C. Pay Gómez, H. Takakura, R. Tamura, M. de Boissieu, J. Phys.: Condens. Matter **25** (2013), p. 205405.

From Colorings to Weavings

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Keywords: hyperbolic tilings, colorings, weavings

Many crystalline nets in the Euclidean space E^3 are constructed from reticulation of the hyperbolic plane H^2. The construction of crystalline three-dimensional Euclidean nets is done by projecting two-dimensional hyperbolic tilings onto a family of triply periodic minimal surfaces (TPMSs)[1]. In this study, we construct weavings in H^2 which can then be used to construct three-periodic patterns by mapping the weavings onto periodic minimal surfaces.

We define a weaving as a simple arrangement of lines in the plane together with a binary relation specifying which line is above the other [2]. We consider weavings of overlapping nets derived from the colorings of tiling $*pqr$ in H^2, which is the tiling of the plane by triangles with interior angles $\pi/p, \pi/q$ and π/r. By abuse of notation, we also use $*pqr$ to denote the corresponding triangle group of the tiling generated by the reflections along the edges of a triangle in the tiling.

To construct overlapping nets, we use the fact that there is a one-to-one correspondence between the set of transitive n-colorings of tiling $*pqr$ and the set of index n subgroups of the triangle group $*pqr$ [3]. Given an n-coloring of tiling $*pqr$, we consider the vertex sets derived from the n types of colored domains, and then two neighboring vertices of the same color are connected by an edge if they are identified to each other; that is, they are mapped to each other by an element of the symmetry group of the colored tiling. This process yields n untangled overlapping nets. We then use some subgroups of the symmetry group of the overlapping nets to generate weavings. Furthermore, we also characterize when two weavings of overlapping nets are equivalent.

1. S. J. Ramsden, V. Robins and S. T. Hyde, Acta Cryst **A65** (2009), p. 81.
2. J. Pach, R. Pollack and E. Wezl, Algorithmica **9** (1993), p. 561.
3. E.D.B Provido, M.L.A.N. De Las Peñas and R. Felix, Acta Cryst **A** (to appear).

Direct observations of local electronic states in Al-based quasicrystals by STEM-EELS

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Keywords: Electronic structure, STEM, EELS

Most quasicrystals (QCs) reveal pseudogaps in their density of states around Fermi level, and hence the stability of QCs have been discussed in terms of energetic gains in electron systems. In fact, many QCs have been discovered by tuning valence electron density. Therefore, understanding electronic structures in QCs may provde an imprtant clue for their stabilization mechanism. Generally, it has been frequently discussed based on an interaction between Fermi surface and Brillouin zone boundary within the framework of nearly free electron model. However, real electronic structures of QCs have not yet been fully understood, particularly being in microscopic-macroscopic relations. In the present work, we investigate local electronic states in Al-based QCs using electron energy loss spectroscopy (EELS) combined with scanning transmission electron microscopy (STEM), by which EELS spectra with sub-Å probe and atomic structure can be obtained simultaneously. We report STEM-EELS results on $Al_{72}Ni_{20}Co_8$ and $Al_{57.6}Cu_{25.9}Ir_{16.5}$ decagonal phases [1].

Energy-loss near edge structures of $L_{2,3}$ edges of Ni and Co alter significantly depend on the local environment. Intensity ratio (L_2/L_3), as commonly correlated with 3d orbital occupancies, becomes larger at the 2-nm cluster centers than their edges. Plasmon loss spectra of the both QCs also appear to vary depending on the local environment. For the decagonal Al-Cu-Ir, principal components analysis clearly shows up the atomic-site dependence of plasmon loss spectra in a two-dimensional map. Qualitatively, there seems to be certain correlations between the plasom peaks and the L-edges, both of which reveal different behaviours at the cluster centers and the edges. Since plasma oscillation is collective motion of valence electrons with several tens of nm-scale, the site dependence of plasmon loss spectra may be caused by inter-band transitions with localized d-states. These results suggest that hybridization strength between Al sp states and transition metal d states is different at the cluster centers and the edges. QCs seem to have unusual electronic structures, which may stabilize their complex quasiperiodic structures.

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1. P. Kuczera, J. Wolny and W. Steurer, Acta Crystallogr. **B68** (2012), 578.

Soft X-ray Emission Study of Al-Co-Ni Quasicrystals

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Keywords: decagonal quasicrystal, soft X-ray emission spectroscopy, electronic structure

Al-Co-Ni alloys form decagonal quasicrystals (d-QC) in a wide concentration range with various structural modifications depending on a Co/Ni ratio [1]. According to a theoretical study [2], a pentagonal Al-transition metal (TM) ring is formed in the center of the decagonal column in Co-rich $Al_{72}Co_{20}Ni_8$, while Ni-rich $Al_{72}Co_8Ni_{20}$ shows symmetry-breaking of the column center to a hexagon-boat-star tiling with Ni-Ni pairs. To clarify the chemical nature bringing their unique atomic arrangements from spectroscopic points of view, we have studied the d-QC TM 3d electronic structures by the TM $L\alpha$ soft X-ray emission spectroscopy (XES) as well as the X-ray photoelectron one (XPS) and a cluster calculation. In this report, we present results of bulk-sensitive XES measurements compared with the previous surface-sensitive XPS measurement [3].

XES measurements were performed at BL2C of Photon Factory, KEK by using the synchrotron light as the excitation source. Much attention was paid to the energy calibration to compare the energy distributions of TM 3d states in studied d-QC. Specimens were prepared by Ar arc-melting and subsequent quenching for Ni-rich d-QC $Al_{72}Co_8Ni_{20}$ and by the Czochralski method for Co-rich one $Al_{72}Co_{16}Ni_{12}$.

The spectral shape and peak position of the Co and Ni $L\alpha$ XES spectra, which show the partial electronic density of states (DOS) of the respective $3d$ states, in the Ni-rich d-QC are not so much different from those in the Co-rich one, while the $3d$ band in the XPS spectra, which represent the total DOS, is shifted from the binding energy E_B of 2.3 eV in the Ni-rich d-QC to 1.8 eV in the Co-rich one. In particular, a double peak feature predicted as the bonding and anti-bonding bands of the Ni-Ni pair in the Ni-rich d-QC by the model cluster calculation [3] is not recognized in the Ni $L\alpha$ XES spectrum. This is partly due to the emphasized Ni-Ni pairs in the model calculation and suggests the predominance of Ni-Al pairs or a strong TM-Al interaction. This may also imply that the d-QC forms as a TM atom is surrounded by Al atoms; additional Co-Co interaction might lead to the pentagonal ring formation in the Co-rich d-QC.

1. S. Ritsch, C. Beeli, H.-U. Nissen & R. Lück, Phil. Mag. A **71** (1995), p. 671.
2. S. Hiramatsu and Y. Ishii, J. Phys. Soc. Jpn. **75** (2006), p. 054602.
3. K. Soda, M. Inukai, M. Kato, S. Yagi, Y.-G. So & K. Edagawa, Phil. Mag. **91** (2011), p. 2510.

Crystalline Approximants in the Al-Pd-Co System

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Keywords: structure, approximant, decagonal, icosahedral, pseudo-Mackay

A great number of complicated intermetallic compounds were reported in binary and ternary alloy systems of Al with transition metals. Al–Pd–Co is one of the most interesting alloy systems, since a variety of crystalline phases associated with quasicrystals has been reported in the conventionally solidified samples [1]. Among these crystalline phases, the structures of ε-phases are closely associated with Al_3Pd (ε_6-phase), which is an important crystalline approximant for the decagonal quasicrystal with a period of 1.6 nm [2]. W-AlPdCo with about 5 mol% Pd showed cell parameters similar to those of W–AlCoNi [3] and its structural information is useful for understanding the columnar unit in the decagonal phase with a periodicity of 0.8 nm. On the other hand, some crystalline phases associated with the icosahedral phase were also found in this Al-Pd-Co system. C_2–phase and F-phase are classified into this category, although each structure has not been fully revealed yet. R-AlPdCo (R-3: a = 2.910 nm, c = 1.319 nm) is another example and its structure indicates two types of pseudo-Mackay clusters similar to those found in 1/1-AlCuRu approximant [4]. In this context, a series of structural investigations of intermetallic compounds in Al–Pd–Co is quite interesting in order to understand the columnar unit for the decagonal phase together with the icosahedral atom cluster for the icosahedral phase. This paper demonstrates our recent results of single crystal structural analysis for approximant phases in Al-Pd-Co.

The small addition of Ge into the ternary Al-Pd-Co alloy encouraged the formation of F-phase and single crystal specimen was picked up from an as-prepared alloy ingot of $Al_{65}Pd_{10}Co_{20}Ge_5$. Single crystal X-ray diffraction study suggested a cubic cell (a = 2.441 nm) and the observed reflections obeyed the extinction rule for the space group *Pa*3. The program package SIR97 was employed for obtaining an initial structural model, and the parameters were refined by the least-squares program SHELXL97. Structural model indicates a pseudo-Mackay cluster around the Co site; however, the pseudo-Mackay cluster in F-phase is different from those found in R-AlPdCo. The structure of W-AlPdCo decagonal approximant also will be discussed at the conference.

1. M. Yurechko, B. Grushko, T. Velikanova, K. Urban, J. Alloy. Compd. **337** (2002), p. 172.
2. Y. Matsuo, K. Hiraga, Philos. Mag. Lett. **70** (1994), p. 155.
3. K. Sugiyama, S. Nishimura and K. Hiraga: J. Alloy. Compd. **342** (2002), p. 65.
4. R. Simura, S. Suzuki, K. Yubuta and K. Sugiyama, Mater. Trans. (2013, in press).

Six-dimensional model of Al-based F-type icosahedral quasicrystals

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Keywords: icosahedral quasicrystals, Al-transition metals, structure model

A structure model, based on a dense packing of clusters of two kinds; the pseudo-Mackay-type and the mini-Bergman-type that were found in the recent structure analysis of a cubic approximant crystal in Al-Pd-Cr-Fe system [1], is proposed for the Al-based F-type icosahedral quasicrystals.

We employ a set of 12-fold packing sites [2], which is a subset vertices of the three-dimensional Penrose tiling (or Ammann tiling) with an edge length of $a_0 \approx 2.81$ Å, for the cluster centers. For F-type ordering, $a = 2a_0 \approx 5.62$ Å is chosen as the icosahedral lattice constant, which is $\tau\,[=(1+5^{1/2})/2]$ times smaller size than that used in a previous model by one of the authors [3] and the same size with a model proposed by Elser [4]. Thus the cluster centers split into even and odd parities. Adjacent clusters are mutually connected either along a two-fold direction with the distance of $b=(4+8/5^{1/2})^{1/2}a_0 \approx$ 7.74 Å or a three-fold direction with $c=(3+6/5^{1/2})^{1/2}a_0 \approx 6.70$ Å. These are the shortest two distances between cluster centers as observed in the approximant crystal. Each b-linkage connects a pair of cluster centers having the same parity, while each c-linkage connects a pair of cluster centers having different parities.

The six-dimensional model consists of three independent occupation domains (ODs) located at (0,0,0,0,0,0), (1/2,0,0,0,0,0) and (1,1,1,1,1,1)/4. Central atoms of pseudo-Mackay-type clusters are generated from the central part of the OD at (0,0,0,0,0,0), and those of mini-Bergman-type clusters are generated from the whole of the OD at (1/2,0,0,0,0,0). The present model can reproduce the cluster structures as well as their connection scheme observed in the approximant crystal. The results of detailed geometrical analysis of the model will be discussed.

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1. N. Fujita, H. Takano, A. Yamamoto, A. P. Tsai, Acta Cryst. A **69** (2013), p. 322–340.
2. C. L. Henley, Phys. Rev. B **34** (1986), p. 797-816.
3. A. Yamamoto, H. Takakura, A. P. Tsai, Phys. Rev. B **68** (2003), p. 094201.
4. V. Elser, Philos. Mag. B **73** (1996), p. 641-656.

Arrangement of TM atoms in an Al-Cu-Co decagonal quasicrystal studied by *C*s-corrected HAADF-STEM

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Keywords: *C*s-corrected STEM, bond orientational order

Modern *C*s-corrected scanning transmission electron microscopy (STEM) has a high resolution to reflect individual atoms in observed STEM images of decagonal quasicrystals. Recent re-examination of Al-TM (transition metal) decagonal quasicrystals and crystalline approximants by a full use of *C*s-corrected STEM with high-angle annular detector dark-field (HAADF) and annular bright-field (ABF) techniques has proposed new structural models formed by bond orientational ordered (BOO) arrangements of TM atoms [1-5], and consequently has disproved previous cluster-based models that are characterized as BOO arrangements of 2 nm clusters. The purpose of the present paper is to re-examine the structure of an annealed $Al_{64}Cu_{22}Co_{14}$ decagonal quasicrystal, which is known to be one of highly ordered decagonal quasicrystals, by *C*s-corrected STEM with HAADF and ABF techniques. A *C*s-corrected STEM study of the Al-Cu-Co decagonal quasicrystal was already performed by Taniguchi and Abe [6], but they discussed only the structure of 2 nm cluster and never touched on the structure of a full area including glue regions between the atom clusters. In observed HAADF-STEM images, individual TM atoms and mixed sites (MSs) of Al and TM atoms are represented as separated bright dots, and consequently arrangements of TM atoms and MSs on two quasiperiodic planes can be directly determined. TM atoms on the two quasiperiodic planes are arranged with pentagonal tiling of an edge-length of 0.76 nm, and also they are located at lattice points in a Penrose lattice of an edge-length of 0.25 nm. Occupation domains of TM atoms in this model have been discussed.

1. A. Yasuhara, K. Saito and K. Hiraga in "Proceedings of Aperiodic 2012", in press.
2. K. Sugiyama, A. Yasuhara and K. Hiraga in "Proceedings of Aperiodic 2012", in press.
3. K. Yubuta, A. Yasuhara and K. Hiraga in "Proceedings of Aperiodic 2012", in press.
4. K. Hiraga and A. Yasuhara: Mater. Trans. **54** (2013), p. 493.
5. K. Hiraga and A. Yasuhara: Mater. Trans. **54** (2013), in press.
6. S. Taniguchi and E. Abe, Phil. Mag. **88** (2008), p. 1949.

Antiferromagnetic order in the Cd_6R approximants

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Keywords: quasicrystals, approximants, magnetism

Many theoretical treatments of spins on aperiodic lattices support the notion of long-range antiferromagnetic order on a quasilattice. However, there has been no experimental confirmation of long-range magnetic order in quasicrystalline systems, and the absence of long-range magnetic order extends to crystalline approximant phases of the icosahedral structures as well. Surprisingly, the 1/1 approximant to the Cd-Mg-R icosahedral phases, Cd_6R, appears to be an exception to the rule.

Here, we will report the results of x-ray resonant magnetic scattering (XRMS) and neutron diffraction measurements on Cd_6R (R = Tb, Ho, Gd) and show that long range antiferromagnetic order is, indeed, realized at low temperature. The Bragg peaks that arise from the antiferromagnetic order are as sharp as those associated with the chemical structure indicating true long-range (> 500 Å) magnetic order. For Cd_6Tb ($T_N = 24$ K), using the Cd^{112} isotope, neutron diffraction measurements show that the magnetic structure is, in fact, more complicated than originally believed. High-resolution x-ray diffraction and XRMS measurements on Cd_6Ho show that there is a previously unreported cubic-to-monoclinic structural distortion below $T_S = 178$ K, and that this system orders antiferromagnetically below $T_N = 8.5$ K. XRMS measurements on Cd_6Gd, likewise, demonstrate long-range magnetic order below $T_N \approx 19$ K.

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Letter frequency in the Kolakoski sequence

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Keywords: Combinatorics on words, Symbolic dynamics, Aperiodic tilings

The classical Kolakoski sequence, despite its name actually first studied by Oldenburger [5], is the sequence on the alphabet $\{1, 2\}$ defined as its own symbols run length sequence. Though its straight forward and easy definition, the sequence rises several intriguing question, which have been open since the 1960:s when Kolakoski formulated them, see [2, 3]. One such question is on the letter frequency. It is conjectures to be $\frac{1}{2}$, but not even its existence is cleared. Slight modifications in the definition of the Kolakoski sequence, opens possibilities to answer similar questions, see [1], where is was also shown that these changes lead to model sets.

We discuss here a highly efficient numerical method of calculation the letter frequency, in the classical as well as in a general Kolakiski sequence defined over a two letter alphabet, as considered in [4].

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1. M. Baake and B. Sing, "Kolakoski(3; 1) is a (deformed) model set", Canad. Math. Bull. 47 (2004), 168–190.
2. W. Kolakoski, "Problem 5304: self generating runs", Amer. Math. Monthly 72 (1965), 674.
3. W. Kolakoski, "Problem 5304", Amer. Math. Monthly 73 (1966), 681–682.
4. J. Nilsson. "A Space-Efficient Algorithm for Calculating the Digit Distribution in the Kolakoski Sequence", J. Integer Seq. 15 (2012), no. 6, Article 12.6.7, 13 pp.
5. R. Oldenburger, "Exponent trajectories in dynamical systems", Trans. Amer. Math. Soc. 46 (1939), 453–466.

Scaling properties of the Thue-Morse diffraction measure

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Keywords: diffraction, dynamical spectrum, Riesz product

We revisit the well-known and much studied Riesz product representation of the Thue-Morse diffraction measure; see [1,2] and references therein. It is also the maximal spectral measure for the corresponding dynamical spectrum in the complement of the pure point part [3].

The known scaling relations are summarised (and references given), and some new findings are explained. In particular, it is shown that only denominators connected with the primes 3 and 5 contribute, together with uncountably many further positions that are Diophantine approximations of them.

1. M. Baake and U. Grimm, “The singular continuous diffraction measure of the Thue-Morse chain”, J. Phys. A: Math. Theor. **41** (2008), p. 422001; arXiv:0809.0580.
2. M. Baake, F. Gähler and U. Grimm, “Spectral and topological properties of a family of generalised Thue-Morse sequences”, J. Math. Phys. **53** (2012), p. 032701; arXiv:1201.1423.
3. M. Queffélec, “Substitution Dynamical Systems – Spectral Analysis”, 2nd ed. (Springer, Berlin) (2010).

Quotient cohomology of certain 1- and 2-dimensional substitution tiling spaces

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Keywords: tiling cohomology, tiling spaces, substitution tiling

The quotient cohomology of tiling spaces, which was introduced in [1], is a topological invariant that relates a tiling space to one of its factors (when seen as tiling dynamical systems). In particular, it is a relative version of the tiling cohomology that distinguishes the factors of a tiling space. In this work, the quotient cohomologies within certain families of substitution tiling spaces in 1 and 2 dimensions are determined. Specifically, we present the quotient cohomologies for the family of the generalised Thue-Morse sequences [2], for the squiral tilings [3], and for the generalised chair tilings, correcting some errors in [1].

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1. M. Barge and L. Sadun, New York Journal of Mathematics **17** (2011), p. 579.
2. M. Baake, F. Gähler and U. Grimm, Journal of Mathematical Physics **53** (2012).
3. M. Baake, F. Gähler and U. Grimm, Journal of Integer Sequences **16** (2013).

Dynamical properties of the visible lattice points

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Keywords: *k*th-power-free lattice points, hull, dynamical system, invariant measure, ergodicity

We consider the visible points of a lattice in Euclidean *n*-space together with their generalisations, the *k*th-power-free points of a lattice [2], and study the corresponding dynamical system that arises via the closure of the lattice translations. This extends previous results obtained in [1,3] for the special case of square-free integers.

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1. F. Cellarosi and Ya. G. Sinai, “Ergodic properties of square-free numbers”, J. Eur. Math. Soc. **15** (2013), 1343-1374.
2. P.A.B. Pleasants and C. Huck, “Entropy and diffraction of the k-free points in n-dimensional lattices”, Discrete Comput. Geom. (2013), accepted.
3. P. Sarnak, “Three lectures on the Möbius function randomness and dynamics (Lecture 1)” (2010).

Discrete tomography: magic numbers for *N*-fold symmetry

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Keywords: Discrete tomography, cyclotomic model set, magic number, *U*-polygon

We consider the problem of distinguishing convex subsets of *n*-cyclotomic model sets Λ by (discrete parallel) X-rays in prescribed Λ-directions. In this context, a ‘magic number’ *m* has the property that any two convex subsets of Λ can be distinguished by their X-rays in any set of *m* prescribed Λ-directions. In [1] it was shown that these numbers exist and that they only depend on the value of *n*; see [2] for a gentle exposition. Moreover, first explicit calculations showed that for pentagonal, octagonal, decagonal and dodecagonal model sets, the least possible such nubers are 11, 9, 11 and 13 in that very order.

In this short note, we report recent progress in the calculation of these numbers which suggests that the least possible magic number for *n*-cyclotomic model sets might just be $N+1$, where N is the least common multiple of *n* and 2.

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1. C. Huck and M. Spieß, J. Reine Angew. Math. **677** (2013), p. 199-224.
2. C. Huck, in “Aperiodic crystals”, eds. S. Schmid *et al.*, (Springer, Dordrecht) (2013), p. 29-34.

Tiling vertices and the spacing distribution of its radial projections

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Keywords: aperiodic tilings, model sets, spacing distribution

In [1], Boca, Cobeli and Zaharescu gave a very elegant representation of the first consecutive spacing distribution when looking at the visible points of the square lattice $\mathbf{Z}^2$. Here one considers the lattice points which are "visible" from the origin. This amounts to selecting those points (x,y) with coprime coordinates. Now place a circle of radius R at the origin and project all points inside onto this circle, effectively reducing the polar coordinate of the point to the angle information. Then sort all these angles and measure the difference between neighbouring ones. In [1], it was proved, even in a more general context, that there exists a limit distribution of the differences when R tends to infinity.

One might now ask the question, if the limit distribution somehow encodes information about the degree of order of the input point set. Or phrased differently, can one quantify how much the distribution varies when exchanging the original lattice with some other locally finite point set? It is known that the set of Poisson distributed points in the plane yields the exponential distribution, in that regard representing the most "unordered" set. This case also seems to the only other one which can be fully understood analytically.

We take a look at the numerical results when using the vertex set of aperiodic tilings in the plane as input (e.g. Ammann-Beenker, rhombic Penrose and chiral Lançon-Billard). In connection with this problem, we also study the visibility property for special aperiodic point sets, generated from a cyclotomic model set description. It will turn out, that these cases resemble the lattice case to some extend.

This is joint work with M. Baake and F. Götze.

1. F.P. Boca, C. Cobeli, A. Zaharescu, Commun. Math. Phys. **213** (2000), p. 433-470 (DOI: 10.1007/s002200000250).

Coincidences of the Shifted Hexagonal Lattice and the Hexagonal Packing

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Keywords: coincidence site lattice, hexagonal lattice, multilattice

A geometric study of twin and grain boundaries in crystals and quasicrystals is achieved via coincidence site lattices (CSLs) and coincidence site modules (CSMs), respectively. Recently, coincidences of shifted lattices and multilattices (i.e. finite unions of shifted copies of a lattice) have been investigated in [1,2]. Here, we solve the coincidence problem for the shifted hexagonal lattice. This result allows us to analyze the coincidence isometries of the hexagonal packing by viewing the hexagonal packing as a multilattice.

1. M. J. C. Loquias and P. Zeiner, J. Phys.: Conf. Ser. **226** (2010), p. 012026.
2. M. J. C. Loquias and P. Zeiner, http://arxiv.org/abs/1301.3689.

On a Family of Random Noble Means Substitutions

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Keywords: Random Substitutions, Dynamical Systems, Diffraction

In 1989, Godrèche and Luck [1] introduced the concept of local mixtures of primitive substitution rules along the example of the well-known Fibonacci substitution and foreshadowed heuristic results on the topological entropy and the spectral type of the diffraction measure of associated point sets.

In this contribution, we present a generalisation of this concept by regarding the so-called 'noble means family', consisting of finitely many primitive substitution rules that individually all define the same two-sided discrete dynamical hull. We report about results in the randomised case on topological entropy, ergodicity of the two-sided discrete hull, and the spectral type of the diffraction measure of related point sets.

This work was supported by the German Research Council (DFG), within the CRC 701.

1. C. Godrèche, J. M. Luck, J. Stat. Phys. **55** (1989), p. 1-28.
2. M. Baake, M. Moll, in “Aperiodic Crystals”, eds. S. Schmid et al., (Springer, Dordrecht) (2013), p. 19-27.

Topology of the Random Fibonacci Substitution Tiling Space

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Keywords: random Fibonacci, locally random substitution, tiling space

In 1998, Anderson and Putnam showed that a substitution tiling space can be represented as inverse limit of an inflation and substitution map on the cellular Andeson-Putnam complex [1]. The cohomology of the tiling space can then be computed as the direct limit of the homomorphism induced by inflation and substitution on the cohomology of the complex.

Gähler and Maloney [2] investigated the cohomology of one-dimensional tiling spaces arising from several substitutions, which are all acting on the same set of tiles. Since each substitution is applied globally, the entropy remains zero.

The next natural goal is to go one step further by studying mixed substitutions that are randomly applied locally, which makes the entropy positive. In this study, we investigate the topology of an example of such system, the random Fibonacci system introduced by Godrèche and Luck in 1989 [3] when studying quasi-crystalline structures and tilings in the plane. They defined the random Fibonacci substitution rule by the generalized substitution

$$\theta : \begin{cases} a & \mapsto & \begin{cases} ba & \text{with probability } p \\ ab & \text{with probability } 1-p \end{cases} \\ b & \mapsto & a \end{cases}$$

1. J.E. Anderson and I.F. Putnam, Ergodic Theory Dynam. Systems 18 (1998), p. 509.
2. F. Gähler and G.R. Maloney, Topology Appl. 160 (2013), p. 703.
3. C. Godrèche and J.M. Luck, J. Stat. Phys. 55 (1989), p. 1.

Triangular spiral tilings

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Keywords: Spiral tiling, triangle, phyllotaxis, paper folding

Phyllotaxis is one of the most classical model of crystallography, and is a source of quasicrystals. Quasicrystals are also applied to figurative art, see [1]. Here we study the topology of spiral tilings [2], which is intimately related to phyllotaxis theory and continued fractions. A quadrilateral spiral tiling is determined by a generating complex number a, $|a|<1$, and a pair of positive integers m,n, that are relatively prime. We give a simple characterization when they give a triangular spiral tiling. When m,n are fixed, the admissible generator a form a curve in the unit disk. The family of triangular spiral tilings with opposed parastichy pairs (m,n) is parameterized by the divergence angle $\arg(a)$, while triangular spiral tilings with non-opposed parastichy pairs are parameterized by the plastochrone ratio $1/|a|$. The generators for triangular spiral tilings with opposed parastichy pairs are not dense in the complex parameter space, while those with-non-opposed parashichy pairs are dense.

The proofs are given in a general setting of spiral multiple tilings, i.e., tilings of the covering space of the punctured plane.

In the conference, we shall also present paper-folding sheets that build spiral towers whose top-down views are triangular tilings. Some are very easy, and some are very hard to build.

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1. A. Hizume and Y. Yamagishi, Journal of Physics A: Math. Theor. **44** (2011), p. 015202
2. T. Sushida, A. Hizume and Y. Yamagishi, Journal of Physics A: Math. Theor. **45** (2012), p. 235203.

Similar submodules and coincidence site modules

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Keywords: CSL, similar sublattices, $\mathbb{Z}$-modules

We consider connections between similar submodules and coincidence site modules of general $\mathbb{Z}$-modules in $\mathbb{R}^d$.

Similar submodules are submodules that are similar to its parent module M, i.e. they are scaled and/or rotated versions of M. Given an isometry R, the intersection $M \cap RM$ is called a coincidence site module, if $M \cap RM$ is a submodule of full rank in M.

Here, we generalize results obtained by S. Glied and M. Baake [1,2] on similar and coincidence isometries of lattices and lattice-like modules. In particular, we show that the factor group $OS(M)/OC(M)$ is Abelian for arbitrary $\mathbb{Z}$-modules M, where $OS(M)$ and $OC(M)$ are the groups of similar and coincidence isometries, respectively. In addition, we derive various relations between the indices of coincidence site submodules and corresponding similar submodules.

1. S. Glied and M. Baake, Z. Krist. **223** (2008), pp. 770-772.
2. S. Glied, Can. Math. Bull. **55** (2011), pp. 98-107.

Monte-Carlo Studies on Magnetic Ordering in Cd_6RE Cubic Approximants

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Keywords: Approximant, Cd-based, Magnetic ordering, Monte-Carlo calculation

Cd_6RE (RE=rare-earth) cubic approximants exhibit antiferromagnetic phase transitions at low temperatures [1]. It is believed that this transition is caused by long-range ordering of the spins of the rare-earth atoms placed on the vertices of icosahedral shells. However, it is not practical to determine the configuration of individual spins by neutron experiments, since Cd possesses high absorption cross section of neutrons. Our objective is to obtain a theoretical prediction for the spin configuration in Cd_6RE at low temperatures.

We adopted a model where classical continuous spins interact through the Heisenberg type exchange interaction. We applied a Monte-Carlo method proposed by Wolff [2] to execute the calculations, instead of the conventional single-flipping method. The positions of the rare-earth ions were given in accordance with the work by Tamura et al [1]. Calculations were made by assuming interactions only between first and second nearest neighbouring spins. We observed the magnetic phase transition to an ordered state with a complex spin structure depending on the interaction parameters. Detailed analysis of the spin structures will be presented. We shall further discuss the possibilities of successive magnetic orderings and metamagnetic behaviours.

1. R. Tamura, Y. Muro, T. Hiroto, K. Nishimoto and T. Takabatake, Phys. Rev. **B 82** (2010), p. 220201.
2. U. Wolff, Phys. Rev. Lett. **62** (1989), p. 361.

Singular continuous to absolutely continuous spectral transition in a family of quasi-one dimensional quasiperiodic lattices

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Keywords: Quasicrystal. Transfer matrix, Green's function

We investigate the electronic energy spectrum of a whole class of Fibonacci and non-Fibonacci quasicrystalline atomic chains [1] generated using the substitution rule $\boldsymbol{L} \rightarrow \boldsymbol{L}^m\boldsymbol{S}^n$, $\boldsymbol{S} \rightarrow \boldsymbol{L}$, and the aperiodic Thue-Morse chain [2] generated according to the rule $\boldsymbol{L} \rightarrow \boldsymbol{LS}$ and $\boldsymbol{S} \rightarrow \boldsymbol{SL}$. Each such chain is *side coupled* to an array of isolated atoms or atomic clusters. The atoms, mimicking single level *Quantum Dots* couple to the chains at special vertices *locally* or *non-locally*.

We work with a tight binding Hamiltonian,

$$H = \varepsilon \Sigma_i \mathrm{c}_i^\dagger \mathrm{c}_i + \Sigma_{<ij>} \mathrm{t}_{ij} (\mathrm{c}_i^\dagger \mathrm{c}_j + \mathrm{h.c.}) , \qquad (1)$$

and prove that definite correlations between the *numerical values* of the dot-chain coupling and the hopping integral along the aperiodic backbone can render the entire energy spectrum *absolutely continuous*, destroying the usual singular continuous character completely. The analysis is based on the study of a possible commutation of various transfer matrices corresponding to the resonating clusters of atoms, and a comprehensive study of the local density of states at various atomic sites using a Green's function formalism.

We substantiate the results by exact calculation of the two terminal transmission coefficient of different quasiperiodic chains side coupled to the single level quantum dots. The stability of the results against a possible fluctuation of the system parameters from the resonant values is studied and discussed. The results hold true even in case of randomly disordered chains and provide a case where the canonical Anderson localization is not observed even in the presence of disorder [3]. Finally, the role of the dot-chain coupling at various length scales are explored within a *real space renormalization group* scheme.

1. M. K. Ali and G. Gumbs, Phys. Rev. B **38** (1988), p. 7091.
2. J. M. Luck, Phys. Rev. B **39** (1989), p. 5834.
3. B. Pal, S. K. Maiti and Arunava Chakrabarti, Europhys. Lett. (2013), (to be published).
4. B. Grushko, Journal of Alloys and Coumpounds **557** (2013), p. 102.

Electric-elastic field for a straight dislocation in one-dimensional hexagonal quasicrystals

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Keywords: electric-elastic, dislocation, one-dimensional hexagonal quasicrystals

Dislocation problems of quasicrystals have solved by using Green's function method. The practice shows the method has its limitation. We need to develop other methods of solution, such as Stroh's method. The alternate approach may have advantages compared to the Green's function method for some actual calculations and might be more suitable for numerical calculation e.g. reducing analytical expressions of the displacement fields induced by straight dislocations in quasicrystals. Moreover, for complicated classes of quasicrystals, no solutions for the dislocation problems have been found by the Green's function method, but these problems can be solved applying our procedure.

The performance of quasicrystal materials is influenced by the presence of defects such as dislocations, inclusions, cracks etc. Such solutions are very convenient to be used in the study of point defects and inhomogeneities in the materials. For an one-dimensional hexagonal quasicrystal with a straight line dislocation parallel to the quasi-periodic axis, the electric-elastic field induced by the straight dislocation can be obtained by superposition of the electric-elastic fields of a pure blade part and a pure screw part. For a blade dislocation, the solution is available in the piezoelasticity of conventional crystals. For a screw dislocation in this quasicrystal of general cross-sections, the electric-elastic field and the image force on the dislocation are given via the generalized Stroh formalism. These provide important information for further studying the deformation and fracture of the new solid phase. They also play an important role in numerical simulations such as the finite element method and the boundary element method.

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Insight into hydrogen storage capacity of Ti-Zr-Ni-based quasicrystals

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Ti-Zr-Ni-based icosahedral quasicrystals are of interest due to their storage of ample hydrogen. However, reported storage abilities of these quasicrystals differ remarkably. To evaluate their reasonable hydrogen capacity, the Bergman cluster structure and the quality in loading hydrogen of such materials are reviewed. The published results about the hydrogen storage are compared and discussed. The cluster structure of a Ti-Zr-Ni quasicrystal is analyzed based on its approximant phase W(Ti-Zr-Ni), demonstrating that H/M=2.89 might be their theoretical maximum to load hydrogen. However, because of incomplete occupancy of tetrahedral interstices with limited size and high site energy in the quasicrystal structure, the top storage would be difficult to reach, which is supported by our experimental results of Ti-Zr-Ni(-Pd) quasicrystals manifested to absorb around 2.2wt.% H_2. With the combination of the theoretical prediction and some reported data, the most likely level of hydrogen concentration in such quasicrystals is speculated.

Phason contribution to the dislocation loop bias in quasicrystals

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Keywords: quasicrystal, dislocation, bias

A number of physical phenomena such as swelling, radiation growth, irradiation creep, etc., occurs in structural materials under irradiation. The driving force for these effects is the rearrangement of point defect fluxes due to the dislocation bias for interstitial atoms. We describe the model for finding dislocation bias in quasicrystals.

In addition to the sinks of radiation defects present in crystals, quasicrystals have phason sinks. Dislocation climb in quasicrystals is associated with the formation of the phason wall due to the lack of translational invariance. In view of this, we consider a simplified model of a circular dislocation loop under irradiation containing a phason disk-like defect inside. This disc-like defect is constantly growing together with the dislocation loop and it is regarded as a neutral absorbing sink. The approximate analytical solution for the capture efficiency of the dislocation loop for radiation point defects is found [1] and compared with the numerical solution of this model problem. The absorbing capacity of the dislocation loop in a quasicrystal is several times greater than that in a crystal due to the contribution of phason defects. The dislocation loop bias for interstitial atoms in a quasicrystal is lower and it significantly depends on the loop radius. Since the swelling rate is proportional to the dislocation bias, quasicrystals are expected to be more resistant to swelling under irradiation.

1. G. N. Lazareva, A. S. Bakai, Journal of Kharkiv National University **1041** (2013), Physical series: “Nuclei, Particles, Fields”, issue 2/58, p. 64.

Transport properties of the Au-Al-Yb quasicrystal and approximant under hydrostatic pressure

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Keywords: Quantum critical phenomenon, mixed valence, heavy fermions, electrical resistivity under hydrostatic pressure

Quantum criticality has been considered to be specific to crystalline materials such as heavy fermions. Very recently, however, the Tsai-type quasicrystal $Au_{51}Al_{34}Yb_{15}$ was reported to show unusual quantum critical behaviour, i.e., the diverging behaviour of the magnetic susceptibility (with an unusual critical index) and the electronic specific heat coefficient as $T \rightarrow 0$ [1]. The geometric structure of the Tsai-type quasicrystal to which this new material belongs is rather well understood [2] but only few is known about its electronic state. Here we report the transport properties of the quasicrystal and its crystalline approximants under hydrostatic pressure.

The quantum critical behaviour that the mixed-valence Au-Al-Yb quasicrystal shows is robust against the application of hydrostatic pressure. Interestingly, the quasicrystal exhibits the non-Fermi liquid like temperature dependence of the electrical resistivity [1]. We have measured the temperature dependence of the electrical resistivity down to about 2 K under pressure up to about 1.5 GPa and observed that the resistivity remains to be of the non-Fermi liquid type and the power law changes with increasing pressure. This means that the non-Fermi liquid feature is also robust against pressure. At the conference we will present the detailed results of the electrical resistivity measurement of the quasicrystal down to lower temperatures together with the results of the approximants.

1. K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura and T. Ishimasa, Nature Materials **11** (2012), 1013.
2. T. Ishimasa, Y. Tanaka and S. Kashimoto, Phil. Mag. **91** (2011), 4218.

Structural phase transition of a series of Cd$_6$M crystalline approximants

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Keywords: approximants, electron diffraction, order-disorder phase transition

An occurrence of an order-disorder phase transition related to the structure of the cluster, was discovered above ~100 K for a series of Cd$_6$M (M = Ca, Sr, Rare earth metals) approximants [1]. The Cd-based quasicrystals and their approximants are made of Tsai-type icosahedral clusters [2]. The Tsai-type icosahedral cluster is composed of four successive shells, which are, from the center, a Cd4 tetrahedron, a Cd20 dodecahedron, a M12 icosahedron and a Cd30 icosidodecahedron. For most of Cd6M, the Cd4 tetrahedron at the center is orientationally disordered at room temperature expect for Cd$_6$Eu [1,2] and Cd$_6$Ce [1,3]. Also, the phase transition has been interpreted as involving orientational ordering of the Cd4 tetrahedron at low temperature. In this work, we have investigated the low-temperature (LT) superstructure and the phase transition temperature of a series of Cd$_6$M (M = Ca, Y, Sr, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) crystalline approximants by transmission electron microscopy as well as electrical resistivity measurements.

For M = Ca, Y, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er and Tm, the LT superstructure is explained by a $\sqrt{2}a \times a \times \sqrt{2}a$ lattice with the space group C2/c. Additionally, no superlattice reflections were observed for non-aged Cd$_6$Ho, and Cd$_6$Er and Cd$_6$Tm. For M = Sr and Yb a $\sqrt{2}a \times 2a \times \sqrt{2}a$ monoclinic lattice with P2/m.

On the other hand, no phase transition is observed for M = Lu, indicating that the Cd4 tetrahedron at the cluster center remains disordered down to the lowest temperature, i.e., 20 K. The LT superstructures are well classified in terms of the atomic radius of the M atom and it is shown that the volume inside the Cd20 dodecahedron plays an important role in the phase transition at low temperatures [3].

1. R. Tamura *et al.*, Jpn. J. Appl. Phys., Part 2 **41** (2002), p. L524.
2. C. P. Gómez and S. Lidin, Phys. Rev. B **68c** (2003), p. 024203.
3. K. Nishimoto, T. Sato, R. Tamura, J. Phys.: Condens. Matter **25** (2013), p. 235403.

Mechanical properties and microstructures of quasicrystal-reinforced Mg-Cd-Yb extrusions

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Keywords: Quasicrystals, Mg alloy, Mechanical property

Icosahedral quasicrystal (i-Qc) forms in wide composition range; $Mg_xCd_{(84-x)}Yb_{16}$ with x=0~60 in the Cd-Mg-Yb system [1]. Recently, we have found that a eutectic reaction occurs involving i-Qc at 460°C and $Mg_{68}Cd_{24}Yb_8$, resulting in a lamellar structure of Mg in i-Qc matrix. There is a clear orientation relationship for the i-Qc and Mg, where i-Qc[21111]//Mg[2-1-10] and i-Qc[221001]//Mg[0001]. The i-Qc and Mg are coexisting in the wide composition range and hence this system is an ideal one to study the contribution of i-Oc in reinforced-Mg alloys [2-4].

Specimens with the compositions of $Mg_{(100-4x)}Cd_{3x}Yb_x$ (x=0, 1, 2, 4, 8) were studied. Extrusions were performed at 300°C with a ram speed of 10 mm /min and extrusion ratio of 37.5: 1. Microstructures were studied with scanning and transmission electron microscopes (SEM, TEM). Mechanical properties were studied by means of tensile and compression tests at room temperature.

With the concentration of Qc, which is proportional to Yb content (x), ultimate tensile strength (UTS) showed 270-366 MPa (yield stress at 0.2% strain: 235-310 MPa) in the range of x=1~4. Elongation was varied from 2% (x=4) to 10% (x=1). Specimen with eutectic composition (x=8) was destroyed before reaching 0.2% strain during tensile test. Pure Mg extrusion (x=0) showed UTS: 176 MPa, 0.2% yield stress: 67 MPa, elongation: 13%. The volume fraction of i-Qc is high (~37%) in $Mg_{84}Cd_{12}Yb_4$, however, it could show some elongation. This might be due to the stable interface between i-Qc and Mg.

1. J. Q. Guo, E. Abe, A. P. Tsai, Phil. Mag. Lett. **82** (2002), p. 27.
2. D. H. Bae, S. H. Kim, W. T. Kim, D. H. Kim, Mater. Trans. **42** (2001), p. 2144.
3. A. Singh, M. Nakamura, M. Watanabe, A. Kato, A. P. Tsai, Scripta Mater. **49** (2003), p. 417.
4. S. Ohhahsi, A. Kato, M. Demura, A. P.Tsai, Mater. Sci. Eng. A **528** (2011), p. 5871.

Physical properties of icosahedral (Au,Cu)-Al-Yb quasicrystals

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Keywords: quasicrystal, intermediate valence, (Au,Cu)-Al-Yb

The icosahedral Au-Al-Yb quasicrystal (QC) was discovered in 2011 [1]. Interestingly, the Yb valence was found to be intermediate between Yb^{2+} and Yb^{3+} [2]. Therefore, it is certainly of a great interest to investigate how the physical property changes when the Yb valence further increases. An application of pressure was performed by Watanuki et al. as an attempt to increase the Yb valence [3].

In this work, we have substituted Cu into the Au site in order to reduce the quasilattice constant a_{6D}. For the experiment, alloy ingots of nominal compositions $(Au_{1-x},Cu_x)_{49}$-$Al_{34}Yb_{17}$ were prepared in an arc furnace. Then, the alloys were melt-spun into thin ribbons. It was found that a_{6D} successfully decreases monotonously as Au is replaced by Cu and a decrease of 2.43% in a_{6D} was obtained at $(Au_{0.4},Cu_{0.6})_{49}$-Al_{34}-Yb_{17}. The change of the magnetic susceptibility and electrical resistivity will be presented in the poster.

1. T. Ishimasa *et al.*, Phil. Mag. **91** (2011), p. 4218.
2. T. Watanuki *et al.*, Phys. Rev. **B 86** (2012), p. 094201.
3. T. Watanuki *et al.*, Phys. Rev. **B 84** (2011), p. 054207.

Inhomogeneous electron localization in icosahedral quasicrystals

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Keywords: quasicrystals, electron structure, localization of electrons

As is well known, the width of pseudo-gap near the E_F of the conduction band in quasicrystals is too large to be an origin of unusually great thermal effects in conductivity, magnetic susceptibility and Hall-constant. Therefore, there is a long standing problem of singular electron states, which ought to be responsible for these effects. Recently the heat capacity contribution associated with thermally induced current carriers (TICC) has been revealed in Al-Cu-Fe i-phases [1,2]. This contribution turned out to be a succession of two Schottky-like heat anomalies connected with short-range order. Within the conventional Schottky model limitations, this means that the TICC origin is the local two-level excitations with characteristic energy of $\delta E_1 \sim 20$ and $\delta E_2 \sim 250$meV. Accordingly, inhomogeneous electron localization due to exchange/covalent pairing may be a fundamental property of i-phases and their approximants. We show that superposition of the pseudo-gap and a few duplets, schematically shown on Fig.1, is suitable for understanding of mixed metal-dielectric properties of quasicrystals on condition that the intra-band and intra-duplet transitions are independent and give additive contributions in all physical properties. Interrelation between of electron localization and complex short-range order is discussed.

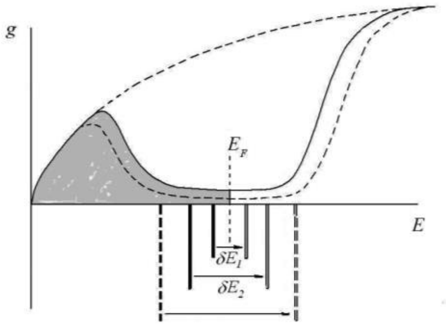

Fig.1

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1. A. Prekul, N. Shchegolikhina, K. Edagawa, Phil.Mag. **91** (2011), p. 2828.
2. A. Prekul, N. Shchegolikhina, A. Gaiduchenko et al, JETP Letters **94** (2011), p. 366.

Enhancement of Power Factor by Fe Substitution for Mn in Al-Pd-Mn Quasicrystals

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Keywords: Al-Pd-Mn, thermoelectric material, power factor

Al-Pd-Mn and Al-Pd-Re icosahedral quasicrystals are suitable for thermoelectric material [1], because these materials exhibit low thermal conductivities about 1-2 $\mathrm{Wm^{-1}K^{-1}}$ at room temperature mainly due to their complex crystal structure, and have large Seebeck coefficients about 90 $\mu\mathrm{VK^{-1}}$ by forming the pseudogap near the Fermi level. As an application of quasicrystals for thermoelectric materials, Pope *et al.* [2] and Kirihara *et al.* [3] have reported the thermoelectric properties of undoped Al-Pd-Mn and Al-Pd-Re, respectively. Our group has proposed the guiding principle of "Weakly Bonded Rigid Heavy Clusters (WBRHCs)" for an improvement of the thermoelectric properties in icosahedral cluster solids [4]. Based on this scheme, we have improved the thermoelectric properties by Ru [5] and Fe [6] substitution for Re in Al-Pd-Re, and Ga substitution for Al in Al-Pd-Mn [7,8].

In this research, we report the highest power factor in quasicrystals through Fe substitution for Mn in Al-Pd-Mn. Although the electrical and magnetic properties below room temperature of Al-Pd-Mn-Fe phase have been reported by Wang *et al.* [9], there is no report on their thermoelectric properties. We found 2/1-approximant phase in Al-Pd-Mn-Fe with the composition of $\mathrm{Al_{71}Pd_{20}(Mn_{0.5}Fe_{0.5})_9}$, which is similar XRD pattern of 2/1-Al-Pd-Mn-Si approximant [10]. This finding will promote further understanding between the crystal structure and properties.

1. E. Maciá, Critical Reviews in Solid State and Materials Sciences **37** (2012), p. 215.
2. A. L. Pope, T. M. Tritt, M. A. Chernikov, and M. Feuerbacher, Appl. Phys. Lett. **75** (1999), p. 1854.
3. K. Kirihara, and K. Kimura, J. Appl. Phys. **92** (2002), p. 979.
4. K. Kimura, J. T. Okada, H. Kim, T. Hamamatu, T. Nagata, and K. Kirihara, Mater. Res. Soc. Symp. Proc. **886** (2006), p. 231.
5. T. Nagata, K. Kirihara, and K. Kimura, J. Appl. Phys. **94** (2003), p. 6560.
6. J. T. Okada, T. Hamamatu, S. Hosoi, T. Nagata, K. Kimura, and K. Kirihara, J. Appl. Phys. **101** (2007), p. 103702.
7. Y. Takagiwa, T. Kamimura, S. Hosoi, J. T. Okada, and K. Kimura, J. Appl. Phys. **104** (2008), p. 073721,
8. Y. Takagiwa, T. Kamimura, J. T. Okada, and K. Kimura, J. Electron. Mater. **39** (2010), p. 1885.
9. C. R. Wang, S. T. Lin, and Y. C. Chen, J. Phys.: Condens. Matter. **6**(1994), p. 10747.
10. K. Sugiyama, N. Kaji, and K. Hiraga, Z. Kristallogr. **213** (1998), p. 90.

Lamelar structure and nanomechanical properties of quasicryslalline alloys Al-Cu-Fe

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Keywords: quasicrystal, transformation, nanomechanical properties

Icosahedral (3D-aperiodic) quasicrystals, including those of the Al-Cu-Fe system, show up high values of elasticity modulus and microhardness and may well take part of dispersion-hardening phases or serve as the base for wear-resistant materials [1,2]. The above listed practical applications call for researches into microscopic properties, which manifest themselves upon micro- and nano-scaled contact impact by the method of nanoindenting. Investigation of the influence of microstructural state of quasicrystalline alloys on their nano-scaled mechanical properties is considered topical. In the Al-Cu-Fe system, the icosahedral phase (ι) undergoes a series of structural transformations into approximant phases [3,4], which can be accompanied by various microstructural effects, such as the formation of lamellae. We study the kinetics of microstructure and phase transformations upon isothermal annealings of quenched quasicrystal-forming alloys $Al_{62.2}Cu_{24.8}Fe_{13}$ and $Al_{61.7}Cu_{25.2}Fe_{13.1}$ whose compositions fall into the stability region for the icosahedral phase. It is shown that at the annealing temperature 550°C, with increasing the duration of annealing and developing metastable transformations of ι-phase into P1-,P2-pentagonal approximant phases, there forms a homogeneous nanosize lamellar structure (ι + P1 + P2) which replaces individual P1-interlayers in the ι-matrix.

The *P-h* diagrams and the AFM and SEM-images of indents taken for two types of alloys with a lamellar and polygrain single-phase i-structure (T_{ann}=650°C) in the load range $5 \leq P_{max} \leq 500$ mN display signs of elastic-plastic behavior. Unlike polygrain alloys with the normal indentation size effect, for the alloys with the lamellar structure there is observed a nonmonotonous dependence hardness-peak load (P_{max}). We find the effect of deformation hardening in the load range $50 \leq P_{max} < 500$ mN with increasing the Meyer's and the plastic hardness, there takes place. The effects discovered are considered to be the result of resistance to plastic deformation from the boundaries of the lamellar structure.

1. F. Fleury, S. Lee, W. Kim and D. Kim, Metals and Mater. Intern. **6** (2000), p.415.
2. J. Dubois, "Useful quasicrystals", (World Scientific Publ., Singapore), (2005), p. 482.
3. N. Menguy, M. Auder, P. Guyot and M. Vacher, Phil.Mag. B **68** (1993), p. 595.
4. M. Quiquandon, A. Quivy, J. Devaud, F. Faudot, S. Lefebvre, M. Bessiere and Y. Calvayrac, J. Phys.: Condens. Matter **8** (1996), p. 2487.

Curie temperature and density of states at the Fermi level for Al-Cu-Fe phases : β-solid state solution – approximants- icosahedral quasicrystals

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Keywords: quasicrystal, approximant, magnetic and electronic properties

In Al-Tm based alloys, the anomalous physical properties (diamagnetism, high electrical resistivity) of quasicrystals and related canonical approximant phases correlate with an increase in the pseudogap effect and are considered to be due to complex cluster local structure with Al*s,p*-Tm*d* covalent binding [1, 2]. In the Al-Cu-Fe system, for which canonical and non-canonical approximants were found [3], anomalies are expected to grow in the series: β-solid state solution and β-based ordered phases (non-canonical approximants) – canonical approximants – icosahedral quasicrystal. In this sequence of phases, the effects of complex cluster local structure become more pronounced. We study how the diamagnetic contribution and the negative Curie temperature (θ) vary for these phases. According to the RKKY mechanism, the Curie temperature, which takes into account the contribution from antiferromagnetic ordering, should be proportional to the density of states at the Fermi level [4].

Low-temperature magnetic susceptibility and low-temperature heat capacity investigations have been performed in the temperature range 1.8 – 400 K. It was shown that the density of states at the Fermi level lowers, the diamagnetic effect grows, and the absolute values of the Curie temperature fall consistently in the following series of Al-Cu-Fe phases: β-solid state solution, β-based ordered η-AlCu(Fe)-phase, canonical approximant P1+P2-phases, icosahedral quasicrystal. The observed drop of the Curie temperature is considered as a result of both the lowering of the density of states at the Fermi level in this series of phases and the decrease in the local magnetic moment values characterizing the degree of covalent binding.

1. P. Lanco, T. Klein, C. Berger, F. Cyrot-Lackmann, G. Fourcaudot and A. Sulpice, Europhys. Lett. **18** (1992), p.227.
2. H. Sato, T. Takeuchi and U. Mizutani, Phys. Rev.B. **70** (2004), p.024210-1.
3. J. Dubois, “Useful quasicrystals”, (World Scientific Publ., Singapore), (2005), p. 482.
4. S. Vonsovskii, “Magnetizm”, (J. Wiley), (1974), p.1256.

Physical properties of bimetallic PdIn catalysts

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Keywords: alloys, selective catalysts, electrical and thermal conduction in crystalline metals and alloys

The bulk physical properties of single-crystalline bimetallic PdIn catalysts have been investigated in correlation with previously studied PdGa [1]. Both compounds are promising for selective catalysis. The bulk is influencing the properties of the surface, so knowledge of the bulk properties of the material is important to connect catalytic properties of the surface to the structural and electronic properties of the bulk. For that purpose we have determined the magnetic susceptibility, electrical resistivity, thermoelectric power, Hall coefficient, thermal conductivity and the specific heat of single crystal of PdIn grown by the Czochralski technique. The results show that PdIn is also a diamagnet with metallic electrical resistivity and moderately high thermal conductivity.

This work was done in collaboration with J. Stefan Institut (Ljubljana), Ludwig-Maximilians-Universität München, Department of Earth and Environmental Sciences, Crystallography Section (München), Institute of Molecular Physics, Polish Academy of Sciences (Poznan), Max-Planck-Institut für Chemische Physik fester Stoffe (Dresden) within the activities of the COST Action CM0904 "Network for Intermetallic Compounds as Catalysts for Steam reforming of Methanol".

1. M. Klanjšek, A. Gradišek, A. Kocjan, M. Bobnar, P. Jeglič, M. Wencka, Z. Jagličić, P. Popčević, J. Ivkov, A. Smontara, P. Gille, M. Armbrüster, Yu. Grin, J. Dolinšek, J. Phys.: Condensed Matter **24** (2012), p. 085703.

1/1-AlReSi approximant crystal: Electric properties, vacancy distribution and chemical bonding

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Keywords: electric properties, microstructure, vacancy concentration, electron density distribution,

To understand the origin of high electrical resistivity of Al-Pd-Re quasicrystal [1], 1/1-AlReSi approximant crystal is one of the suitable candidates, because both consist of the same structure unit, that is, Mackay icosahedral cluster. 1/1-AlReSi approximants exhibit peculiar transport properties with changing Re concentration [2]; $Al_{73}Re_{17}Si_{10}$ exhibits high electrical resistivity and its negative temperature dependence below room temperature, while $Al_{73}Re_{15}Si_{12}$ exhibits positive temperature coefficient of resistivity. Therefore, to elucidate the origin of the electric properties of 1/1-AlReSi approximants contribute further understandings of those for the related quasicrystal.

The remaining and important problem, the same as seen in Al-Pd-Re quasicrystals, is the porous microstructure after arc-melted and annealed AlReSi approximants. Recently, the electric and thermal properties of poly-crystalline Al-Pd-Re quasicrystals are discussed with their porous microstructure and oxidization [3] or sample's composition [4]. The microstructure of arc-melted and annealed AlReSi approximants is sensitive to the nominal composition; the sample with high Re concentration ($Al_{73}Re_{17}Si_{10}$) contains a lot of pores (relative density ~55%) while the sample with low Re concentration ($Al_{73}Re_{15}Si_{12}$) does not contain such pores (relative density ~95%). Therefore, it is important to investigate the effect of improvement of microstructure on the electric properties below room temperature, especially in high Re contained sample with high electrical resistivity. We found that the microstructure itself does not influence on the temperature coefficient of resistivity. In turn, the difference in vacancy concentration detected by positron annihilation spectroscopy has an influence on the electric properties of AlReSi approximants. Also, we will present the electron density distribution of metallic sample by MEM/Rietveld analysis, and discuss the chemical bonding nature compared with that of non-metallic sample [5].

1. H. Akiyama *et al.*, Jpn. J. Appl. Phys., Part 2 **32** (1993), L1003.
2. R. Tamura, T. Asao, S. Takeuchi, Phys. Rev. Lett. **86** (2001), p. 3104.
3. J. Dolinšek, P. J. McGuiness, M. Klanjšek, I. Smiljanić, A. Smontara, E. S. Zijlstra, S. K. Bose, I. R. Fisher, M. J. Kramer, and P. C. Canfield, Phys. Rev. B **74** (2006), p. 134201.
4. Y. Takagiwa, T. Kamimura, S. Hosoi, J. T. Okada, K. Kimura, Z. Kristallogr. **224** (2009), p. 79.
5. K. Kirihara, T. Nagata, K. Kimura, K. Kato, M. Takata, E. Nishibori, and M. Sakata, Phys. Rev. B **68** (2003), p. 014205.

RKKY interactions and low-temperature behaviour of spins in quasiperiodic tilings

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Keywords: magnetism, RKKY interactions, Monte Carlo simulation, Ising model

Understanding the magnetic properties of complex materials like quasicrystals still poses many open questions. According to experimental results the dominant interactions in rare-earth quasicrystals are based on the RKKY mechanism, which is a long-range indirect exchange interaction between the localized rare-earth atoms mediated by the conduction electrons.

The poster presents results for the structure of the RKKY interactions for selected two and three-dimensional quasiperiodic model systems. The interaction energies are computed by a continued fraction expansion of the Green's functions for these quasiperiodic tilings.

Based on the exchange interactions we study the mechanism of the alignment of magnetic moments in quasiperiodic tilings with Monte Carlo simulations. In particular, we are interested in the structure of the magnetic ground state as well as the low-temperature behaviour for Ising spins.

Pulse ultrasonic investigations of acoustic waves propagation in single-quasicrystalls $Ag_{42}In_{42}Yb_{16}$

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Keywords: single-quasicrystalls, acoustic waves, echo-pulse method

Results macroscopic elasticity investigations of some quasicrystalls, and also degrees of isotropy of their elastic properties are considered in [1]. The main experimental method of examinations described in [1] the article is the method of ultrasonic resonance spectroscopy. Application of the specified method is stipulated, including, negligible linear dimensions of the researched samples.

At the same time, at present there are examples of single-quasicrystalls growth with linear dimensions from several millimeters to centimeters. For such samples more common procedures for the definition of elastic wave's velocities and elastic constants become applicable. The echo-pulse method [2] is one of such methods.

In our work by Bridgman method have been grown single-quasicrystalls composition $Ag_{42}In_{42}Yb_{16}$ with linear dimensions nearly 1 cm. The growth results completely correlate with the results obtained by authors [3]. The synthesized samples were used for conduction of X-ray diffractional investigations. They show presence of the fifth order axes and confirm icosahedral symmetry.

For acoustic measurements we used samples with the shape of rectangular parallelepipeds with linear dimensions about 5 mm. On these samples by echo-pulse method [2] velocities of longitudinal and shear bulk acoustic waves (BAW) were measured. The measurements on 30 MHz frequency were carried out. Measurement accuracy of BAW velocities of absolute values is 10^{-4}. The measured values of velocities in researched samples are about 3270 m.p.s. for longitudinal and 1700 m.p.s. for shear BAW. The obtained data allows to make judgments about anisotropy of the researched single-quasicrystalls.

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1. M. A. Chernikov, Physics-Uspekhi **48** (2005), p. 411.
2. P. P. Turchin, A. A. Parfenov, N. A. Tokarev, A. E. Nesterov, A. Yu. Tarasova, K. S. Aleksandrov, Journal of I.I. Polzunov Altai State Technical University. **3/1** (2011), p. 143.
3. C. Cui, A. P. Tsai, Journal of Crystal Growth **312** (2009), p. 131.

Electronic transport of the $Sc_{57}TM_{13}$ 1/1 approximants

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Keywords: approximants, electrical resistivity, Sc-TM

$Sc_{57}TM_{13}$ (TM = Ru, Rh, Ir, Pt) are binary 1/1 crystal approximants composed of the MI-type clusters [1,2] which have no chemical disorder [1]. The temperature dependence of the electrical resistivity of $Sc_{57}TM_{13}$ is known to exhibit a variety of behaviours depending on the type of TM [3]. In this study, we have investigated the effect of the sample quality on the electrical resistivity of $Sc_{57}TM_{13}$ with different TM.

Alloys with compositions $Sc_{81.8}TM_{18.2}$ were prepared using Sc (99.95 %) and TM (99.9 %) in an arc furnace under Ar, and then wrapped by a Mo foil and annealed for 72 h at 1223 K in a sealed quartz tube under Ar. The electrical resistivity was measured for the annealed samples by the four-probe method at 0.5 ~ 300 K.

The electrical resistivity was confirmed to be very high for all TM, e.g., 150~350 μΩcm although they have no chemical disorders. The ρ_{LT}/ρ_{290K} ratio was found to show different values among different systems ($Sc_{57}Ru_{13}$: 0.4, $Sc_{57}Rh_{13}$: 0.8, $Sc_{57}Ir_{13}$: 0.5, $Sc_{57}Pt_{13}$: 0.75). In addition, an upturn in the electrical resistivity was observed at low temperatures below 9 K for $Sc_{57}Pt_{13}$. Detail of the results will be discussed in the poster presentation.

1. K. Cenzual, B. Chabot and E. Parthe, Acta Crystallogr. C **41** (1985), p. 313.
2. V. N. Eremenko, V. G. Khorujaya, P. S. Martesenyuk and K. Ye. Korniyenko, J. of Alloys and Compounds **217** (1995), p. 213.
3. Y. G. So, K. Edagawa and R. Tamura, Phil. Mag. **87** (2007), p. 2957.

Lattice dynamics of the decagonal approximant $Al_{13}Co_4$ phase

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Keywords: quasicrystals, approximants, lattice dynamics, phonons dispersions, ab initio calculation (DFT), inelastic neutron scattering, thermal conductivity.

The lattice dynamics of quasicrystals has been the subject of both theoretical and experimental investigations since their discovery [1].

In the long wavelength regime, acoustic modes have been predicted to be best visible around strong Bragg peaks, acting as Brillouin zone centers. For higher wave vectors, the theory predicts that the modes are critical, that is to say they are neither extended as in simple crystals and no localized as in disordered systems [2]. Experimentally phonon have been studied in different quasicrystallines systems. For all of them, acoustic modes are well defined for wavevector smaller than 3 nm^{-1}, and then broaden rapidly as the result of a mixing with other excitations [3].

We will present a combined experimental and atomic scale simulation study of the lattice dynamics of the $Al_{13}Co_4$ phase (orthorhombic, 102 atoms in the unit cell) [4] which is a periodic approximant to the decagonal phase. A particular attention will be given to eventual differences between the periodic and 'quasiperiodic' directions.

Inelastic neutron scattering measurements carried out on a large single grain on a triple axis spectrometer will be compared to atomic scale simulation. We will in particular compare the dispersion relationship but also the intensity distribution of the $S(Q,\omega)$ scattering function which is a very sensitive test [3]. Simulation are carried out either using DFT based calculations or empiracal oscillating pair of potential [3]. Both simulations are in very good agreement with the experiment.

Results will be compared with the phonon thermal conductivity for which a rather weak anisotropy has been observed [6]. Finally a vibrational mode analysis, extracted from the simulation, will be also presented.

1. D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Phys. Rev. B **53** (1984), p. 1951-1954.
2. T. Janssen, G. Chapuis and M. de Boissieu, in "Aperiodic Crystals", (Oxford University Press, Oxford) (2007).
3. M. de Boissieu, S. Francoual, M. Mihalkovic, K. Shibata, A. Q. R. Baron, Y. Sidis, T. Ishimasa, D. Wu, T. Lograsso, L. P. Regnault, F. Gähler, S. Tsutsui, B. Hennion, P. Bastie, Ta. J. Sato, H. Takakura, R. Currat and A.-P. Tsai, Nature Materials **6** (2007), p. 977-984.
4. J. Grin, U. Burkhardt and M. Ellner, Journal Alloys Compounds **206** (1994), p. 243.
5. B. Zhang, V. Grämlich and W. Steurer, Zeitschrift für Kristallographie **210** (1995), p. 498-503.
6. P. Gille, B. Bauer, M. Hahne, A. Smontara and J. Dolinšek, Journal Crystal Growth **318** (2011), p. 1016–1020.
7. J. Dolinšek, M. Komelj, P. Jeglič, S. Vrtnik, D. Stanić, P. Popčević, J. Ivkov, A. Smontara, Z. Jagličić, P. Gille and Yu. Grin, Physical Review B 7**9** (2009), p. 184-201.

In-situ observation of Co rearrangement of near-surface skin layer in $Al_{70}Ni_{15}Co_{15}$ quasicrystal

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Keywords: decagonal quasicrystal, near-surface skin layer, Co depletion

Very recently, before/after annealing, atomic rearrangement on the surface of Al-Co-Cu decagonal quasicrystal was observed by low-energy ion scattering [1]. Al enrichment on the surface is originated from the surface stabilization. On the other hand, diffuse scattering in $Al_{70}Ni_{15}Co_{15}$ was measured [2]. The atomic short-range order (SRO) diffuse scattering was coupled with a phason.

High temperature experiment using anomalous X-ray scattering was performed on the ORNL beam line X14A of the National Synchrotron Light Source in Brookhaven National Laboratory. An energy spectrometer was attached on the six-circle diffractometer. A single quasicrystal of $Al_{70}Ni_{15}Co_{15}$ is selected in this study. Near the Co K-edge, kinetics of diffuse scattering at 807 °C showed the decrease of atomic SRO. At the same time, some weak Debye rings appeared in a vicinity of Bragg reflections (Fig. 1). The Debye rings were observed only near the Co K-edge. Therefore, a small amount of polymerization is relating to Co depletion near the surface. Off-Bragg powder rings correspond to a little difference of lattice constants. We calculate scattering volume ratio of bulk to a near-surface skin layer considering absorption correction using a rod-shape of the sample. The thickness of the skin layer is estimated to be 1.7 nm. The deformed skin layer is also seen on the β_1–β_2 phase transition in V_2H [3].

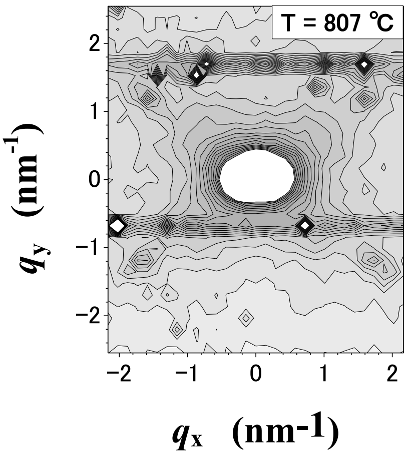

Fig. 1 SRO diffuse scattering (t=1.2 h).

1. R. Zenkyu, J. Yuhara, T. Matsui, S. Shah Zaman, M. Schmid and P. Varga, Phys. Rev. B **86** (2012), p. 115422.
2. H. Abe, N. Tamura, D. Le Bolloc'h, S. C. Moss, Y. Matsuo, Y. Ishii and J. Bai, Mater. Sci. Eng. **299-302** (2000), p. 294.
3. J. Trenkler, H. Abe, P. Wochner, D. Haeffner, J. Bai, H. D. Carstanjen and S. C. Moss, Model. Simul. Mater. Sci. Eng. **8** (2000), p. 269.

Dynamical low-energy electron diffraction study of the 5-fold surface of i-Al-Pd-Mn

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Keywords: quasicrystal, Al-Pd-Mn, LEED, diffraction, surface structure

A low-energy electron diffraction (LEED) experiment was performed on the 5-fold surface of icosahedral quasicrystalline Al-Pd-Mn at 88 K in order to make a quantitative determination of its surface structure. A large data set with a total energy range of 4500 eV was obtained. A large data set is important for solving complex structures with many parameters. For comparison, data sets for simple surfaces are typically less than 1000 eV, and the largest data set we have ever used, for the Al13Co4(100) surface, was about 20,000 eV.

The data were analyzed using a 2/1 periodic approximant structure as the model, with 136 atoms per unit cell, using the SATLEED program for the computations. This method has been applied before to other quasicrystalline surfaces [1,2,3]. Earlier LEED experiments on this surface had employed several significant approximations that averaged over the positions of sets of atoms. [4,5]. This is the first LEED analysis for this surface to consider individual atom positions.

The best-fit structure has a Pendry R-factor of 0.40, which indicates a moderate level of agreement, not unexpected for a complex structure such as this. The structure is essentially a truncation of the bulk structure, although there are some significant displacements of the surface atom positions from the bulk-like positions. This study represents the most complete study of the surface structure of 5-fold i-Al-Pd-Mn to date, and provides a starting point for more extensive investigations.

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1. K. Pussi, N. Ferralis, S. Curtarolo, M. Gierer, M. Mihalkovic, M. Widom, C. J. Jenks, P. Canfield, I. Fisher and R. D. Diehl, Phys. Rev. B **73** (2006), p. 184203.
2. K. Pussi and R. D. Diehl, Z. Kristallogr. **224** (2009), p. 1–4.
3. K. Pussi, M. Gierer and R. D. Diehl, J. Phys. Condens. Mat. **21** (2009), p. 474213.
4. M. Gierer, M. A. Van Hove, A. I. Goldman, Z. Shen, S. L. Chang, C. J. Jenks, C. M. Zhang, P. A. Thiel, Phys. Rev. Lett **78** (1997), p. 467.
5. M. Gierer, M. A. Van Hove, A. I. Goldman, Z. Shen, S. L. Chang, P. J. Pinhero, C. J. Jenks, J. W. Anderegg, C. M. Zhang, P. A. Thiel, Phys. Rev. B **57** (1998), p. 7628.

Surface stability of quasicrystals and related approximants

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Keywords: quasicrystals, surface structure, scanning tunnelling microscopy (STM)

The structure of quasicrystals and related approximants is described in terms of three dimensional atomic clusters as building blocks. When prepared by the usual method of ion-bombardment and annealing, their surface produces atomically flat terraces at specific bulk planes. Different physical factors have been considered to explain the selection of bulk planes at the surface [1-3], based on investigations on similar class of Al-based quasicrystals or single grain samples with specific surface orientations. We have extended the surface study to a polygrain icosahedral (*i*-) Al-Pd-Re quasicrystal and Cd-Yb family systems, which allows deeper understanding of surface stability of these materials.

Scanning tunnelling microscopy from the polygrain *i*-Al-Pd-Re quasicrystal with random grain orientation predominantly shows the formation of large terraces along the twofold planes. This indicates that the twofold surface, which has the highest atomic density, is the most stable among all the crystallographic surfaces. This observation is in contrast with previous reports [4] that the fivefold surface of *i*-Al-Pd-Mn is more stable than other high symmetry surfaces. The stability of the fivefold *i*-Al-Pd-Mn surface was explained in terms of atomic density and Al content [3].

The high symmetry surfaces of the *i*-Ag-In-Yb [5, 6] quasicrystal are formed at bulk planes intersecting the centre of rhombic triacontahedral (RTH) clusters, the building blocks of the system. These planes have moderate atomic density and contain mostly In and Yb, elements having lower surface free energy than Ag. The (100) surface of the Ag-In-RE (RE= Gd, Tb) approximants develops facets. The facet planes are not dictated by high symmetry axes of the RTH cluster but these are formed along the planes containing high density of cluster centres. The atomic density along the facet planes is generally low. The combination of these results indicates that no universal model can be used to describe the stability of surfaces of quasicrystals and related approximants.

1. M. Gierer, M. A. Van Hove, A. I. Goldman *et al.*, Phys. Rev. Lett. **78** (1997), p. 467.
2. Z. Papadopolos, G. Kasner, J. Ledieu, *et al.*, Phys. Rev. B **66** (2002), p. 184207.
3. H. R. Sharma, V. Fournée, M. Shimoda *et al.*, Phys. Rev. Lett. **93** (2004), p. 165502.
4. Z. Shen, W. Raberg, M. Heinzig, C. J. Jenks, V. Fournée *et al.*, Surf. Sci. **450** (2000), p. 1.
5. H. R. Sharma, M. Shimoda, K. Sagisaka *et al.*, Phys. Rev. B **80** (2009), p. 121401.
6. C. Cui, P. J. Nugent, M. Shimoda, J. Ledieu, V. Fournée, A. P. Tsai, R. McGrath, H. R. Sharma, J. Phys.: Condens. Matter **24** (2012), p. 445011.

Surface topography of single quasicrystals

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Keywords: quasicrystals, surface topography, decorations

Surface topography of faceted icosahedral Al-Cu-Fe and decagonal Al-Cu-Co single quasicrystals has been investigated by the scanning electron microscopy (SEM) using primary and secondary electrons. The selected area diffraction (SAD) was also applied. The polyhedral equilibrium single grains of the icosahedral ψ phase of an Al-Cu-Fe alloy, for which the nominal composition was 65 at. % Al, 20 at.% Cu and 15 at.% Fe were obtained in a helium atmosphere using the Bridgman-Czochralski-Growth (BCG) apparatus equipped with an induction furnace. The decagonal $Al_{73.5}Cu_{17.5}Co_9$ single quasicrystals have been obtained by inclined front crystallization technique.

Both types of single quasicrystals exhibited a decorations on their facets, however the character of decorations was totally different. Two stages of decorations has been developed on icosahedral $Al_{60}Cu_{26}Fe_{14}$ quasicrystals: cellular primary decorations and secondary fractal like decoration. Surface decorations on decagonal $Al_{73.5}Cu_{17.5}Co_9$ quasicrystals formed a kind of irregular stars placed on the neighbouring islands.

There was no evident difference in chemical composition between the inner dodecahedra, primary cellular decorations as well as the secondary fractal like decorations.

1. M. Surowiec, W. Bogdanowicz, J. Krawczyk, B. Formanek, M. Sozanska, Phil. Mag. **91** (2011), p. 2458.
2. C. Beeli and H.-U. Nissen, Phil. Mag. B, **68** (1993), p. 487.

Leaching of Al-based polygrain quasicrystalline and related crystalline surfaces

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Keywords: leaching, hydrogen storage, catalyst

The potential application of quasicrystals as catalysts has been investigated by Tsai's group after alkaline leaching quasicrystal powder. The leached surface shows a relatively high specific surface area and a high density metallic sites for catalysis like Raney nickel catalysts [1-2]. The leaching of icosahedral Al-Cu-Fe quasicrystal yields Cu and Fe nano-particles on the top of the quasicrystalline surface [3]. These nano-particles are believed to be responsible for catalytic reactions. However, the role played by the supporting quasicrystal in the activity is not fully understood and the optimization of the catalytic activity is currently limited to heuristic approaches.

In the present investigation, we have studied the leaching on poly- grain Al (Al-Cu-Fe, Al-Pd-Re and Al-Pd-Mn) base quasicrystalline as well as crystalline (B2 phase) alloys surface by 10 mole NaOH solution. The surface was leached at varying times from 30 mins to 8 hours and subsequently characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (SEM) and energy dispersive x-ray (EDX) analysis. Leaching of the samples at 30 mins generated a homogeneous layer and further leaching (1-8 hours) yielded nano size particles on the surface. The spherical microstructure has been observed on Al-Cu-Fe crystalline surface whereas on quasicrystlline surface a petal like microstructure was appeared. The implications of the evolution of the different microstructures in the context of structure, stability and activity will be discussed. The results will be compared with the microstructure of leached poly-grain samples containing a mixture of different surface orientations.

1. T. Tanabea, Satoshi Kameoka, A. P. Tsai, Applied Catalysis A **384** (2010), p. 241.
2. T. Tanabe, Satoshi Kameoka, A. P. Tsai, J Mater Science **46** (2011), p. 2242.
3. T. P. Yadav, M. Lowe, R. Tamura, R. McGrath, and H.R. Sharma in "Aperiodic Crystals", eds. S. Schmid *et al.*, (Springer, Dordrecht) (2013)

Leaching of mechanically activated Al-Cu-Fe icosahedral quasicrystalline phase and its catalytic application

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Keywords: leaching, hydrogen storage, catalyst

The powder of thermally stable icosahedral (*i*) Al–Cu–Fe quasicrystal leached with NaOH aqueous solutions shows excellent activity for steam reforming of methanol [1-2]. The leaching treatments yield Cu and Fe nano-particles on the top of the quasicrystalline surface. These nano-particles are believed to be responsible for catalytic reactions. To find out the role played by the supporting quasicrystalline phase in the catalytic activity, the leaching of well-oriented surface of single grain *i*-Al-Cu-Fe was studies recently [3].

In the present investigation, we have leached $Al_{65}Cu_{20}Fe_{15}$ as grown icosahedral quasicryslline alloy as well as 40 hours mechanically activated alloys with 10 mole NaOH aqueous solutions. The mechanical activation of as grown icosahedral quasicryslline was done with low intensity (200 rpm) of milling with a ball to powder ratio of 40:1. The X-ray diffraction, scanning electron microscopy, transmission electron microscopy, differential thermal analysis and energy-dispersive x-ray analysis were employed to characterize the as grown and mechanically activated samples. The 2 hour leached as grown and mechanically activated Al_{65}Cu20Fe15 alloys was subjected for catalyst application in MgH_2 hydrogen storage materials. The catalytic effect of leached alloy on the de/rehydrogenenation characteristics of MgH_2 has been studied. The onset decomposition temperature for leached icosahedral quasicrystal catalyzed MgH_2 is found to be ~ 250°C which gets reduced to ~220°C for leached mechanically activated icosahedral quasicrystale catalyzed MgH_2. The hydrogenation behaviour including absorption kinetics will be discussed and presented in detail.

1. T. Tanabea, Satoshi Kameoka, A. P. Tsai, Applied Catalysis A **384** (2010), p. 241.
2. T. Tanabe, Satoshi Kameoka, A. P. Tsai, J Mater Science **46** (2011)**,** p. 2242.
3. T. P. Yadav, M. Lowe, R. Tamura, R. McGrath, and H. R. Sharma in “Aperiodic Crystals”, eds. S. Schmid *et al.*, (Springer, Dordrecht) (2013)

$Au_{10}M_4Zn_{89}$ (M=Cr, Mo): A fully ordered complex intermetallic compound analysed by TOPOS

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Keywords: complex metallic alloys, crystal chemistry, X-ray diffraction, “Nanoclustering” procedure

The crystal chemistry of the ternary Au-M-Zn (M=Cr, Mo) alloys were studied by synthesis, single crystal X-ray diffraction, and electronic structure calculations. The binary phases-$CrZn_{17}$ or $MoZn_{20.44}$ [1] are disordered exhibiting a complex interplay of occupational and positional disorders. The inclusion of Au proves to be very site specific, and at the limiting composition $Au_{10}M_4Zn_{89}$ (M=Cr, Mo), structures are completely ordered. Electronic structure calculations of $Au_{10}M_4Zn_{89}$ (M=Cr, Mo) by using the tight-binding linear muffin-tin orbital atomic-spheres approximation (TB-LMTO-ASA) method, indicate that the observed chemical composition and atomic distributions lead to the presence of a pronounced pseudogap at the Fermi level in the density of states and this is consistent with the Hume-Rothery interpretation of γ-brasses, in general [2,3]. The structure of the ordered $Au_{10}M_4Zn_{89}$ (M=Cr, Mo) compound has been described by using the algorithm of automatic geometric and topological analysis that is implemented into the program package TOPOS as the “Nanoclustering” procedure [4]. The structure is largely tetrahedrally close packed, but an octahedral arrangement of atoms is incompatible with tetrahedral close packing. The structure can also be described as an arrangement of nested polyhedral units, centered at sites of high symmetry points. A closer inspection of the atomic arrangements in $Au_{10}M_4Zn_{89}$ (M=Cr, Mo) reveals that the cluster description may conveniently be expanded to 28-atom shells.

This presentation will discuss about the synthesis, crystal and electronic structure calculations of the ternary Au-M-Zn (M=Cr, Mo) alloys.

1. T. Nasch, W. Jeitschko, J. Solid State Chem. **143** (1999), p. 95-103.
2. W. Hume-Rothery, J. Inst. Metals **35** (1926), p. 295.
3. S. Thimmaiah, G. J. Miller, Chem. Eur. J. **16** (2010), p. 5146-5471.
4. V. A. Blatov, Struct. Chem. **23** (2012), p. 955-963.

The reinforcement distribution in the CQ composites of Al-Cu-Fe alloys obtained by the Bridgman method

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Keywords: icosahedral quasicrystals, composites, directional solidification, fibrous reinforcement

The composites are currently one of the main structural materials in the aerospace, automotive and engineering industries. The fibrous composites with single-crystalline matrix and reinforcement contained quasicrystalline phases have a great importance as materials for the components of internal combustion engines and gas turbines due to their specific mechanical and thermal properties. Quasicrystalline phases possess good stability at high temperatures, low coefficient of sliding friction and high hardness, but unfortunately can be brittle [1,2].

The analysed composites were obtained by the Bridgman method through solidification of $Al_{61}Cu_{27}Fe_{12}$ (at.%) alloy with two pulling down rates of 0.07 and 0.5 mm/min. [3,4]. The microstructure of composites with crystal matrix and quasicrystal reinforcement (CQ composites) were studied. The crystalline β-phase was the matrix and the quasicrystaline *i*-phase was the reinforcement of obtained CQ composites. The shape and spatial distribution of reinforcement fibres in the samples solidified with pulling rate of 0.5 mm/min. were specified. Some geometrical relations of the fibres arrangement were defined. Obtained composite samples were subjected to X-ray phase analysis, optical and scanning electron microscopy observations, chemical microanalysis and the Laue diffraction. Changes in microstructure of composites obtained with pulling rates of 0.07 and 0.5 mm/min were defined.

1. G. Laplanche, A. Joulain, J. Bonneville, R. Schaller and T. El Kabir, J. Alloy Compd. **493** (2010), p. 453
2. J. M. Dubois „Useful quasicrystals”, (World Scientific, Singapore, 2005)
3. J. Krawczyk, W. Bogdanowicz, Solid State Phenom. **203-204** (2013), p. 48
4. J. Krawczyk, W. Bogdanowicz and T. Goryczka, Phil. Mag. **90** (2010), p. 3987

Superconductors, LnT_2Zn_{20} (Ln = La, Pr, T = Ru, Ir): Their Crystal Structures

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Keywords: Crystal structure, Superconductor, Cluster compound

In recent years, the cluster compounds and/or the compounds having cage-like substructure have attracted much attention not only in chemistry field but also in field of solid-state physics, to show rich interesting properties, since the discovery of fullerenes and fullerides. For example, in solid-state field, these compounds (especially, having rattled atoms in the cluster/cage structure) show various kinds of physical properties such as strong electron-phonon coupling superconductivity [1], heavy fermion behaviour [2], and thermoelectricity with glass-like thermal conductivity [3].

In 2010, we found new superconducting compounds; LnT_2Zn_{20} (Ln = La, Pr, T = Ru, Ir), showing superconducting transitions at Tc around 0.2 K ($LaRu_2Zn_{20}$), 0.6 K ($LaIr_2Zn_{20}$), and 0.05 K ($PrIr_2Zn_{20}$). Especially, $PrIr_2Zn_{20}$ is the second example of superconductor in the intermetallic compounds containing Pr atom. [4] Before taking superconducting state, these compounds take structural transitions, but do not have any magnetic transitions. At room temperature, the crystal structure of these compounds basically takes cubic $CeCr_2Al_{20}$-type structure (Fd-3m). [5] Details of the crystal structure are not so clear.

To understand the detail of this crystal structure, we carried out single-crystal diffraction technique at 293 K. Our used single crystals are grown by Zn self-flax method. [6] In the structure, *Ln* atom locates in the cage structure formed by 16 Zn atoms. On the other hand, *T* atom is surrounded by 12 Zn atoms forming another cage structure. Both *Ln* and *T* atoms locate at crystallographically independent sites. However, some of Zn sites show the site disordering behaviour. More details will be presented.

1. E. D. Bauer, N. A. Frederick, P.-C. Ho, V. S. Zapf, and M. B. Maple, Phys. Rev. B **65** (2002), p. 100506.
2. See, for example, J. Phys. Soc. Jpn. **77** (2008), Suppl. A, and references therein.
3. Ed. M. G. Kanatzidis, S. D. Mahanti, and T. P. Hogan, “Chemistry, Physics and Materials Science of Thermoelectric Materials: Beyond Bismuth Telluride”, (Kluwer Academics/Plenum Publishers, New York) (2003)
4. T. Onimaru, K. Matsumoto, Y. F. Inoue, K. Umeo, Y. Saiga, Y. Matsushita, R. Tamura, K. Nishimoto, I. Ishii, T. Suzuki, and T. Takabatake, J. Phys. Soc. Jpn. **79** (2010), p. 033704.
5. T. Nasch, W. Jeitschko, and U. C. Rodewald, Z. Naturforsch. B **52** (1997), p. 1023.

Phase equilibria investigation of Al-Co complex metallic alloys

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Ternary Al-Co-TM alloys (TM = Cu, Pd, Ni, Fe) are an interesting group of materials since their phase equilibria consist of complex intermetallic phases, including stable quasicrystals and quasicrystalline approximants [1]. For their phase diagram construction and identification of reactions, the binary Al-Co system plays an important role. The Al-Co phase diagram has been intensively studied by Gödecke [2] and Grushko [3]. Despite of many similarities in both published phase diagrams, they differ in several details. The major difference is in the description of phase transformations occurring in the $Al_{13}Co_4$ family, lying between Al_5Co_2 and Al_9Co_2 phases. Our work is therefore focused on the experimental re-investigation of Al-Co phase diagram between Al_5Co_2 and Al_9Co_2 compounds. Seven complex metallic alloys with nominal composition of $Al_{71}Co_{29}$, $Al_{72}Co_{28}$, $Al_{73}Co_{27}$, $Al_{74}Co_{26}$, $Al_{75}Co_{25}$, $Al_{75.5}Co_{24.5}$, and $Al_{76}Co_{24}$ were prepared and investigated at near-equilibrium conditions. The alloys were long-term annealed at 800 - 1200°C and subsequently quenched to fix their high-temperature microstructures. Annealing temperatures were chosen with respect to the results of differential scanning calorimetry. The samples were studied by a combination of X-ray diffraction, scanning electron microscopy including energy dispersive X-ray spectroscopy and electron backscatter diffraction.

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1. B. Grushko, T. Velikanova, Calphad **31** (2007), p. 217-232.
2. T. Gödecke, M. Ellner, Z. Metallkd. **87** (1996), p. 854-864.
3. B. Grusko, R. Wittenberg, K. Bickmann, C. Freiburg. J. Alloy Compd. **233** (1996), p. 279-287.

Varied Linear Phason Strain and Its Induced Domain Structure in Quasicrystalline Precipitates of Zr-Al-Ni-Cu-Nb Bulk Metallic Glass Matrix Composites

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Quasicrystalline precipitates in ZrAlNiCuNb alloy [1] were systematically studied by transmission electron microscopy. Electron diffraction patterns show that precipitates always contain various linear phason strains [2, 3], caused by which the diffraction spots' shifting can be divided into two types, parallel and perpendicular to the incident beam direction. The latter one can be subdivided into transverse and longitudinal shifting. Experimentally observed spots' shifting induced by linear phason strains can be parallel, transverse, longitudinal or mixed. After meticulous measurement, quantitative fitting and calculation of the diffraction spots' shifting, the phason strain matrices were determined. Within some single grains, nanoscale domain structures formed as a result of linear phason strain variants along different directions with equal probability. These phason strain variants can counterbalance each other to produce low macroscopic strain for the whole grain. In a unique case, phason strain induces subtle opposite displacements along the incident beam direction, leading to the breaking of central symmetry in the electron diffraction pattern. This study will enrich the knowledge of linear phason strain and may also deepen the understanding about the intrinsic characteristic of quasicrystals and its related bulk metallic glass matrix composites.

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1. Y. F. Sun, C. H. Shek, B. C. Wei, W. H. Li and Y. R. Wang, J. Alloy Compd. **403** (2005), p. 239.
2. P. A. Bancel and P. A. Heiney, J. Phys. Colloques **47** (1986), p. C3-341.
3. J. E. S. Socolar and D. C. Wright, Phys. Rev. Lett. **59** (1987), p. 221.

Novel metadislocations and stacking faults in the complex metallic alloy ε_6-Al-Pd-Mn

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In complex metallic alloys (CMAs), a class of intermetallic phases characterized by high structural complexity and large lattice parameters, conventional mechanisms of plastic deformation are prone to failure. The key for understanding the deformation mechanism in CMAs are so called metadislocations, a novel kind of dislocations first observed in the ε_6-phase of the CMA Al-Pd-Mn [1]. In this specific alloy different types of metadislocations can be categorised with regard to the number of associated phason halfplanes. Up to now detailed microstructural information regarding the core structure could be solely derived for a single type of metadislocation with 10 phason planes [2].

Here present state of the art aberration-corrected high resolution scanning transmission electron microscopy studies on Al-Pd-Mn which allow for straightforward interpretation of various types of metadislocations on the atomic level. Dissociation of the core of a metadislocation with 16 phason planes was observed. Furthermore, the atomic structure of novel stacking faults and dislocations was investigated.

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1. H. Klein *et al.*, Phys. Rev. Let. **82** (1999), 3468.
2. M. Heggen, M. Feuerbacher, Acta. Mater. **61** (2013), 3851.

Elastodynamics of wave-telegraph type for quasicrystals

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Keywords: equations of motion, waves, phason frictional forces

The aim of this work is to propose the elastodynamic model of wave-telegraph type for the description of dynamics of quasicrystals [1]. According to this model, phonons are represented by undamped waves, and phasons by waves damped in time and propagating with finite velocity. Therefore, the equations of motion for the phonon fields are of wave type and for the phason fields are of telegraph type. The main advantage of this model is its ability to describe the damping of the phason waves with respect to the time, and to overcome the paradox of the infinite velocity propagation which is implied by the diffusion equation. Proceeding to the modelling of damped phason waves, the concept of phason frictional forces is used. In this context, anisotropic effects of the damped waves can also be captured. To gain more insight into the significance of this model, qualitative (mathematical and physical) differences and similarities with existing models (elastodynamics of wave type and elasto-hydrodynamics of quasicrystals) are presented and discussed.

We derive the equations of motion for the displacement fields in the theory of incompatible and compatible elastodynamics of wave-telegraph type of quasicrystals [2]. The incompatible case is important, for instance, for the study of dislocations and elastoplasticity while the compatible case is important for the study of dynamics of cracks, elastic waves, body forces, as well as dispersion relations in quasicrystals. In the framework of incompatible elastodynamics of wave-telegraph type, the plastic fields are taken also into account, since a dislocation is the elementary carrier of plasticity.

1. E. Agiasofitou and M. Lazar, The elastodynamic model of wave-telegraph type for quasicrystals, Submitted (2013).
2. E. Agiasofitou and M. Lazar, On the equations of motion of dislocations in quasicrystals, Submitted (2013).

Periodicity and scaling in diffraction patterns of selected aperiodic structures

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Keywords: diffraction; quasicrystals; modulated structure

Aperiodic structures, including modulated structures and quasicrystals, do not exhibit translational invariance, what is the essential feature distinguishing them from classical crystals. However their diffraction patterns are exclusively composed of many periodic series of diffraction peaks [1]. For a selected series of peaks their individual intensities form a curve called the envelope curve for this series. The full diffraction pattern can be used to restore the analytical form of the envelope curve. Translating the envelope curve into respective values in extra space dimension (usually called the perpendicular space of the diffraction vector) one can restore the full diffraction pattern of the structure. The envelope curves not only reproduce the intensities of diffraction peaks, but also indicate the points that are most prone to be involved in phase changes of the structure factor.

Periodic series of diffraction peaks allow the construction of a periodic reference lattice allocated to the physical space. The periodicity of the reference structure does not implicate the periodicity of the structure itself, as there is no such periodicity in the physical space. However one can use the reference lattice to construct probability distributions of the atomic positions calculated with respect to the reference lattice nodes. These probability distributions are periodic, and their period is determined by the period of the reference lattice. For classical crystals such probability distributions are discrete objects and they directly describe the decoration of the elementary cell. For quasicrystals these distributions are continuous and they form the so called average elementary cell. The knowledge of the average elementary cell allows complete reconstruction of the full diffraction pattern of the examined object.

Another property that distinguishes between various structure types is the scaling. It is best shown for the quasicrystalline structures, where one can encounter the so called TAU2 scaling. There is a linear dependence between the atomic positions of decorating atoms in two different average elementary cells: one calculated for the k_0 wave vector and the other calculated for $q_0 = \tau \cdot k_0$, where τ is the so called golden number. It generates a linear relation between the coordinates, with the proportionality coefficient equal to $(-\tau^2)$. The knowledge of the envelope curve for a given series of peaks, the resulting phase relations between the peaks and the coordinate scaling essentially simplify the structure factor formula and allow the structure fitting in the physical space.

1. Wolny, J. *et al.*, Israel J. Chem. 51 (2011) p. 1275-1291.

Structure model for icosahedral quasicrystal based on Ammann tiling

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Keywords: icosahedral quasicrystals, structure modelling, Ammann tiling, Average Unit Cell,

The quasicrystalline family is most widely represented by icosahedral phases (*i*-QCs). However only few *i*-QCs structures has been solved and refined – eg. [1,2], where the structure solution based on higher-dimensional and cluster analysis were used. Here, the another method, called statistical approach using the Average Unit Cell (AUC) concept [3], is presented. The most significance of this method is that is works in real space only. As a starting model the Ammann tiling (AT) is used, where two structural units appear – prolate and oblate rhombohedra (as two rhombuses in 2D Penrose tiling). The statistical method was recently successfully applied to decagonal quasicrystals by Kuczera *et al.* [4,5].

The poster presents the results of applying the statistical method to the description of structure of *i*-QCs. The structure factor for empty Ammann lattice was found and the agreement with higher-dimensional description and numerical diffraction pattern was proven [6,7]. The attempt to decoration scheme was done. The AUC was divided for regions belonging to certain orientations of rhombohedra in real space. The derivation of the structure factor for freely decorated AT is in progress.

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1. A. Fang, H. Zou, F. Yu, R. Wang, X. Duan, J. Phys.: Condens. Matter **15** (2003), p. 4947–4960.
2. H. Takakura, C. P. Gomez, A. Yamamoto, M de Boissieu, A. P. Tsai, Nature Materials **6** (2007), p. 58-63.
3. J. Wolny, Phil. Mag. A **77** (1998), p. 395-412.
4. P. Kuczera, J. Wolny, F. Fleischer, W. Steurer, Phil. Mag. **91** (2011), p. 2500-2509.
5. P. Kuczera, J. Wolny, W. Steurer, Acta Crystallogr. A **68** (2012), p. 578-589.
6. J. Wolny, B. Kozakowski, P. Kuczera, R. Strzalka, A. Wnek, Isr. J. Chem. **51** (2011), p. 1275-1291.
7. R. Strzalka J. Wolny, P. Kuczera, Aperiodic Crystals, S. Schmid *et al.* (eds.), Springer (2013), DOI: 10.1007/978-94-007-6431-6_27.

Structure factor for the Generalized Penrose Tiling

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Keywords: quasicrystals, structure factor, Generalized Penrose Tiling

In this paper the work on Generalized Penrose Tiling (GPT) is presented. The GPT can be considered a promising alternative for Penrose Tiling (PT) as a model for decagonal quasicrystal refinement procedure, particularly in the statistical approach (also called the Average Unit Cell (AUC) approach) [1]. The statistical method using PT has been successfully applied to the structure optimization of various decagonal phases [2,3]. The application of the AUC concept to the GPT will be presented.

In the *n*D approach, PT is obtained by projecting a 5D hypercubic lattice through a window consisting of four pentagons, called the atomic surfaces (AS), in the perpendicular space. The vertices of these pentagons together with two additional points form a rhombicosahedron. The GPT is an extension of the PT. It is generated by projecting the 5D hypercubic lattice through a window consisting of five polygons (decagons and pentagons) in perpendicular space. These polygons are obtained by shifting the original pentagons related to PT along the body diagonal of the rhombicosahedron [4,5]. In other words, the higher dimensional projection strip is shifted in 5D space. This leads to a change in the shape of AS, depending on the shift parameter. The structural building units are still thick and thin rhombuses, but the matching rules and the tiling changes.

The derivation of the analytical formula for structure factor for the empty GPT lattice (with no decoration) is made similarly to the calculation for the PT [6]. In the AUC concept the probability distribution for rhombuses of PT can be obtained as an oblique projection of the AS on the physical space. This holds true also for the GPT. The derivation of the AUC distribution for a given type of rhomb in a given orientation of an arbitrarily chosen GPT will be presented. In the PT, these distributions are triangular, whereas in the case of the GPT they are triangular (originating from the pentagonal AS) or hexagonal (originating from the decagonal AS). The AUC of GPT for shift parameters 0.2 and 0.5 has also been calculated.

1. J. Wolny, Phil. Mag. **77** (1998), p. 395.
2. P. Kuczera, J. Wolny, F. Fleischer, W. Steurer, Philos. Mag. **91** (2011), p. 2500.
3. P. Kuczera, J. Wolny, W. Steurer, Acta Cryst. B **68** (2012), p. 578.
4. W. Steurer, S. Deloudi „Crystallography of Quasicrystals", (Springer) (2009).
5. K. N. Ishihara, A. Yamamoto, Acta Cryst. A **44** (1988), p. 508.
6. B. Kozakowski, J. Wolny, Acta Cryst. A **66** (2010), p. 489.

Diffraction patterns of icosahedral quasicrystal using Average Unit Cell approach

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In our work we calculate diffraction patterns for a quasicrystal with icosahedral symmetry [1] along 2-fold, 3-fold and 5-fold axes and present as sections for $k_{z\|} = 0$, where $k_{z\|}$ axis is always symmetry axis. The Ammann tiling as a model structure with one-atom decoration and the statistical method based on a concept of the Average Unit Cell (AUC) [2] is used.

For calculating the intensities of diffraction peaks we computed a structure factor assuming that an atomic scattering factor is constant for every atom. Calculation is carried out for 77 000 points in a physical space obtained by cut-and project method. The diffraction pattern is computed for peaks with indices of range -5 to 5.

To measure the effectiveness of the AUC-based approach we compare intensities of peaks obtained by a numerical calculation and by a statistical method. The distribution in the AUC for icosahedral quasicrystal is obtained by an oblique projection of the atomic surface onto a physical space [2,3]. To compare the results obtained from both methods we calculate the coefficient. For every diffraction pattern the coefficient of determination is close to 0.99, what allows to conclude that the statistical approach is equivalent to other methods.

1. P. J. Steinhardt, D. Levine, Phys. Rev. B **34** (1986), p. 596-616.
2. J. Wolny, Acta Cryst. A **54** (1998), p. 1014-1018.
3. J. Wolny, B. Kozakowski, P. Kuczera, L. Pytlik, R. Strzalka, A. Wnek, Isr. J. Chem. **51** (2011), p. 1275-1291.

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