



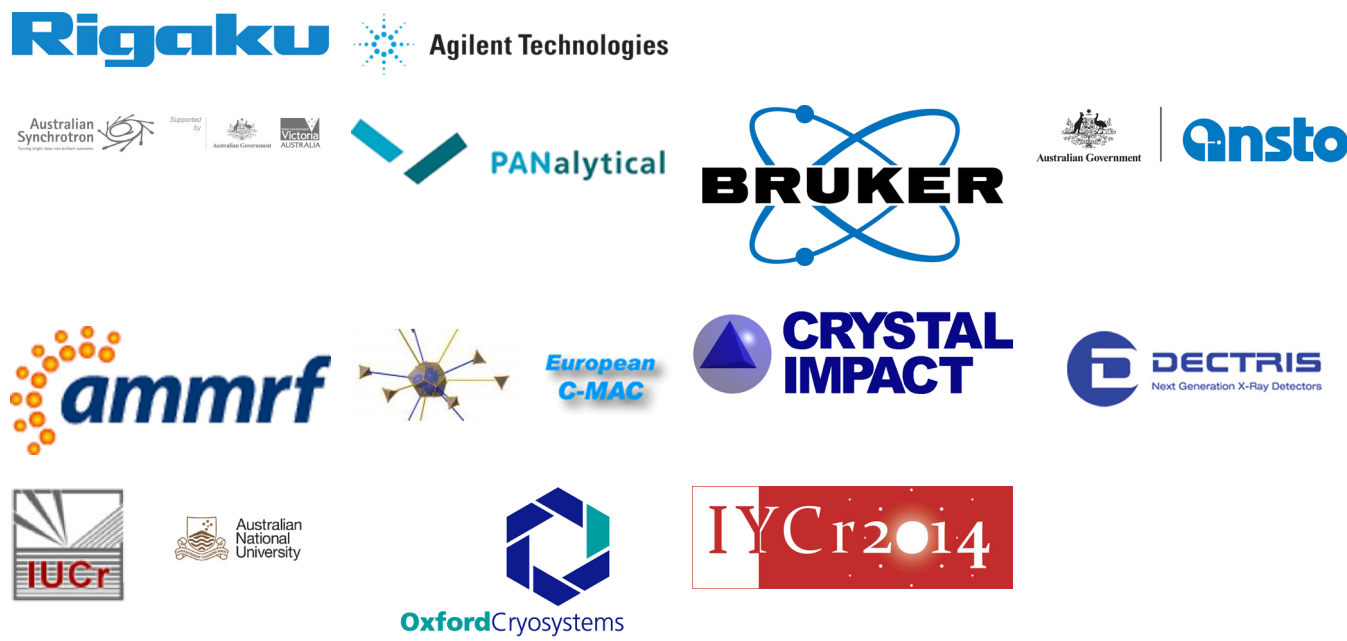
Aperiodic 2012

PROGRAM BOOKLET



Cairns
AUSTRALIA
2 - 7 September 2012

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Aperiodic2012

Conference Program

Sunday 2nd September

14.00 Registration (The Hotel Cairns) until 20.00

Tutorials (Chair - Hans-Rainer Trebin)

14.30	An-Pang Tsai	<i>Stable quasicrystals and their contribution</i>
15.30	Ted Janssen	<i>Fifty years of crystallography of aperiodic crystals</i>
16.30	Patricia Thiel	<i>Surface science of quasicrystals</i>
18.00	Welcome Reception	

Monday 3rd September

Session One - Methods (Chair - Akiji Yamamoto)

8.45	Opening	
9.00	Lukas Palatinus (Invited)	<i>Ab initio structure of incommensurate structures from electron diffraction data</i>
9.40	Andrew Stewart	<i>Extending automated diffraction tomography to aperiodic systems</i>
10.00	Gervais Chapuis	<i>Some extensions of the superspace approach to material science</i>
10.20	Janusz Wolny	<i>Real space structure factor for different aperiodic structures</i>
10.40	Coffee	

Session Two - QCs & Approximants (Chair - Cesar Pay Gómez)

11.10	Pawel Kuczera	<i>The structure of Al-Cu-Me (Me = Co, Rh, Ir) quasicrystals</i>
11.30	Taylan Örs	<i>Structure analysis of decagonal ZnMgDy quasicrystal</i>
11.50	Hiroyuki Takakura	<i>Structure refinement of a ternary icosahedral $Mg_{41}Cd_{41}Yb_{18}$ quasicrystal</i>
12.10	Sven Hovmöller	<i>Structures of pseudo decagonal (PD) approximants in Al-Co-Ni</i>
12.30	Nobuhisa Fujita	<i>F-type icosahedral quasicrystals in Al-based alloys: New insights from a structural analysis of a large cubic approximant</i>

12.50 **Lunch**

Session Three - Modulated Structures I (Chair - Olivier Pérez)

14.20	Phillipe Rabiller	<i>Phase transitions in aperiodic composite crystals</i>
14.40	Nobuo Ishizawa	<i>Pseudo-commensurate $\text{GdBaCO}_2\text{O}_{5+\delta}$ and its phase transition at elevated temperatures</i>
15.00	Laure Bourgeois (Invited)	<i>High-resolution (scanning) transmission electron microscopy of nano-chessboard and other modulated phases</i>
15.40	Coffee	

Session Four - Modulated Structures II (Chair - Gervais Chapuis)

16.10	Luis Elcoro (Invited)	<i>Analysis of uniform superlattice ordering in two dimensions using the superspace</i>
16.50	Chris Ling	<i>Oxide ionic conduction and the three dimensionally incommensurate structure of Type II $\text{Bi}_2\text{O}_3\text{-Nb}_2\text{O}_5$</i>
17.10	Fengxia Wei	<i>3+2 dimensional incommensurate structures of melilites $[\text{Ca}(\text{La},\text{Nd})]_2[\text{Ga}]_2[\text{Ga}_2\text{O}_7]_2$</i>
17.30	Pablo Bereciartua	<i>Superspace description of the system $\text{Bi}_{2(n+2)}\text{Mo}_n\text{O}_{6(n+1)}$</i>

Poster Session

18.00 - 20.00 **Poster Session**

Tuesday 4th September

Session One - Mathematics (Chair - Uwe Grimm)

9.00	Michael Baake (Invited)	<i>Spectral properties of a family of random substitution systems</i>
9.40	Peter Zeiner	<i>Well-rounded lattices</i>
10.00	Michael Whittaker	<i>The fractal dual of the pinwheel tiling</i>
10.20	Johannes Roth	<i>Geometric properties of N-fold quasicrystals</i>
10.40	Coffee	

Session Two - Surfaces & 2D (Chair - Ronan McGrath)

11.10	Hem Sharma (Invited)	<i>Quasicrystalline thin films of single elements and molecules</i>
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11.50	Marian Krajči	<i>Catalytic properties of fivefold surfaces of quasicrystal approximants</i>
12.10	Junji Yuhara	<i>Composition and local atomic arrangement of decagonal Al-Co-Cu quasicrystal surfaces</i>
12.30	Lunch	

Session Three - Self Assembly (Chair - Ron Lifshitz)

14.20	Sharon Glotzer (Invited)	<i>Soft matter quasicrystals: Design rules from computer simulation</i>
15.00	Kobi Barkan	<i>Controlling the self-assembly of soft quasicrystals</i>
15.20	Tomonari Dotera	<i>Quasicrystals formed by hard-core/square-shoulder particles</i>
15.40	Coffee	

Session Four - Magnetism (Chair - Nilay K Mukhopadhyay)

16.10	Ryuji Tamura (Invited)	<i>Structural and magnetic ordering in Cd-based crystalline approximants</i>
16.50	Alan Goldman	<i>Antiferromagnetic order in the quasicrystal approximant, Cd_6Tb</i>
17.10	Andrew Goodwin	<i>Paramagnetic structure from magnetic diffuse scattering</i>

Poster Session

18.00 - 20.00 **Poster Session**

Wednesday 5th September

Session One - Nobel Lecture (Chair - An-Pang Tsai)

9.00	Dan Shechtman (Invited)	<i>The discovery of quasi-periodic crystals</i>
10.00	Coffee	

Session Two - Modulated Structures III (Chair - Siegbert Schmid)

10.30	John Claridge	<i>Modulations, modes, materials and crystal chemistry</i>
10.50	Tilo Söhnel	<i>Modulated structures in mixed transition metal - Main group metal clusters</i>
11.10	Thanh-Ha Nguyen	<i>The first SC-XRD system using a CMOS APS detector</i>
11.30	Lunch	

Excursion

12.40 Excursion Green Island (The Reef Fleet Terminal)

Conference Dinner

19.30 Conference Dinner

Thursday 6th September

Session One - Metallurgy & Alloys (Chair - Marian Krajčí)

- 9.00 Nilay K Mukhopadhyay *Studies on inverse Hall-Petch behavior in nanostructured $Al_{62.5}Cu_{25}Fe_{12.5}$ quasicrystals*
- 9.20 Pavol Priputen *Evolution of phases in selected Al-Co-Cu complex metallic alloys under near-equilibrium conditions at 800-1150°C*
- 9.40 Julia Dshemuchadse *Structural characteristics of complex intermetallics*
- 10.00 Uichiro Mizutani *Hume-Rothery stabilization mechanism in low-temperature phase Zn_6Sc Approximant and e/a determination of Sc, Y and La in Sc-X, Y-X and La-X (X=Zn, Cd and Al) alloy systems*
- 10.20 Coffee

Session Two - Tilings (Chair - Franz Gähler)

- 10.50 Antoine Julien
(Invited) *Complexity of cut and project tilings*
- 11.30 Uwe Grimm *Squirals and their diffraction*
- 11.50 Thomas Fernique *Tilings: When periodicity enforces aperiodicity*
- 12.10 Rima Al Ajlouni *Octagon-based quasi-crystalline formations in Islamic architecture*
- 12.30 Conference Photo
- 12.50 Lunch

Session Three - Dynamics (Chair - Marc de Boissieu)

- 14.20 Yasushi Ishii *Dynamic structure factors for two-dimensional quasicrystals*
- 14.40 Holger Euchner *Tetrahedron dynamics in the i-MgScZn quasicrystal and its 1/1 cubic approximant $ScZn_6$*
- 15.00 Hans-Rainer Trebin *Confirmation of the random tiling hypothesis for a decagonal quasicrystal*

15.20 **Michael Schmiedeberg** *Phason dynamics in light-induced colloidal quasicrystals*

15.40 **Coffee**

Session Four - Physical Properties (Chair - Janusz Wolny)

16.10 **Vicenta Sánchez** *Extended and localised states in generalized Fibonacci lattices:
A real-space renormalization study*

16.30 **Stefanie Thiem** *Quantum diffusion in separable d-dimensional quasiperiodic
tilings with golden and silver mean*

16.50 **Chumin Wang** *Light transmission in aperiodic multilayers of porous silicon*

17.10 **Koichi Kitahara** *Thermoelectric properties of icosahedral quasicrystals and
cubic approximant crystals in Al-Cu-Ru system*

17.30 **Tsunehiro Takeuchi** *Development of thermal-rectifier using Al-based quasicrystals*

19.00 **CAC Meeting**

Friday 7th September

Session One - Diffuse Scattering (Chair - Hiroyuki Takakura)

9.00 **Tsunetomo Yamada** *Diffuse scattering and phason modes in the Zn-Sc
icosahedral quasicrystal*

9.20 **Richard Welberry** *Diffuse scattering resulting from macromolecular frustration*

9.40 **Akiji Yamamoto** *Diffuse scattering of decagonal Al-Cu-Co and Ni-rich
Al-Ni-Co quasicrystals II simulations*

10.00 **Hannes Krüger** *Diffuse scattering in $\text{KAlSiO}_4\text{-O1}$*

10.20 **Arkadiy Simonov** *Interpretation of diffuse scattering from single crystals with
direct 3D PDF fitting*

10.40 **Coffee**

Session Two - Chem & Bio Crystals (Chair - Gloria Borgstahl)

11.10 **Jeffrey Lovelace** *Incommensurately modulated protein crystals*
(Invited)

11.50 **Kirsten Christensen** *New challenges in chemical crystallography*

12.15 **Summary**

12.45 **Closing Comments** Ray Withers

13.00 **Close**

Tutorials

Stable quasicrystals and their contribution

An-Pang TSAI

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Sendai 980-8577, Japan*

Discovering new materials is an important and a never-ending issue in any field of materials science. This is especially crucial for the community of quasicrystals, since a new sample can allow ones to solve atomic structure, to understand physical properties and to develop application. We have been devoting to finding stable quasicrystals since 1987 and had some success in discovering stable quasicrystals and in the mean time a plausible stabilization mechanism of quasicrystal emerged from these discoveries. In this overview, I will review briefly the path of discovering stable quasicrystals and describe their contribution on structure and application at each stage.

Fifty years of crystallography of aperiodic crystals

Ted Janssen

Theoretical Physics, University of Nijmegen, Nijmegen, The Netherlands.

The development of the crystallographic description of aperiodic crystals will be discussed from a historic point of view. The field started in the early sixties of last century with magnetic structures and became broader and broader with the discovery of modulated crystals [1], incommensurate composites, quasicrystals [2] and incommensurate magnetic structures. The common crystallographic formulation for all these systems is that in superspace. Introducing this higher-dimensional space, the problem is transformed to a lattice period structure determination in that higherdimensional space. The various features for the different classes of aperiodic crystals and the difference between them will be discussed. Finally, one may ask the question 'What else is there to be done?'

Janssen

Tutorial: Surface Science of Quasicrystals

Patricia A. Thiel

*The Ames Laboratory, and the Departments of Chemistry, and of Materials
Science & Engineering, at Iowa State University, Ames, Iowa USA*

This talk deals with the ways in which our understanding of solid surfaces has been both enriched and challenged by quasicrystals. Surface properties of the metallic quasicrystals originally generated interest because they were unusual. For instance, among Al-rich alloys, the Al-based quasicrystalline phases exhibit puzzling resistance to surface oxidation. Also, Al-rich quasicrystals have surprisingly good and promising catalytic properties (e.g. for steam reforming of methanol). Perhaps most famously, they exhibit low friction. Comparisons with crystalline materials have established that these features are deeply related to the quasiperiodic atomic structure.

Surface science has elucidated some of these unusual features, and has discovered others. The first topic that will be addressed is their low friction, when measured with techniques that probe macroscopic scales (conventional pin-on-disk tribometers) to nanoscopic scales (atomic force microscopy). The second is oxidation, and the third is metal nanocluster structure. The third has been an area of rich discovery. Metal nanocluster structure at quasicrystal surfaces—and at surfaces of related complex metallic phases—can be influenced by quantum size effects, by preferential nucleation at trap sites, and by the terrace inhomogeneity that is present for many surfaces of these materials.

Oral Presentations

***Ab initio* structure solution of incommensurate structures from electron diffraction data**

L. Palatinus^a, M. Klementová^a and P. Boullay^b

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^b *CRISMAT, CNRS UMR 6508, 14050 Caen, France.*

Ab initio solution of crystal structures from electron diffraction data has a long history, but despite the large body of work done on the topic it had remained a challenge until recently. A breakthrough in the field has been achieved by combining two techniques: precession electron diffraction (PED) [1,2] and electron diffraction tomography [3]. With this approach it has become possible to solve crystal structures on regular basis.

The method can be, in principle, applied also to the *ab initio* structure solution of incommensurately modulated structures. However, these structures pose additional challenges. The satellite reflections are, in general, weaker than the main reflections and it is thus more difficult to extract structural information from their weak signal. Moreover, the modulation functions are continuous, and it is intrinsically more difficult to extract the shape of a continuous function from a noisy electron diffraction data than to determine just the positions of atoms.

Despite of these challenges we have demonstrated that a successful solution of incommensurately modulated structures from PED data is possible. Using a combination of in-house software for integration of electron diffraction data from modulated structures and the program Superflip [4] for structure solution in superspace we succeeded to solve two challenging modulated structures – copper silicide-germanide exhibiting very complicated two-dimensional modulation [5], and Bi₅Nb₃O₁₅ – an Aurivillius-related phase with a surprising stacking of structural motifs.

- [1] R. Vincent, P.A. Midgley, *Ultramicroscopy* **53** 271 (1994).
- [2] C. S. Own, L. D. Marks, W. Sinkler, *Acta Cryst. A* **62** 434 (2006).
- [3] U. Kolb, T. Gorelik, C. Kübel, M.T. Otten, and D. Hubert, *Ultramicroscopy* **107** 507 (2007).
- [4] L. Palatinus, G. Chapuis, *J. Appl. Cryst.* **40** 786 (2007).
- [5] L. Palatinus, M. Klementová, V. Dřínek, M. Jarošová and V. Petříček, *Inorg. Chem.* **50** 3743 (2011).

Extending automated diffraction tomography to aperiodic systems

A. A. Stewart^a E. Mugnaioli^a, T. E. Gorelik^a, and U. Kolb^a

^a Institute for Physical Chemistry, *Johannes Gutenberg University, Mainz, 55128, Germany.*

The technique of Automated Diffraction Tomography (ADT) [1] is an innovative approach to electron crystallography, this method has the advantage of obtaining a more complete coverage of reciprocal space therefor making it easier to identify disorder, space groups, as well as a obtain a far greater completeness of the data set than can be obtained by zone diffraction patterns alone. When ADT is coupled with precession the volume of reciprocal space can be fully integrated, making it easier to solve crystal structures using direct methods and further increases the coverage of reciprocal space. The greater coverage his has led to the easier identification of light and heavy atoms during structure solution using direct methods, whereas zonal patterns often only find the heavy atom positions within a structure.

So far ADT has primarily been applied extensively to periodic systems with only one example of the methodology being applied to an aperiodic system [2]. Given the advantages in quantity and quality of the data acquired by the ADT method, there are some compelling reasons to use it for structure identification and classification as well as enhancing the chance of structure solutions *via* direct methods for aperiodic systems.

We will present an extension of the data processing routines for automated diffraction tomography which will allow for the possibility of identifying modulated structures within a 3 dimensional diffraction volume, including, determining the main and/or satellite vectors, and the associated indexing and intensity extraction of the data.

[1] E. Mugnaioli, T. Gorelik, and U. Kolb, *Ultramicroscopy* **109**, 758-765 (2009).

[2] L. Palatinus, *et al.*, *InOrg. Chem.*, **50**, 3743-3751 (2011)

Some extensions of the superspace approach to material science

Alla Arakcheeva^a and G. Chapuis,^{a,b}

^a*Phase Solutions Ltd, Lausanne, Switzerland.*

^b*Ecole polytechnique Fédérale de Lausanne, BSP, 1015 Lausanne, Switzerland.*

Since the introduction of the superspace approach to describe the symmetry of incommensurately modulated structures, the concept has greatly evolved and many new and useful applications have been proposed in the literature. We would like to present a few examples of applications, which are of interest in material science.

- 1) Structure-property correlation. Based on the $\text{Na}_x\text{Eu}_{2/3-x/3}\text{MoO}_4$ ($0.134 < x < 0.25$) series consisting of 6 incommensurately modulated compounds, it has been found that the characteristic luminescence parameters correlate with the number of Eu^{3+} dimers (distant by 3.95 Å), but not directly with the composition x of the materials as considered before [1].
- 2) The solid-solution concept. $\text{Na}_x\text{Eu}_{2/3-x/3}\text{MoO}_4$ compounds are conventionally considered as a solid-solution of Eu in NaMoO_4 . In the interval $0.134 < x < 0.25$, each composition is characterized by a specific structure and all of them can be derived from a single superspace model. Hence, they can be considered as a family of related compounds. This example points to a possible reconsideration of the solid-solution concept.
- 3) The extension of the structure-type concept. Any incommensurately modulated structure is excluded from the classical definition. However, both 3D and $(3+d)\text{D}$ ($n = 1, 2, 3$) structures, which are characterized by a unique superspace group, by a specific number of atoms in a specific basic unit cell occupying a specific Wyckoff sites, can be considered as a higher dimension structure type [2].
- 4) The commensurate composite concept [3]. One- or two-dimensional composites can much better explain the electronic properties of possibly all of the onerespectively, two-dimensional electronic systems. It is illustrated with the example of the well-known quasi-one dimensional metallic system BaVS_3 .

[1] A. Arakcheeva, D. Logvinovich *et al.* *Chemical Science* **3**, 384 (2012).

[2] A. Arakcheeva and G. Chapuis. *Acta Cryst.* **B64**, 12 (2008).

[3] A. Arakcheeva, G. Chapuis *et al.* *Acta Cryst.* **B59**, 324 (2003).

Real Space Structure Factor for Different Aperiodic Structures

J. Wolny, P.Kuczera, R. Strzalka and A. Wnek

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Computer Science, Krakow, Poland.

The statistical approach to the description of aperiodic structures using the concept of the so called Average Unit Cell (AUC) is presented [1]. The use of this method is shown for different 1D [2,3], 2D [4] and 3D [1] structures. We start with the presentation of the basic ideas for 1D simple sinusoidal modulation (1q) [2] and the Fibonacci chain [3] (a 1D model of a quasicrystalline structure). Up to now the AUC concept has been most thoroughly studied for 2D decagonal quasicrystals [4,5]. The idea of structure factor derivation for the decorated Penrose tiling, a quasilattice for the description of decagonal quasicrystals, is presented. Some examples of structure refinement of decagonal phases are discussed [5]. The potential of the cluster description of decagonal structures is also presented [6,7]. The AUC construction and structure factor derivation is shown for the 3D Amman-Kramer-Neri tiling, which is a model quasilattice for the description of icosahedral phases. The AUC concept can also be extended to the structures with singular-continuous Fourier spectrum. An example for the 1D Thue-Morse is studied [8]. It is also shown [9] that for the 2D random tiling there is a continuous phase transition at critical concentration. Critical behaviours for scaling of diffraction intensities is also discussed [9].

- [1] J. Wolny *et al.*, *Israel J. Chemistry* 51, 1275-1291 (2011).
- [2] G. Urban, J. Wolny, *Ferroelectrics* 250, 131-134 (2001).
- [3] P. Buczek, L. Sadun, J. Wolny, *Acta Physica Polonica* B36, 919-933 (2005).
- [4] B. Kozakowski, J. Wolny, *Acta Crystallogr.* A66, 489-498 (2010).
- [5] P. Kuczera, J. Wolny, F. Fleischer, W. Steurer, *Philos. Mag.* 91, 2500 (2011).
- [6] P. Gummelt, *Geometriae Dedicata* 62, 1-17 (1996).
- [7] A. Dabrowska, B. Kozakowski, J. Wolny, *Acta Crystallogr.* A61, 350-357 (2005).
- [8] J. Wolny, A. Wnek, J. L. Verger-Gaugry, *J. Comput. Phys.* 163, 313-327 (2000).
- [9] J. Wolny, L. Pytlik, B. Lebech, *J. Phys.- Condens. Mat.* 2, 785-795. (1990).

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

P. Kuczera^{a,b}, J. Wolny^a and W. Steurer^b

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^b Laboratory of Crystallography, ETH Zurich, Switzerland.

The structure refinement of three decagonal phases: Al-Cu-Co, Al-Cu-Rh, Al-Cu-Ir will be presented. The synchrotron diffraction experiments were performed at the Swiss – Norwegian beam line at ESRF, Grenoble, France. All three decagonal phases show ~4 Å periodicity (two atomic layers per period). A computer program SUPERFLIP [1] based on the charge-flipping algorithm was used for the initial phasing of the data and obtaining the electron density maps. These maps were used for deriving a Rhombic Penrose Tiling (RPT) model with a tiling edge-length of ~17 Å. The decoration of the unit tiles is based on the ~32 Å cluster proposed by Hiraga & Oshuna [2]. The decoration of RPT with Hiraga clusters is such, that the cluster centers form the Pentagonal Penrose Tiling of an edge-length of ~20 Å. The Hiraga cluster can be considered as a *supercluster* built of 5 clusters proposed by Deloudi et al. [3]. Such a structure explains well the strong Patterson peaks of ~20 and ~32 Å occurring for all three phases. The structure refinement was performed in the real space using the so-called Average Unit Cell approach. This method allows a purely 3D optimization of a quasicrystalline structure and has been previously used for a variety of decagonal phases in the Al-Ni-Co system [4-6]. Our work shows the first solution of a quasicrystal as a ternary alloy (Rh and Ir phases). The final *R*-values are reasonable, the structure is consistent with TEM images and the chemical composition agrees well with the EDX measurements.

[1] L. Palatinus, G. Chapuis, *J. Appl. Crystallogr.* **40**, 786 (2007).

[2] K. Hiraga, T. Ohsuna, K.T. Park, *Phil. Mag. Lett.* **81**, 117 (2001).

[3] S. Deloudi, F. Fleischer, W. Steurer, *Acta. Crystallogr. B* **67**, 1 (2011).

[4] P. Kuczera, J. Wolny, F. Fleischer, W. Steurer, *Philos. Mag.* **91**, 2500 (2011).

[5] P. Kuczera, B. Kozakowski, J. Wolny, W. Steurer, *J. Phys. Conf. Ser.* **226** (2010).

[6] J. Wolny, B. Kozakowski, P. Kuczera, H. Takakura, *Z. Kristallogr.* **223**, 847 (2008).

Structure Analysis of Decagonal ZnMgDy Quasicrystal

T. Örs and W. Steurer

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In this study, the first structure analysis of the ZnMgRE (Rare Earth) family of decagonal quasicrystals (d-ZnMgDy) based on single crystal X-ray diffraction data is performed. Crystals were grown in samples having the nominal composition $\text{Zn}_{57.6}\text{Mg}_{40.8}\text{Dy}_{1.6}$. These samples were prepared by induction melting followed by annealing at 375°C for 10 months and quenching to room temperature. X-ray diffraction experiments were carried out both in-house (Oxford Xcalibur PX diffractometer, CCD detector, Mo K α radiation) and at the Synchrotron facility in Swiss-Norwegian Beam Line, ESRF, Grenoble ($\lambda=0.6980$ Å).

The Laue group is determined as $10/mmm$ and no systematic extinctions were observed. The direct space quasilattice parameters are $a_{1-4} = 4.626(8)$ Å and $a_5 = 5.214(5)$ Å. SUPERFLIP program package [1] (based on charge flipping and low density elimination algorithms) was used for structure solution. Reconstructed electron density shows structural motifs similar to previous HRTEM studies [2].

Initial modeling based on Penrose tiling shows that the structure differs significantly from the well-studied Al-TM (transition metal) type of decagonal phases. One important difference is that the structure exhibits additional occupation domains (OD), which create edge centering positions for a regular rhomb or pentagonal tiling. The modeling of this new type of OD by using the higher dimensional approach will be discussed. The results obtained with a cluster covering model will also be presented.

[1] L. Palatinus and G. Chapuis, *J. App. Cryst.* **40**, 786 (2007).

[2] E. Abe, T. J. Sato and A. P. Tsai, *Phil. Mag. Lett.* **77**, 205 (1998).

Structure Refinement of a Ternary Icosahedral $\text{Mg}_{41}\text{Cd}_{41}\text{Yb}_{18}$ Quasicrystal

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^b *IMRAM, Tohoku Univ., Sendai 980-8577, Japan.*

The detailed atomic structures of ternary quasicrystals (QCs) that are considered as derivative structures from a parent binary QC are important, because not only for their structures themselves, but also for their role to give a clue to an understanding of the stability of QCs. We report here the results of the structure analysis of the ternary icosahedral $\text{Mg}_{41}\text{Cd}_{41}\text{Yb}_{18}$ QC [1] using single crystal x-ray diffraction data. It was confirmed that this ternary QC is isostructural to the binary icosahedral Cd-Yb QC [2] from the analysis of the phase-retrieved electron densities by the low-density elimination method. In the structure refinement, in order to properly handle the possible chemical order of the constituent elements at the rhombic triacontahedral (RTH) cluster level, a revised 6D model of the binary icosahedral Cd-Yb QC [3], in terms of subdivision of the occupation domains (ODs), has been applied to the present ternary QC. The 6D model is composed of three non-equivalent occupation domains (ODs) disposed at (0,0,0,0,0,0), (1,1,1,1,1,1)/2 and (1,0,0,0,0,0)/2 as it was before. The structure refinement indicated that Mg preferentially occupies the OD at (0,0,0,0,0,0). This means that Mg atoms replace Cd atoms at the threefold and fivefold vertices of the outer most shell of a RTH cluster and at the vertices of the dodecahedron shell inside the cluster. These preferential sites for Mg are intimately linked to each other by the connection scheme of the RTH clusters in the QC.

- [1] J. Q. Guo, E. Abe, A. P. Tsai, *Phil. Mag.* **82**, 27-35 (2002).
- [2] A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura, T. J. Sato, *Nature* **408**, 537 (2000).
- [3] H. Takakura, C. P. Gómez, A. Yamamoto, M. de Boissieu, A. P. Tsai, *Nature Mater.* **6**, 58-63 (2007).

Structures of pseudo decagonal (PD) approximants in Al-Co-Ni

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^c*PGI-5, Forschungszentrum Jülich, Germany*

One of the richer systems for quasicrystals and their approximants is the Al-Co-Ni system. A large series of pseudo-decagonal (PD) approximants have been found. Only two of them, PD4 and PD8, have been solved by X-crystallography. We report here the structures of PD1, PD2, PD3 and PD5, solved from the limited information that is provided by electron diffraction patterns, unit cell dimensions and high resolution electron microscopy images.

In electron microscopy (EM) images of all these approximants, a characteristic wheel with 2 nm diameter is seen. The atomic details of this wheel became clear when PD4 was solved by single crystal X-ray diffraction (Oleynikov et al. 2006).

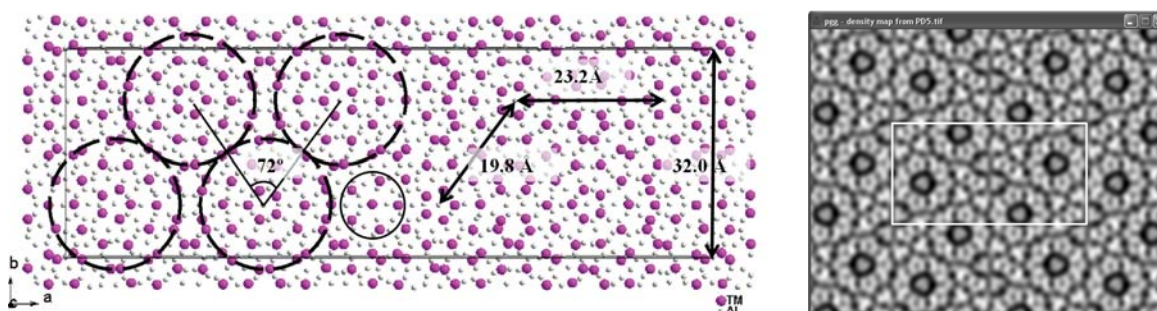


Figure 1. (left) Structure of PD4 from X-ray crystallography [1]. The vertical unit cell dimension $b = 32.0\text{\AA}$ is shared by several PD compounds. The other two important distances are centre-to-centre between two adjacent wheels; 19.8 Å if they intersect and 23.2 Å if they are separated by 3.4 Å. All these distances and angles are found frequently throughout the PD series. The small circle marks a pentagon. After [3].

(right) Structure of PD5, derived from EM images and crystallographic image processing [2]. Six wheels are packed as a squeezed hexagon inside the unit cell [3].

[1] Oleynikov, P., et al. PD4 structure, *Philosophical Magazine* **86** (2006) 457-462.

[2] Hovmöller, S. CRISP program, *Ultramicroscopy* (1992) **41**, 121-135.

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F-type Icosahedral Quasicrystals in Al-based Alloys: New Insights from a Structural Analysis of a Large Cubic Approximant

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The structure analysis of an approximant crystal could provide crucial information on the kinds of clusters as well as their packing nature in a relevant quasicrystal (QC). Synthesis of a stable approximant to a QC is thus of fundamental importance. However, for F-type icosahedral QC's in Al-based alloys, e.g., i-Al-Pd-Mn and i-Al-Cu-Fe, a suitable approximant has been hardly reported, possibly due to the extraordinary stability of the QC itself. This unsatisfactory situation motivates us to search for new stable approximants to i-Al-Pd-Mn by substituting a blend of Cr and Fe for Mn, thus allowing a fine adjustment of the electron concentration. The attempt succeeds in synthesizing a new stable approximant at a certain mixing ratio between Cr and Fe, where fine single crystals with facets are obtained via slow cooling from the melt. The specimen is then subjected to single-crystal X-ray diffraction and *ab initio* structure refinement, leading to a complete structural solution with the space group of *Pa-3* and the lattice constant of 40.5 Å. All the atoms are described by two kinds of clusters [1], denoted by M and B, without a need for glue atoms. The cluster centers of 128 M's and 136 B's are located at the vertices of a canonical cell tiling, which corresponds to the 2x2x2 superstructure of the 3/2-packing [2]. This is the first decoration model of a real approximant to Al-based F-type icosahedral QCs using a canonical cell tiling. A straightforward generalization of the model leads to a number of hypothetical approximant structures, some of which may also realize. The present results altogether would provide new insights into the atomic structure of F-type icosahedral QCs and their approximants.

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Phase transitions in aperiodic composite crystals

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These last decades, the concept of order has broadened to analyze materials which have long-range order with symmetries that are incompatible with periodicity. These aperiodic compounds are described in the frame of a higher-dimensional analogue of the physical space called crystallographic superspace [1]. Phase transitions occur through modifications of the superspace parameters and/or symmetry, which may involve the physical or the internal one.

Aperiodicity in composite materials may appear rather naturally due to the possible misfit of the host and the guest parameters along their crystallographic directions. This may happen with ions in channels, the famous example being the mercury chains in the AsF_6 host frame [2]. More surprising examples are given by simple metals, where the same atom plays the role of the host and of the guest, defining the so-called self-hosting [3]. These compounds may reveal one dimensional liquid state for the guest molecules. Another kind of family concerns supramolecular crystals with long guest molecules which cannot fit their parameter to the one of the host sub-system. A prototype series is given by the alkane chains confined in honeycomb-like urea sublattices.

In this talk, we will present symmetry breakings which concern these aperiodic composites. There, new degrees of freedom concern the structural organization, leading to completely unexpected phases [4-6].

[1] T. Janssen, G. Chapuis, M. de Boissieu, *Aperiodic Crystals: From Modulated Phases to Quasicrystals*, (Oxford Univ. Press, Oxford, 2007).

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Pseudo-Commensurate $\text{GdBaCo}_2\text{O}_{5+\delta}$ and Its Phase Transition at Elevated Temperatures

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Structural changes in the giant magnetoresistance compound $\text{GdBaCo}_2\text{O}_{5+\delta}$ with $\delta \sim 0.35$ were studied by the single-crystal X-ray diffraction in the temperature range between 300 and 500 K. The basic structure of the compound is a double-layered perovskite type, having an alternating layer sequence of $[\text{GdO}_\delta]$ - $[\text{CoO}_2]$ - $[\text{BaO}]$ - $[\text{CoO}_2]$ along the c axis. The crystal belongs to $P4/mmm(\alpha 00)0000(0\alpha 0)0000$ with $\alpha = 0.3368(1)$ according to the notation for five-dimensional superspace groups [1]. The room temperature structure was refined using Jana2006 [2] to $R = 2.16\%$ for all observed 2216 reflections consisting of 331 main reflections ($R = 1.72\%$), 1039 first-order satellites ($R = 1.99\%$) and 846 second-order ones ($R = 3.60\%$). The crystal has the oxygen deficiency which occurs only in the $[\text{GdO}_\delta]$ layer, though it causes many positional modulations of constituting atoms in association with a valence fluctuation of Co between +2 and +3. Since α was very close to $1/3$, the structure was also solved and refined by the conventional three-dimensional approach assuming a $3 \times 3 \times 2$ cell of $P4/mmm$ symmetry, and the results obtained by the two approaches were compared. The crystal undergoes a first-order phase transition into a commensurate $1 \times 2 \times 2$ structure of orthorhombic $Pmmm$ at around 400 K. The high temperature form has another geometrical arrangement about the deficient O atoms in the $[\text{GdO}_\delta]$ layer. Complementary electron diffraction studies [3] using the conventional and Lorentz electron microscopes revealed mutually different behaviors about the phase transition. Our present X-ray results obtained at zero magnetic field agreed with those obtained by the Lorentz electron microscope.

- [1] H. T. Stokes, B. J. Campbell and S. van Smaalen, *Acta Cryst.* **A67**, 45-55 (2011).
- [2] V. Petricek, M. Dusek and L. Palatinus, Jana2006, Czech Republic (2006).
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High-Resolution (Scanning) Transmission Electron Microscopy of Nano-Chessboard and Other Modulated Phases

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Perovskites often display complex and highly ordered nanoscale modulations arising from a subtle interplay between structural and chemical factors. Striking examples of such ordering are the so-called "nano-chessboard" phases, which include the $\text{Li}_{0.3}\text{Nd}_{0.567}\text{TiO}_3$ (LNT) defect perovskite [1]. The exact nature of the modulation at the atomic scale is still in debate. Similarly, the structure and its relationship with properties of many novel perovskite-related materials developed as potential high-performance and lead-free ferroelectric materials remain unclear. Aberration-corrected transmission electron microscopy (TEM) and scanning (S)-TEM studies of several such phases will be presented. In particular, our attempts to separate local strain and chemical aspects of the LNT structure will be described. An extension of a recent investigation [2] in the incommensurately modulated $\text{Bi}_{1-x}\text{Ca}_x\text{Fe}_{\text{III}}\text{O}_{3-x/2}$ (BCF) will also be presented.

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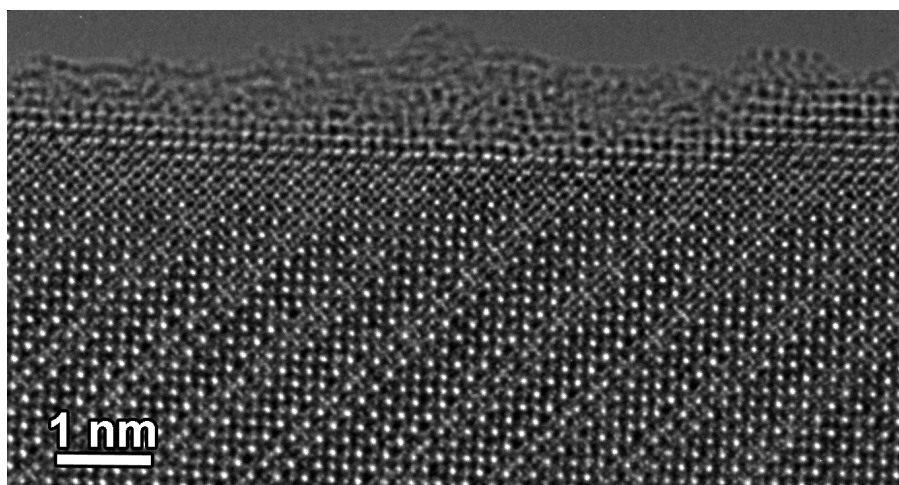


Fig. 1: Modulated BCF structure viewed along [100] by transmission electron microscopy.

Analysis of Uniform Superlattice Ordering in Two Dimensions using the Superspace

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Uniform configurations of minority motifs (or defects) in two dimensions are investigated using the square lattice as a working example. An effective repulsive interaction between the minority motifs is considered to find, for each composition, the distribution of defects that minimizes the energy. While in 1D systems, any reasonable repulsive interaction gives the same distribution of defects, which can thus be undoubtedly considered as the most uniform distribution of defects, in 2D the distribution with the lowest energy depends on the interaction. We have to talk then in this case of pseudouniform orderings. In general, the ordered superlattices are built by the concatenation or intergrowth of basic tiles constituted by simple monatomic supercells. Three different kinds of superlattice orderings have been identified: stripe-like, checkerboard and snub-square orderings, all having a very simple superspace description with simple relations between composition and modulation wave vector(s). Stripe-like and checkerboard arrangements are easily described in a (2+1)D space using crenel functions to represent the atoms and the defects. Snub-square orderings require a (2+2)D superspace model with step-like 2 dimensional atomic domains. In all the cases the closeness condition is fulfilled. These ideas can be used to describe the structure of systems exhibiting compositional patterning at the nanoscale (i.e., nano-chessboard and nano-diamond patterns), as an alternative to the so far assumed *ordered* phase segregation.

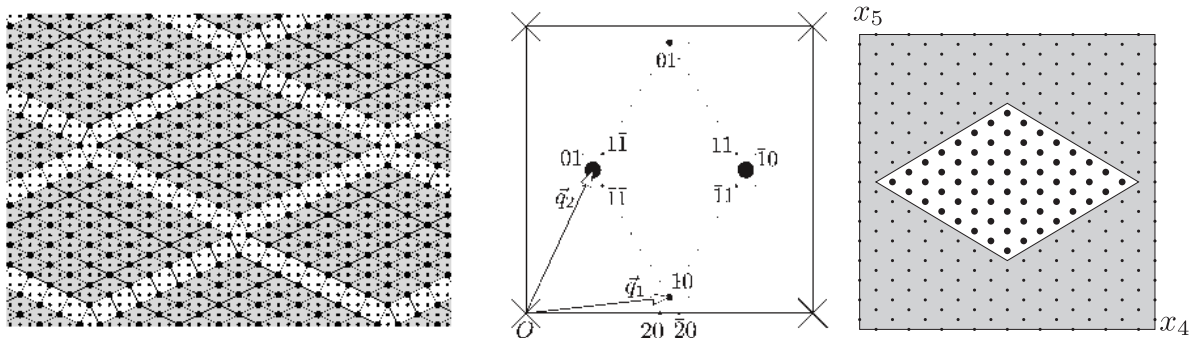


Fig.: (a) Snub-square structure with $x=32/135$ proportion of vacancies (big dots), (b) Diffraction pattern of (a) and (c) Step-like 2D atomic domain in superspace.

Oxide ionic conduction and the three dimensionally incommensurate structure of Type II $\text{Bi}_2\text{O}_3\text{--Nb}_2\text{O}_5$

C.D. Ling^a, S. Schmid^a and V. Petricek^b

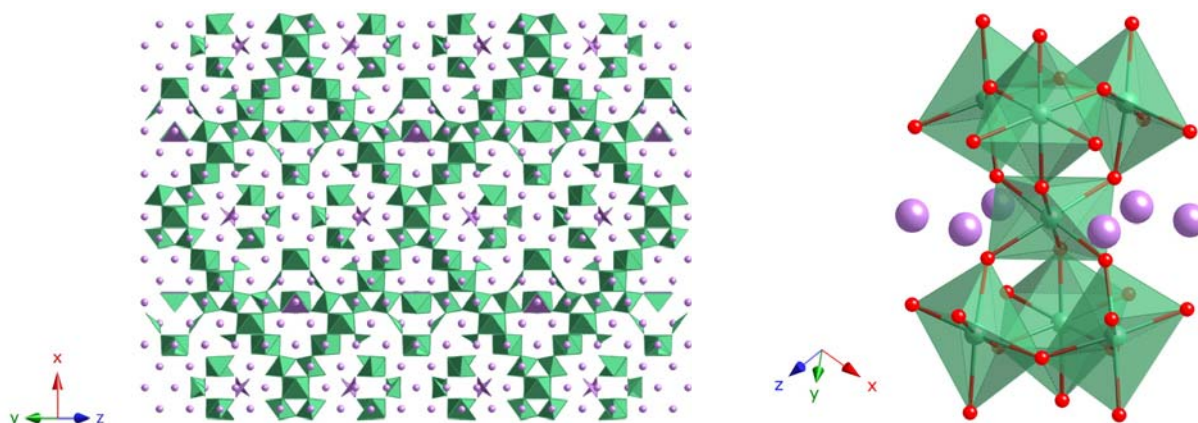
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We have grown a large (cm-scale) crystal of the Type II phase in the $\text{Bi}_2\text{O}_3\text{--Nb}_2\text{O}_5$ pseudo-binary system by a novel refluxing floating-zone method. We collected high-quality single-crystal neutron diffraction data, against which we freely refined its three-dimensionally incommensurate modulated structure. [1] The structure can be described in terms of a hypothetical pyrochlore-type phase $\text{Bi}_2\text{Nb}_2\text{O}_7$, in which the chains of corner-connected NbO_6 octahedra along the four $\langle 110 \rangle$ directions are smoothly pulled apart in an infinitely adaptive manner, leaving wide continuous fluorite-type bismuth-rich channels in between. Refined anharmonic atomic displacement parameters show that these channels are essentially identical to cubic $\delta\text{-Bi}_2\text{O}_3$, the best oxide ionic conductor known; [2] and impedance measurements confirm that the Type II phase is indeed a better oxide ionic conductor than the Type III phase, which forms in the same compositional range but lacks these wide continuous channels. This is only the third “six dimensional” structure to be refined, the first using neutrons, and the first in which the 6D structure plays an integral role in an important physical property: intermediate temperature oxide ionic conduction.

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3+2 Dimensional Incommensurate Structures of Melilites:



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Melilite-type $[\text{Ca}(\text{La},\text{Nd})]_2[\text{Ga}]_2[\text{Ga}_2\text{O}_7]_2$ gallates are promising ion conducting electrolytes for deployment in solid oxide fuel cells. Strong anisotropic displacements of oxygen arise from the structural misfit between the interlayer $\text{Ca}/(\text{La},\text{Nd})$ cations and the $[\text{Ga}]-[\text{Ga}_2\text{O}_7]$ tetrahedral layers. A model employing 2D modulation achieves bond lengths and bond angles that preserve satisfactory bond valence sums [1,2]. The melilites belong to the tetragonal superspace group $P\bar{4}2_1m(\alpha,\alpha,0)00s(\bar{\alpha},\alpha,0)000$, where α depends on compositions, onto which modulation vectors are superimposed: $\mathbf{q}_1 = \alpha(\mathbf{a}^* + \mathbf{b}^*)$, $\mathbf{q}_2 = \alpha(-\mathbf{a}^* + \mathbf{b}^*)$. Both displacive and occupational modulations made contribution. Through this mechanism, melilites are primed to accommodate mobile oxygen interstitials, suggesting a rational approach to crystallochemical tailoring that will enhance ionic diffusion and optimize electrolyte performance.

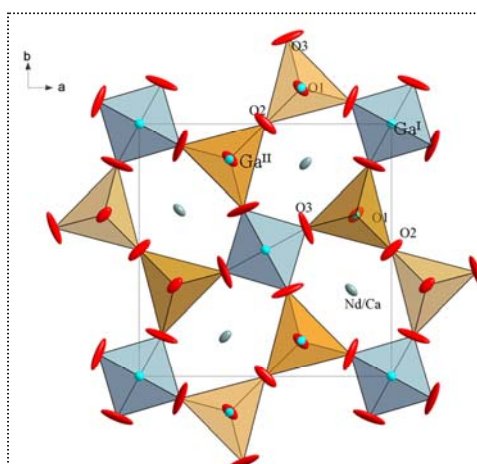


Figure 1. Melilite average structure

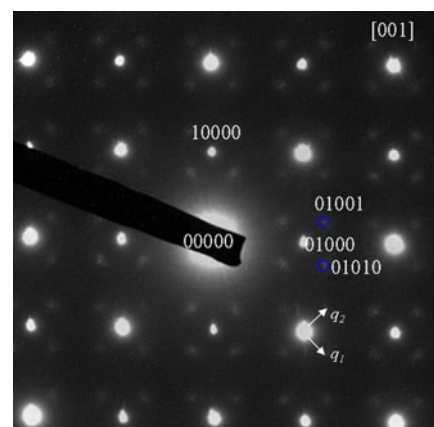


Figure 2. <001> zone diffraction pattern

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Superspace description of the system $\text{Bi}_{2(n+2)}\text{Mo}_n\text{O}_{6(n+1)}$

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The family of compounds with generic formula $\text{Bi}_{2(n+2)}\text{Mo}_n\text{O}_{6(n+1)}$ ($n=3, 4, 5, 6$) [1] has been described within the superspace formalism using the Aurivillius structure of the compound Bi_2MoO_6 as reference. The superspace description of this system requires two models, depending on the parity of the parameter n . In both cases the average unit cell is given by the vectors $\{\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F\}$ associated with the unit cell of the fluorite-like structure of the compound $\delta\text{-Bi}_2\text{O}_3$. Odd members ($n=3$ and 5) present a superspace group $F2(\alpha 0 \gamma)$ with a modulation vector $\mathbf{q}_o = \frac{1}{3n+4}(-2\mathbf{a}_F^* + 2(n+1)\mathbf{c}_F^*)$.

However, a different modulation vector $\mathbf{q}_e = \frac{1}{3n+4}(\mathbf{a}_F^* + (2n+3)\mathbf{c}_F^*)$ is necessary for the even members ($n=4$ and 6), implying the superspace group $F2/m(\alpha 0 \gamma)0s$.

In both models the occupational modulations for Bi and Mo atoms are represented by complementary crenel functions, which give rise to the cationic distribution proposed for these compounds [2]. Another feature of both models is that the atomic domains representing O atoms associated with Mo coordination environments exhibit very large positional modulations.

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Spectral properties of a family of random substitution systems

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The classic Fibonacci substitution has a random extension that produces Meyer sets with entropy. This was originally introduced in a 1989 paper by Godrèche and Luck, and can be generalised to noble means substitutions. Here, some basic properties are reviewed, including entropy, ergodicity and diffraction.

Well-rounded lattices

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A lattice is called well-rounded, if its lattice vectors of minimal length span the underlying space. Their importance is due to their close relationship to perfect lattices. As the lattices used in cut and project schemes are usually well-rounded it is interesting to have a closer look on them in this context.

Here we concentrate on well-rounded sublattices of highly symmetric lattices. We present criteria for the existence of well-rounded sublattices and discuss their relationship to coincidence site lattices. We determine the well-rounded sublattices of several important lattices, count their numbers for a given index and encode this information in suitable Dirichlet series, which allows us to determine the asymptotic growth rate of the number of well-rounded sublattices.

This is joint work with M. Baake (Bielefeld, Germany) and R. Scharlau (Dortmund, Germany).

The Fractal Dual of the Pinwheel Tiling

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The Pinwheel tiling of the plane, discovered by J. Conway and C. Radin [2], is a substitution tiling with tiles appearing in an infinite number of distinct orientations. The nature of the pinwheel substitution system gives rise to fixed points within each tile of the tiling. Piecing these fixed points together and iterating the substitution gives rise to an iterated function system, which produces fractals [1]. For the Pinwheel tiling, each tile in the tiling has an iterated function system within it, and piecing all these fractals together gives a new tiling of the plane by tiles with fractal boundaries. We call this new tiling the fractal dual of the Pinwheel tiling.

In the Pinwheel tiling, tiles appear in an infinite number of orientations; this is revealed in the fractal dual of the Pinwheel tiling by an infinite number of orientations in every edge of the new tiles. The fractal dual of the Pinwheel tiling is mutually locally derivable with the original Pinwheel tiling and provides the first example of a Pinwheel tiling that “forces its border.”

I will not assume any knowledge of fractal geometry and the presentation will be self-contained.

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Geometric Properties of N-fold Quasicrystals

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Quasicrystals of n -fold planar symmetry possess sites, called flowers or stars, with $2n$ - or n -fold point symmetry. The flowers are very predominant in fivefold quasicrystals and play an important role for example in the stabilization of colloidal quasicrystals [1,2]. We have determined the number of stars directly up to $n=11$. We observe that if n increases, the number of stars decreases more than exponentially. Thus we argue that the tiling patches with very high n (up to 30) which many groups study experimentally should not be called quasicrystals since they do not form a representative sample due to their small size.

Laser potentials, which are generated by the superposition of harmonic waves, exhibit local isomorphism classes much like rhombus tilings. While the classes are known for tilings [3], we determine them for n -fold symmetric laser fields and show how many free parameters exist.

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Quasicrystalline Thin Films of Single Elements and Molecules

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We have studied the growth of thin film of various elements (e.g., Pb, Bi, Sb, Cu) and molecules (i.e., Pentacene and C₆₀) on the surface of icosahedral Ag-In-Yb quasicrystal using various surface science techniques, namely, scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and x-ray photoelectron spectroscopy (XPS).

The deposited Pb grows in quasicrystalline order up to second layer. Such quasicrystalline bilayer structure is observed for the first time. Higher coverage yields fivefold-twinned hexagonal Pb islands with (111) surface orientation. The islands are of specific heights (magic heights), which correspond to the stacking of four-six atomic layers of the bulk Pb, possibly due to the confinement of electrons in the islands. Sb yields quasicrystalline monolayer and partial second layer, which is also in quasicrystalline order. At high coverage, a disorder film is produced. Bi forms quasicrystalline monolayer, structure of which is slightly different from that of the Pb and Sb film. No Bi sticks on the surface after formation of a monolayer. The structure of the films can be understood in terms of substrate atomic structure [1-3]. The experimental results will be compared with first-principles calculations. We will also demonstrate an example of quasicrystalline molecular thin film formed on the surface substrate. The observed model structures of single elements quasicrystalline thin films can be used to investigate the influence of atomic order in physical properties.

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Catalytic properties of fivefold surfaces of quasicrystal approximants

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Recently it has been shown that some low order approximants to decagonal or icosahedral quasicrystals provide excellent activity and selectivity for hydrogenation of alkynes. Our recent works on $\text{Al}_{13}\text{Co}_4$ [1] and AlPd [2] compounds demonstrated that the catalytically active surfaces in both cases are surfaces with the (pseudo)five-fold symmetry. Ab-initio DFT calculations have been used to identify the reaction centers and to construct a detailed atomistic scenario for the acetylene to ethylene hydrogenation. It was found that the activity of the catalysts is not promoted by the transition metal (TM) atoms alone but by a cluster of Al atoms centered by a slightly protruding TM atom. In the present contribution we extend our studies to other related compounds and demonstrate that local configurations of Al and TM atoms favorable for selective catalysis of the hydrogenation reactions naturally appear at Al-TM surfaces with the pentagonal symmetry.

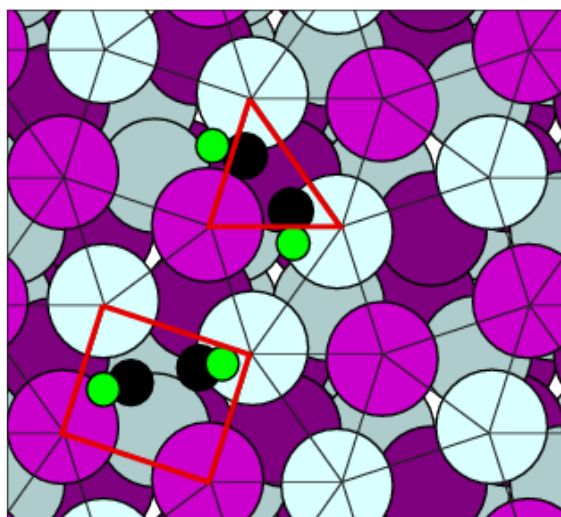


Figure 1. The structure of the pseudo-fivefold surface of the AlPd B20 compound can be described by a rectangle-triangle tiling. The adsorption sites of acetylene in some triangular and rectangular tiles are the catalytically active centers (enhanced) for a hydrogenation reaction.

□

[1] M. Krajčí and J. Hafner, *J. Catal.* **278**, 200 (2011).

[2] M. Krajčí and J. Hafner, *J. Phys. Chem.*, **DOI: 10.1021/jp212317u** (2012).

Composition and local atomic arrangement of decagonal Al-Co-Cu quasicrystal surfaces

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^b Institut für Angewandte Physik, Technische Universität Wien, Vienna, Austria.

The surface structures of decagonal quasicrystals have been studied by scanning tunneling microscopy (STM), showing several types of clusters with fivefold symmetry. However, a structural model has not been obtained because of the difficulty to determine the composition quantitatively. So far, the surface composition of the Co-rich d-Al-Co-Ni quasicrystal has been investigated by Auger electron spectroscopy (AES) and low energy ion scattering (LEIS), indicating that Al atoms segregate to the surface on annealing [1], but others have suggested a bulk terminated structure without any surface reconstruction [2].

In this paper, we investigated the composition of decagonal Al-Co-Cu surface by AES and LEIS. The surface compositions after annealing were Al-richer and Co-poorer than those after sputtering or bulk composition [3]. Two types of the characteristic clusters were observed by STM [4]. Structural optimization using *ab initio* calculations based on density functional theory (DFT) was performed on several compositional models, which are based on the W-(AlCoNi) bulk model [5].

The surface structures of two types of the characteristic clusters were determined by comparison of the STM image and the simulated image of the structures obtained by DFT (Fig.1). The topmost layer was composed of Al and Cu atoms, and the compositional ratio was consistent with the AES and LEIS results.

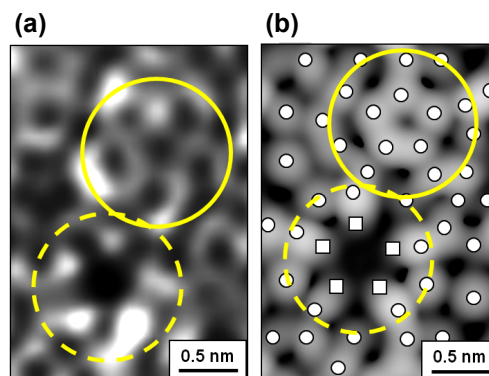


Fig.1 (a) Negative-bias simulated STM image with the atomic arrangement of the topmost layer (Al : ○, Cu : □) shown as overlay. (b) Negative-bias experimental STM image of the d-Al-Co-Cu surface.

[1] J. Yuhara *et al.*, Phys. Rev. B **70** (2004) 024203.

[2] N. Ferralis *et al.*, Phys. Rev. B **69** (2004) 153404.

[3] R. Zenkyu *et al.*, Phys. Rev. B submitted (2012).

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[5] M. Mihalkovič and M. Widom, alloy database at <http://alloy.phys.cmu.edu/>

Soft Matter Quasicrystals: Design Rules from Computer Simulation

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The surprising recent discoveries of quasicrystals and their approximants in soft materials - including dendrimers, block copolymers, nanoparticle suspensions and hard colloids - poses the intriguing possibility that these structures can be realized in a broad range of nano- and micro-scale assemblies. In this talk, we review recent reports of quasicrystals in computer simulations of hard polyhedra, micelles, and amphiphilic nanoparticles. We present an example of a degenerate quasicrystal of anisotropic hard dimers in which the degeneracy lies in the orientation of dimer axis, rather than the usual tiling degeneracy. We demonstrate the robustness of the dodecagonal quasicrystal to particle imperfections, including size polydispersity, shape, and other features arising in nanoparticle synthesis. We show how in all of these cases the structures are entropically stabilized, and form in the absence of any explicit attraction. We show that these entropic forces manifest, in the case of hard faceted particles, in the form of effective directional entropic bonds. Based on our findings, we propose a simple design heuristic for assembling quasicrystals and approximants in soft matter systems that can explain quasicrystal formation in micellar and related materials.

- [1] A.S. Keys and S.C. Glotzer, *Phys. Rev. Lett.* **99**, 235503 (2007).
- [2] A. Haji-Akbari, M. Engel, et al. and S.C. Glotzer, *Nature* **462**, 773 (2009).
- [3] S.C. Glotzer and A.S. Keys, *Nature* **454**, 420 (2008).
- [4] A. Haji-Akbari, M. Engel, and S. C Glotzer, *Phys. Rev. Lett.* **107**, 215702 (2011).
- [5] S.C. Glotzer and M. Engel, *Nature* **471**, 309 (2011).
- [6] C.R. Iacovella, A.S. Keys and S.C. Glotzer, *PNAS* **108**, 20935 (2011).
- [7] P.F. Damasceno, M. Engel and S.C. Glotzer, *ACS Nano* **6**, 609 (2012).
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Controlling the Self-Assembly of Soft Quasicrystals

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A large number of soft-matter systems have been shown in recent years to form ordered phases with dodecagonal symmetry. These systems vary in the length scales of their building blocks from several to hundreds of nanometers, and include, among others, dendrimers [1], star polymers [2], block copolymer micelles [3], and nanoparticles [4] (see [5] for a recent review). As argued in Aperiodic 2006 [6], we have recently established [7] that the stability of single-component soft quasicrystals can be attributed to the existence of two natural length scales in their isotropic pair potential, along with an effective three-body interaction arising from entropy. We demonstrate here how one can use this understanding to design the pair potentials of single-component systems and control the self-assembly of various desired structures, including quasicrystals. We apply similar principles to the design of pair potentials for controlling the self-assembly of multi-component systems, such as [3], and verify that our design principles indeed work using numerical simulations. Finally, we show that the numerical scheme that we use can also provide a platform for the study of the dynamics of these soft quasicrystals.

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- [3] S. Fischer *et al.*, *PNAS* **108**, 1810 (2011).
- [4] D.V. Talapin *et al.*, *Nature* **461**, 964 (2009).
- [5] T. Dotera, *Isr. J. Chem.* **51**, 1197 (2011).
- [6] R. Lifshitz and H. Diamant, *Phil. Mag.* **87**, 3021 (2007).
- [7] K. Barkan, H. Diamant and R. Lifshitz, *Phys. Rev. B* **83**, 172201 (2011).

Quasicrystals formed by hard-core/square-shoulder particles

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One of the new frontiers of quasicrystal (QC) research in the 21st century are the various soft QCs seen, e.g., in polymer, micellar, and dendrimer systems [1]. Here we report the formation of 10-fold, 12-fold, and 18-fold QCs in Monte Carlo simulations of two-dimensional hard-core/square-shoulder particles (Fig. 1) [2]. Despite the purely repulsive and isotropic pair interaction, this system displays a variety of aperiodic phases which are characterized by bond-orientational order arising from the competition between the hard-core and soft-shoulder length scales.

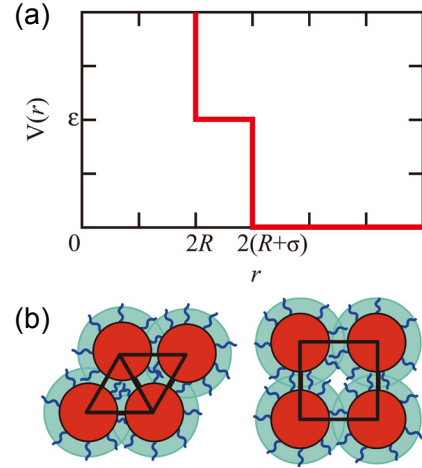


Figure 1. Hard-core/soft-shoulder pair potential (a). The two structural elements of QCs formed by core-shell particles: Equilateral triangles and squares (b).

We scanned the phase diagram for QCs by varying temperature, the packing fraction ρ , and the shoulder-to-core ratio $\lambda = 1 + \sigma/R$; here σ is the thickness of the shoulder and R is the core radius. Table 1 shows the ranges of λ and ρ where QCs are formed at certain temperature.

QC	λ	ρ
18-fold	1.25-1.30	0.77
12-fold	1.35-1.47	0.77
10-fold	1.47-1.62	0.52-0.6

Table 1. Ranges of shoulder-to-core ratio λ and packing fraction ρ required for QC formation.

We observed that the 18-fold QC is closely related to the 12-fold random QC, since it is composed of equilateral triangles and 80°-100° rhombi so that all angles involved are multiples of 20°.

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- [2] M. A. Glaser, G. M. Grason, R. D. Kamien, A. Košmrlj, C. D. Santangelo, and P. Ziherl, *EPL* **78**, 46004 (2007).

Structural and Magnetic Ordering in Cd-based Crystalline Approximants

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Since the fascinating discovery of quasicrystals (QCs) by Shechtman *et al.*[1] particular attentions have been paid to their unique atomic structure as well as the physical properties intrinsic to QCs. Amongst all the icosahedral (*i*) QCs, substantial works have been performed on stable ternary *i*-QCs such as *i*-Al-Cu-Fe and *i*-Al-Pd-Mn QCs because of their high structural perfection. The discovery of stable binary *i*-Cd-Yb and *i*-Cd-Ca QCs by Tsai *et al.*[2] has opened up a new era for the quasicrystal researches on both the structure and properties since these *i*-QCs and approximants (APs) are not only structurally ordered but also chemically ordered. Subsequent works have shown an occurrence of a unique low-temperature structural transition associated with the dynamical motion of a tetrahedron inside an icosahedral cluster in a series of Cd₆M APs[3], which is classified into a “nondiffusive order-disorder transition”. In addition to the unique structural transitions, the Cd₆M APs are also found to exhibit long-range magnetic orders [4] at low temperatures unlike ternary magnetic *i*-QCs and APs where spin-glass-like freezing has been observed without exception. Most of the magnetic Cd₆M APs exhibit an antiferromagnetic transition with rich metamagnetic anomalies accompanying salient hysteresis in *M-H* curves below T_N . The presentation will be focused to both the structural and magnetic ordering in the Cd₆M APs and the interplay between the structural transition and the magnetism will be discussed.

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- [2] Tsai *et al.*, *Nature* 408, **537** (2000).
- [3] Tamura *et al.*, *Jpn. J. Appl. Phys.* **41**, L524 (2002).
- [4] Tamura *et al.*, *Phys. Rev. B* **82**, 220201(R) (2010).

Antiferromagnetic order in the quasicrystal approximant, Cd_6Tb .

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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 there is strong evidence that the geometry or topology of the quasilattice frustrates magnetic ordering. 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.[1] Here, we will report the results of x-ray resonant magnetic scattering measurements on Cd_6Tb and show that long range antiferromagnetic order is, indeed, realized below $T_N = 24 \pm 1$ K.[2] The Bragg peaks that arise from the antiferromagnetic order are as sharp as those associated with the chemical structure, providing a lower limit for the magnetic correlation length of approximately 500 Å. Viewing the structure as a body-centered cubic packing of Tsai clusters, we find that the Tb ions associated with the icosahedral cluster at the corner of the unit cell are antiferromagnetically correlated with the Tb ions associated with the icosahedral cluster at the body-center of the unit cell.

[1] R. Tamura, Y. Muro, T. Hiroto, K. Nishimoto, and T. Takabatake, *Phys. Rev. B* **82**, 220201(R) (2010).

[2] M.G. Kim, G. Beutier, A. Kreyssig, T. Hiroto, T. Yamada, J.W. Kim, M. de Boissieu, R. Tamura, and A. I. Goldman, submitted to Physical Review B.

Paramagnetic Structure from Magnetic Diffuse Scattering

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The paramagnetic state plays a central role in many areas of contemporary solid-state physics: examples include the emergence of high-temperature superconductivity from spin liquid phases [1], magnetic monopole formation in spin ices [2], and the ongoing search for new physics in quantum spin liquids [3]. The suppression of long-range spin periodicity in cooperative paramagnets means that no magnetic Bragg peaks are observed. Instead, the magnetic contribution to the neutron scattering pattern is a smoothly varying function of reciprocal space. We have recently shown that the structural information contained within this diffuse magnetic scattering can be extracted using a reverse Monte Carlo (RMC)-based approach [4]. This talk will begin with an outline of our methodology in the context of fitting both to powder-averaged and to single-crystal magnetic diffuse scattering, before describing the results of recent diffuse scattering studies of two canonical systems: paramagnetic MnO and Co-doped beta-Mn.

- [1] A. T. Boothroyd, P. Babkevich, D. Prabhakaran and P. G. Freeman, *Nature* **471**, 341 (2011)
- [2] C. Castelnovo, R. Moessner and S. L. Sondhi, *Nature* **451**, 42 (2008).
- [3] F. L. Pratt, *et al.*, *Nature* **471**, 612 (2011).
- [4] J. A. M. Paddison and A. L. Goodwin, *Phys. Rev. Lett.* **108**, 017204 (2012).

The Discovery of Quasi-Periodic Crystals

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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 a 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 crystallographic community of this 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 Crystallography. 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 were published, a result of the 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 discuss their structure as well as some of their properties and uses.

[1] D. Shechtman, I. Blech, Met. Trans. 16A (June 1985) 1005-1012.

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Modulations, Modes, Materials and Crystal Chemistry

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Janner and Jansen first demonstrated the equivalence between the superspace description of incommensurate structures and the mode description phonon modes[1], however with few exceptions[2] this is rarely exploited in the description of modulated structures. The following will use the available tools including ISODISTORT[3] and the Bilbao crystallographic server[4] in order to discuss the crystal chemistry of two families of perovskite oxides:

(i) Modulated bismuth A site perovskites. $\text{Bi}_2\text{Mn}_{4/3}\text{Ni}_{2/3}\text{O}_6$ we have previously described the room temperature phase in 3+2 dimensional space group $\text{Ibmm}(0-p0,q00)\text{mm.ss}$ ($\sqrt{2}a_p \times 2a_p \times \sqrt{2}a_p$; $p,q \sim \frac{1}{2}$). [5] The phase $\text{Bi}_2\text{Mn}_{2/3}\text{Ti}_{2/3}\text{Ni}_{2/3}\text{O}_6$ crystallizes in the same superspace group. Its room temperature structure based combined synchrotron X-ray and time of flight neutron diffraction will be discussed together with the lack of B site ordering. $\text{Bi}_2\text{CoTiO}_6$ is a metastable high pressure double perovskite showing no cation order but does show an incommensurate modulation. Combined refinements show that this material crystallizes in the polar superspace group $\text{I2cm}(0p0)000$ ($p \sim -2/3$). By combining both superspace and mode based descriptions the relationships between these phases and doped BiFeO_3 systems will be explored.

(ii) $\text{A}'\text{A}''\text{B}'\text{B}''\text{O}_6$ derivatives here the development of quantitative models for the stripe phases observed in NaLaMgWO_6 will be discussed via both mode based model building and superspace refinements of HRPD data of the $\text{Na}_{1-x}\text{La}_{1+x/3}\text{MgWO}_6$ phases.

[1] A. Janner, T. Janssen, *Phys. Rev. B*, **15**, 643-658 (1977).

[2] J.M. Perez-Mato, D. Orobengoa, M.I. Aroyo, M. I. *Acta Cryst.* **A66**, 558–590 (2010).

[3] B. J. Campbell, H. T. Stokes, D. E. Tanner, and D. M. Hatch, *J. Appl. Cryst.* **39**, 607-614 (2006).

[4] Bilbao Crystallographic Server: <http://www.cryst.ehu.es>

[5] J.B. Claridge, *et al.*, *J. Am. Chem. Soc.* **131**, 14000-14017 (2009).

Modulated Structures in Mixed Transition Metal - Main Group Metal Clusters

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Mixed tin - transition metal cluster compounds form novel nano-scale clusters with a wide variety of different combinations of metals and resulting architectures which are size tunable. Two examples will be discussed in more detail in this presentation. The central and most striking structural feature of all these stannates is the formation of transition metal centered Sn₆-octahedra, as it is also observed in Ir₁₀CoSn₄₅O₄₅ and Ir₃Sn₈O₄. Ir₁₀CoSn₄₅O₄₅ can be described as an addition of CoO to Ir₁₀Sn₄₅O₄₄, a compound containing endless fivefold chains formed by Ir centered corner-linked Sn₆-octahedra. To get a deeper understanding of the real structure of Ir₁₀Sn₄₅O₄₄ HRTEM investigations have been performed. Ir₁₀Sn₄₅O₄₄ shows strong one-dimensional disordered stacking of ordered nanoscale clusters with an ordered polytype which shows a doubling of the lattice constant *c* in comparison to the undoped ternary compound Ir₁₀Sn₄₅O₄₄. As the building blocks of this artificially layered material two different (00l) layers A (undistorted) and B (distorted) could be found. These A and B layers have the thickness of a cluster layer formed in Ir₁₀Sn₄₅O₄₄ (≈ 1.8 nm). The stacking of the layers along [001]* is in a random order, but domains with preferred AA- (BB-) and AB sequences can be observed. In bright-field images these lamellas were pictured as broad stripes. As expected the Fourier transform of images of layers containing a random stacking order show very strong diffuse signals along [001]*.

In Ir₃Sn₈O₄, the oxygen poorest of all compounds in this group of clusters, IrSn₆ octahedra are partly side-linked in contrast to most of the other compounds in this group. This compound shows an incommensurately modulated structure due to very strong Ir-Ir interactions within the condensed IrSn₆ octahedra. This paper gives an overview about the preparation, crystallographic and spectroscopic characterization of this new group of cluster compounds.

The first SC-XRD system using a CMOS APS detector

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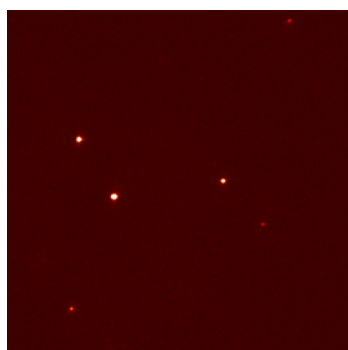
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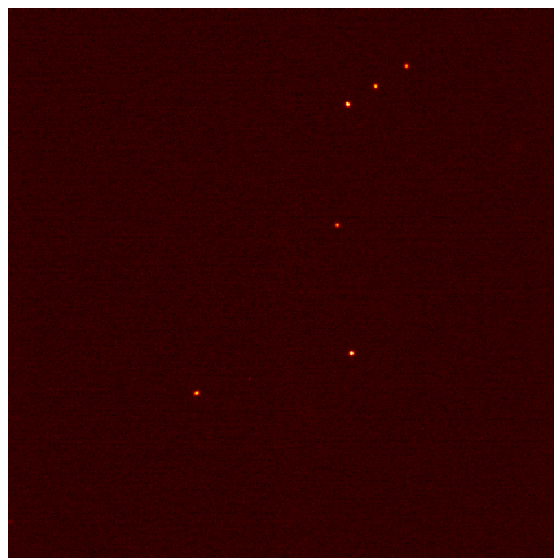
Although synchrotron radiation beam time has become readily available in many regions, modern crystallography more than ever relies on in-house, high-end systems for SC-XRD structure investigations. Very recently, the D8 CRYSTALLOGRAPHY SOLUTIONS family became available addressing these demands. The systems feature the latest generation of microfocus X-ray sources, X-ray optics and dedicated software. However, the most significant contribution to the improved data quality, typically resulting in lower R-values, often observed within a shorter exposure time, can be assigned to the PHOTON 100 detector.

Rapid advances in CMOS sensor technology have enabled the development of first CMOS active pixel sensor for X-ray crystallography. Compared to conventional CCD detectors CMOS technology offers a number of features, such as sensor size, sensitivity, zero blooming, making it superior. CMOS technology also allows shutterless read-out, which removes the effect of mechanical jitter from the data.

Details of the design concept of the D8, including comparisons of CMOS and CCD technology as well as a number of examples on the investigation of challenging solid state chemistry samples in will be presented.



Diffraction pattern using an APEX II (left) and a PHOTON 100 (right) at $2\theta = 90^\circ$: The size ratio between the shown diffraction images represents the difference in the active area of the compared detectors.



Studies on Inverse Hall-Petch behavior in nanostructured $\text{Al}_{62.5}\text{Cu}_{25}\text{Fe}_{12.5}$ quasicrystals

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In the present investigation a single phase $\text{Al}_{62.5}\text{Cu}_{25}\text{Fe}_{12.5}$ icosahedral phase produced by spray forming was mechanically milled in planetary ball mill at 100 rpm up to 80 h in controlled atmosphere in order to synthesize nano-quasicrystalline phases up to 20 nm crystallite size. The microhardness tests were conducted on the powders obtained from various milling experiments. It was found that the microhardness increases initially and then decreases with the decrease of grain size. The grain size dependent hardness was clearly noticed. More interestingly, inverse Hall-Petch (HP) behavior was reported for the first time in quasicrystalline materials. The Al-Fe-Cu quasicrystalline materials exhibit both the Hall-Petch and Inverse Hall-Petch relation in the nanoscale regime. The transition from HP to IHP is found to be around 40 nm grain size. The increase of the hardness with the decrease of grain size i.e. in the HP region can be attributed to the difficulty of dislocation movement and other defects such as shear bands at smaller grain size but still the role of grain boundary may not be significant. The softening of the nano-quasicrystalline materials at lower grain size is due to the fact the grain boundary play an important role by way of grain boundary sliding, grain rotation and grain movement. The mechanistic diffusion during the indentation may also cause to soften the materials. Efforts will be made to understand these features in the context of structural complexities and plasticity of quasicrystalline phases.

Evolution of phases in selected Al-Co-Cu complex metallic alloys under near-equilibrium conditions at 800-1150°C

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The work is focused on the experimental investigation of intermetallic phases in $\text{Al}_{60}\text{Co}_{29}\text{Cu}_{11}$, $\text{Al}_{63}\text{Co}_{24}\text{Cu}_{13}$, and $\text{Al}_{67}\text{Co}_{20}\text{Cu}_{13}$ complex metallic alloys at near-equilibrium conditions. The alloys were long-term annealed at temperatures between 800 and 1150°C and subsequently rapidly cooled to fix their high-temperature microstructures. Annealing temperatures were chosen reflecting the results of DTA analysis. Particular samples were studied by X-ray diffraction, scanning electron microscopy including energy dispersive X-ray spectroscopy and electron backscatter diffraction, and transmission electron microscopy. In the microstructures of particular samples various combinations of D, B2, m, Al_5Co_2 , and $\Theta\text{-Al}_2\text{Cu}$ phases were identified depending on both bulk metal composition and thermal history. The obtained results were used to construct partial isothermal sections of the Al-Cu-Co phase diagram for temperatures used in the investigation.

Structural Characteristics of Complex Intermetallics

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Complex compounds can be found in a large variety of intermetallic systems. They are usually categorised according to the number of atoms per unit cell, which amounts to hundreds or even thousands in some cases [1]. Several quasicrystal approximants and some modulated structures can be found among these compounds, which occur preferably in highly-symmetric lattices. Therefore we are concentrating on cubic [2] and hexagonal structures.

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

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

- [1] T. Weber, J. Dshemuchadse, M. Kobas, M. Conrad, B. Harbrecht, W. Steurer, *Acta Cryst. B* 65, 308-317 (2009).
- [2] J. Dshemuchadse, D. Y. Jung, W. Steurer, *Acta Cryst. B* 67, 269-292 (2011).

Hume-Rothery Stabilization Mechanism in Low-Temperature Phase Zn_6Sc Approximant and e/a Determination of Sc, Y and La in Sc-X, Y-X and La-X (X=Zn, Cd and Al) Alloy Systems

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By making full use of the first-principles FLAPW-Fourier method, the present authors [1, 2] have recently demonstrated the Hume-Rothery stabilization mechanism to hold true not only for RT-type Al-Mg-Zn and Al-Li-Cu 1/1-1/1-1/1 approximants but also for MI-type 1/1-1/1-1/1 approximants including Al-Mn, Al-Re-Si, Al-Cu-Fe-Si etc. The FsBz interactions involving the set of {543}+{550}+{710} lattice planes with $|G|^2=50$ are found to be commonly responsible for causing a pseudogap at the Fermi level. The aim of the present work is to extend the approach above to Tsai-type 1/1-1/1-1/1 approximant and to confirm if the Hume-Rothery stabilization mechanism holds for a whole series of 1/1-1/1-1/1 cubic approximants.

Ishimasa et al. [3] revealed that the Zn_6Sc 1/1-1/1-1/1 approximant transforms into an ordered structure containing 336 atoms per unit cell with space group B2/b at low temperatures. We performed FLAPW electronic structure calculations with subsequent FLAPW-Fourier analysis. The square of the Fermi diameter, e/a and e/uc and critical reciprocal lattice vector $|G|^2$ are determined. The present work is extended further to all intermetallic compounds existing in Sc-X, Y-X and La-X (X=Zn, Cd and Al) binary alloy systems to determine e/a values for them. From this, we could determine the effective e/a for three transition metal elements Sc, Y and La in the periodic table.

[1] M. Inukai, E.S. Zijlstra, H. Sato and U. Mizutani, *Phil. Mag.* **91**, 4247 (2011).

[2] U. Mizutani, M. Inukai, H. Sato and E.S. Zijlstra, *Phil. Mag.* in print (2012).

[3] T. Ishimasa et al., *Phil. Mag.* **87**, 2887 (2007).

Complexity of cut and project tilings

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Cut-and-project tilings are an important source of examples for quasi-periodic tilings, as the Penrose tilings or Octagonal tilings can be described in this way. They can be seen as a multidimensional analogue of Sturmian sequences or cubic billiard sequences. In this talk, I will present the construction of cut-and-project tilings (with canonical acceptance domain), and give a few results on their complexity function. The complexity function, which was well studied for one-dimensional words, gives a quantitative measure of the order or disorder of an quasi-periodic tiling, as it counts the number of patches of a given size. Furthermore, I will explain how the growth of the complexity function is related with the topology of the tiling space.

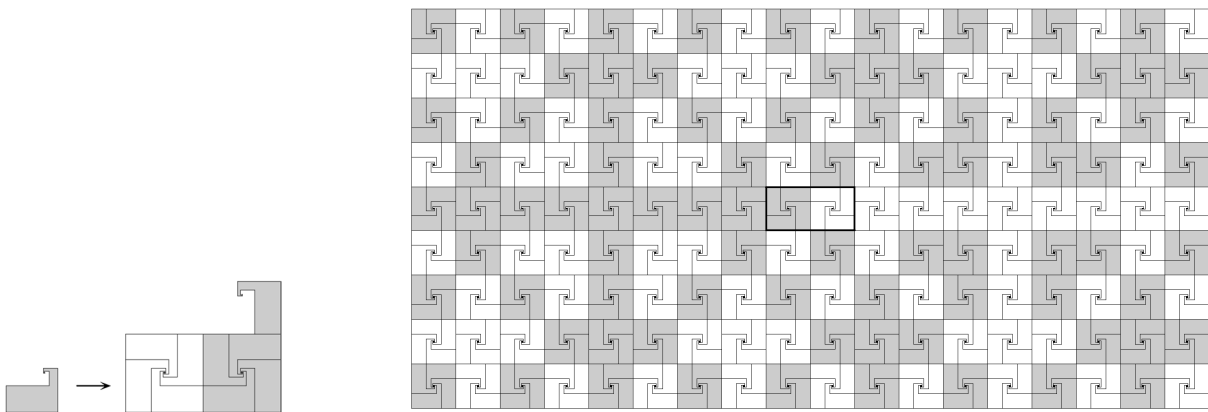
Squirals and their Diffraction

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The Thue-Morse system is a paradigm for singular continuous diffraction. Recently, we showed [1] that it is possible to show singular continuous diffraction for a whole family of generalised Thue-Morse sequences. This can be extended beyond the one-dimensional case. Here, we consider the squiral tiling, which is a planar inflation tiling shown below. Its inflation rule (also shown below) is equivalent to a simple bijective block substitution rule, and the squiral tiling is MLD (mutually locally derivable) with a two-colouring of the square lattice. The block inflation leads to a lattice dynamical system with interesting properties. In particular, it can be viewed as a two-dimensional generalisation of the Thue-Morse system. For balanced weights, the squiral tiling shows purely singular continuous diffraction. The dynamical spectrum is of mixed type, with pure point and singular continuous components. We outline a constructive approach that admits a generalisation to a large class of bijective block substitutions in any dimension.



- [1] M. Baake, F. Gähler and U. Grimm, Spectral and topological properties of a family of generalised Thue-Morse sequences, *J. Math. Phys.* **53**, 032701 (2012); arXiv:1201.1423.

Tilings: When Periodicity Enforces Aperiodicity

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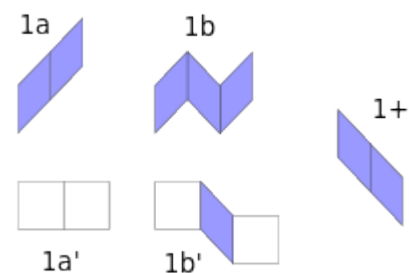
^b *LIPN, University of Paris, France.*

A tiling is aperiodic if it is non-periodic but can nevertheless be described only by local constraints (the first such tiling was found by Robert Berger in 1964). Aperiodic tilings intend to model how the non-periodicity of quasicrystals can be enforced by finite range energetic interactions, and a complete characterization of them could be seen as an extension of the classic crystal system to a “quasicrystal system”.

Some large classes of tilings have already been characterized, such as substitutive tilings [1] or computable tilings [2]. These approaches however lead to huge sets of complicated local constraints – thus somehow unrealistic regarding quasicrystals.

Here, instead, we follow an approach initiated by Leonid Levitov [3] and notably pursued by Le [4]. The idea is to enforce the periodicity of some projections of the tiling (seen in the reciprocal space), with the non-periodicity coming “for free” from classic algebraic geometry results. This yields a general method to design rather light local constraints for many tilings based on algebraic irrationalities.

In this talk, we will mainly focus on a worked out example which should reach a large public, namely an octogonal tiling characterized by forbidden small patterns like those on the figure (right). A general result will also be given (in more technical terms).



- [1] C. Goodman-Strauss, *Annals of Mathematics* **147** (1998)
- [2] Th. Fernique and M. Sablik, to appear in *Proc. of CiE'12* (2012)
- [3] L. Levitov, *Communications in Mathematical Physics* **119** (1988).
- [4] T. T. Q. Le, *Communications in Mathematical Physics* **150** (1992)

Octagon-based Quasi-crystalline Formations in Islamic Architecture

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The unexpected discovery of ancient Islamic ornaments with quasi-crystalline symmetries has triggered significant discussion and a number of debates on the mathematical sophistication of Islamic geometry and its generating principles. Astonishingly, eight centuries, before its description in the West, ancient artists had constructed patterns with perfect quasi-crystalline formations [1]. Recent studies have provided enough evidence to suggest that ancient designers, by using the most primitive tools (a compass and a straight edge) were able to resolve the complicated long-range principles of quasi-crystalline formations [1,2]. Derived from these principles, a global multi-level structural model is presented that is able to describe the global long-range translational and orientational order of 8-fold and 16-fold quasi-crystalline symmetries in Islamic Architecture (fig.1).

This new method can be used as a general guiding principle for constructing infinite patches of octagon-based quasi-crystalline formations, including Ammann-Beenker tiling [3], without the need for local strategies (matching, scaling, etc.) or complicated mathematics. In addition, this novel method provides an easy tool for scientists, mathematicians, teachers, designers and artists, to generate and study a wide range of octagon-based quasi-crystalline formations.

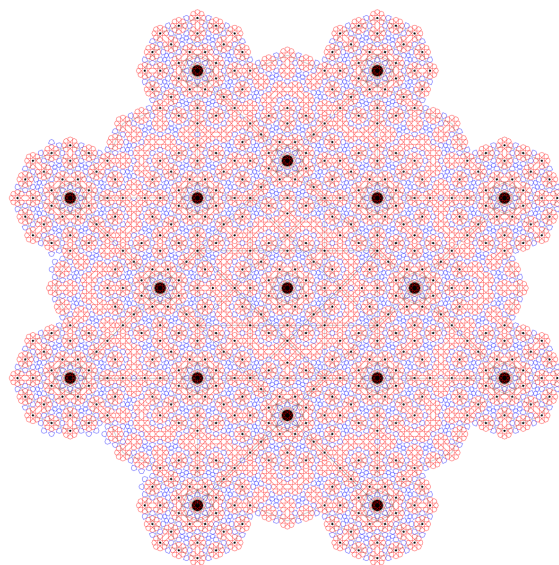


Figure 1: The global quasi-periodic empire of an ancient octagonal pattern in Morocco.

- [1] R. Al Ajlouni, *Acta Crystallographica Sec. A*, **68**, 235 (2012).
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- [3] F. Gahler and H. Jeong, *J. Phys. A: Math. Gen*, **28**, 1807 (1995).

Dynamic Structure Factors for Two-dimensional Quasicrystals

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Quasicrystals (QCs) are long-range ordered materials with rotational symmetry incompatible with translational order. Soon after the discovery of QCs, the concept of phason was proposed, and various structural characteristics in real QCs are now understood in terms of spatial variation of the phason variables. In particular, the long-wavelength phason fluctuations observed as diffuse scatterings provide one of the strong evidences that the hydrodynamic continuum theory of the phason describes the exotic nature of QCs correctly. Recently we have studied the dynamic structure factor for two-dimensional decagonal (10-fold) quasicrystals based on the hydrodynamic model, and discussed the possibility to observe the phasonic dynamics in scattering experiments [1]. Quasicrystalline structures are obtained also in metamaterials such as Faraday waves on liquid surfaces, photonic structures generated by laser beams, and some soft materials. The quasicrystalline ordering in metamaterials is usually two-dimensional, and the rotational symmetry is more variable. In addition, although the phasonic dynamics is very slow for metallic QCs, it could be in a reasonably accessible range for metamaterials. To provide theoretical information for possible experimental observation of the phasonic dynamics in metamaterials, we extend the calculations of the structure factor based on the hydrodynamic model for the decagonal case to other rotational symmetries such as octagonal (8-fold) and dodecagonal (12-fold) ones. The different symmetries lead to different elastic response. We shall discuss characteristic line shapes of the dynamic and static structure factors.

[1] A. Chatzopoulos, H.-R. Trebin and Y. Ishii, *submitted to Phys. Rev. B*.

Tetrahedron Dynamics in the i-MgScZn quasicrystal and its 1/1 cubic approximant ScZn₆

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Both, the i-MgScZn QC and its ScZn₆ 1/1 approximant consist of triacontahedral clusters, arranged on a non-periodic and a bcc lattice, respectively. These clusters are of icosahedral symmetry, except for the innermost shell, which is a symmetry-breaking tetrahedron [1]. Due to the reduced symmetry of this tetrahedral shell it can occupy several equivalent orientations inside a triacontahedral cluster.

In the ScZn₆ 1/1 approximant this gives rise to an order-disorder phase transition during which the tetrahedra orient anti-parallel along the [110] direction of the cubic high temperature phase [2], while in the QC no such transition is evidenced.

We present a combined experimental and simulation study of the tetrahedron disorder in the ScZn₆ 1/1 approximant and the i-MgScZn QC. For both systems neutron scattering experiments strongly indicate the tetrahedron disorder to be dynamic in nature. These experimental findings are interpreted by molecular dynamics simulations, using oscillating pair potentials, indeed evidencing that the tetrahedra are exposed to constant reorientations, which in case of the 1/1 approximant freeze in at the phase transition temperature.

[1] M. de Boissieu et al., *Nature Materials*, 6, 977 - 984 (2007)

[2] T. Ishimasa et al., *Phil. Mag.*, 87, 2887 - 2897 (2008)

Confirmation of the Random Tiling Hypothesis for a Decagonal Quasicrystal

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Quasiperiodic tilings carry phason degrees of freedom, which show up as local structural rearrangements present in equilibrium. The random tiling hypothesis of Henley and Elser [1,2] states, that the resulting configurational entropy stabilizes a quasicrystal at elevated temperatures and leads to a periodic crystal at low temperatures. Although the random tiling hypothesis has been confirmed previously in discrete tiling models, it has so far not been investigated in models of freely moving particles. Here, we study the role of entropy for a monatomic two-dimensional decagonal model quasicrystal, whose atoms interact by a double-well Lennard-Jones-Gauss pair potential [3]. We calculate the free energy of the system, which can be split up into a phonon part and a configurational (phason) part. The phonon part of the free energy is calculated with molecular dynamics using the Frenkel-Ladd method [4] combined with thermodynamic integration. For the configurational part a new Ising-type model of uncorrelated flips is employed in Monte Carlo simulations. We observe that the free energy takes a square-gradient form of the phason displacement as predicted by the random tiling hypothesis and determine phason elastic constants over a large range of temperatures. The free energy calculations confirm a phase transition from an entropically stabilized decagonal random tiling phase to an energetically stabilized periodic crystal. At the transition temperature one of the phason elastic constants changes sign. Thus, for the first time, a virtual quasicrystal confirms all predictions of the random tiling hypothesis in a fully atomistic model.

- [1] V. Elser, *Phys. Rev. Lett.* **54**, 1730 (1985)
- [2] C. L. Henley, *J. Phys. A* **21**, 1649 (1988)
- [3] M. Engel and H.-R. Trebin, *Phys. Rev. Lett.* **98**, 225505 (2007)
- [4] D. Frenkel and A. J. C. Ladd, *J. Chem. Phys.* **81**, 3188 (1984)

Phason dynamics in light-induced colloidal quasicrystals

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We study a 2D charge-stabilized colloidal suspension in an external potential with quasicrystalline symmetry. In experiments the potential is realized by five, seven, or more interfering laser beams. Such a colloidal system is an attractive model system for studying the dynamics or ordering of atomic systems leaving aside chemical details of the interactions between atoms.

We employ our colloidal model system to study the properties of phasons. Phasons like phonons in the light-induced quasicrystal can be controlled by changing the phases of the laser field. We perform Brownian dynamics simulations to unravel single-particle dynamics as well as correlated phasonic flips when a constant phasonic drift is applied to the quasicrystalline potential. Single colloids exhibit characteristic trajectories along different directions that are given by their starting positions. We are able to define a characteristic area for phononic and phasonic displacement and demonstrate that each particle trajectory can then be predicted by mapping it into this area. Our observations help to get a deeper insight into the properties of phasonic displacements in colloidal as well as in atomic quasicrystals.

Extended and Localized States in Generalized Fibonacci Lattices: A Real-Space Renormalization Study

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Structural disorders in a solid can deeply modify the nature of its electronic states. It is well known that they are all extended in periodic systems and localized in randomly disordered systems of one and two dimensions [1]. However, the degree of localization in other aperiodic systems is still an unclear subject. In particular, a generalization of the Fibonacci chain can be obtained by using the substitution rules $A \rightarrow A^m B^n$ and $B \rightarrow A$, being m and n positive integer numbers. In this work, we prove that the aperiodic chains with $n = 1$ satisfy the Pisot criterion [2] and then are quasiperiodic. Furthermore, starting from an off-diagonal tight-binding Hamiltonian we extend a previously developed renormalization method [3] to address the density of states and electric conductivity in the generalized Fibonacci lattices. Both analytical and numerical results confirm the existence of transparent states with a unity transmittance in some of these lattices. In addition, the spectral-averaged transmittance shows a power-law decay with the system length when $n = 1$ and a quicker decay for other cases. It would be worth mentioning that for all the cases the spectral-averaged transmittance is neither a constant as in periodic systems nor an exponential decay as in randomly disordered ones. Finally, an analysis of multidimensional systems, such as aperiodic nanowires, by means of the convolution technique [3] will also be presented.

This work has been partially supported by UNAM-IN119011 and CONACyT-131596. Computations were performed at Bakliz and Kanbalam of DGCTIC, UNAM.

[1] E. Abrahams, et al., Phys. Rev. Lett. 42, 673 (1979).

[2] J.M. Luck, C. Godreche, A. Janner, and T. Janssen. J. Phys. A 26, 1951 (1993).

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Quantum Diffusion in Separable d-Dimensional Quasiperiodic Tilings with Golden and Silver Mean

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Understanding the relations between the atomic structure and the physical properties of materials remains one of the elementary questions of condensed-matter physics further emphasized by the discovery of quasicrystals. To address this challenge we present results for the electronic structure and the transport properties in quasiperiodic separable tight-binding models in one, two, and three dimensions. First, we investigate a class of one-dimensional quasiperiodic chains, in which the atoms are coupled by weak and strong bonds aligned according to the golden-mean and the silver-mean sequences. The associated d-dimensional quasiperiodic tilings are constructed from the direct product of d such chains, which yields either the square/ cubic metallic-mean tilings or the generalized labyrinth tilings. This allows us to consider rather large systems numerically.

The electronic transport is studied by means of the scaling behavior of the mean square displacement and the return probability of wave packets with respect to time. The results reveal the occurrence of anomalous diffusion for these systems. By extending a renormalization group approach, originally proposed for the golden-mean chain, we show also for the silver-mean chain as well as for the higher-dimensional labyrinth tilings that in the regime of strong quasiperiodic modulation the wave-packet dynamics are governed by the underlying quasiperiodic structure. Further, we also discuss lower bounds for the scaling exponent of the width of the wave packet and propose a modified lower bound for the absolute continuous regime.

Light transmission in aperiodic multilayers of porous silicon

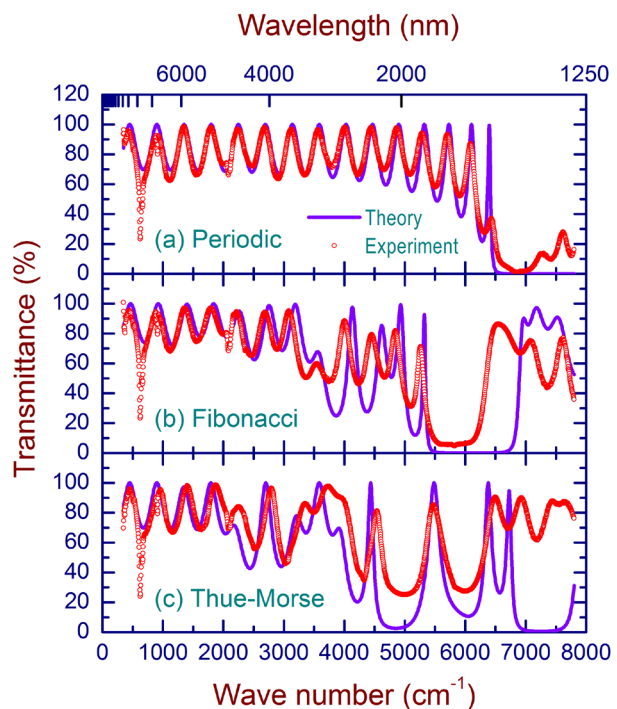
Alessio Palavicini and Chumin Wang

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Porous silicon is a nanostructured material and exhibits efficient photo- and electroluminescence in the visible range at room temperature, as well as a tunable refractive index determined by its porosity. Porous silicon samples can be obtained by etching a crystalline silicon wafer in a solution of hydrofluoric acid [1]. In this work, we report the fabrication of porous silicon aperiodic multilayers alternating layers with high and low porosities, which correspondingly produce high and low refractive indices. The free-standing multilayers were formed following three different sequences: periodic, Fibonacci and Thue-Morse. These aperiodic structures were verified by scanning electron microscopy and the light transmission spectra (open circles in the figure) were measured by means of Fourier-transform Infrared spectroscopy. On the other hand, we calculate the light transmittance of aperiodic porous silicon multilayers by using the transfer matrix method for all directions of incidence and a wide range of wavelengths. The experimental measurements are compared with theoretical predictions (solid lines in the figure). In addition, an analysis of infrared absorption peaks at 517, 625, 910 and 2087 cm^{-1} due to the molecular vibrations at pore surfaces reveals the presence of hydrogen and oxygen atoms. Finally, the efficiency as an omnidirectional mirror for each structure is also assessed.

This work has been partially supported by UNAM-IN117411 and CONACyT-131596. Computations were performed at Kanbalam of DGCTIC, UNAM.

[1] R. Cisneros, H. Pfeiffer, and C. Wang, *Nanoscale Res. Lett.* **5**, 686 (2010).



Thermoelectric Properties of Icosahedral Quasicrystals and Cubic Approximant Crystals in Al-Cu-Ru System

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One of practical applications of Al-based icosahedral quasicrystals is to be used for thermoelectric materials, because they possess relatively large Seebeck coefficients ($\sim 100 \mu\text{VK}^{-1}$) and glass-like low thermal conductivities ($\sim 1 \text{Wm}^{-1}\text{K}^{-1}$). For a better understanding of the physical properties of quasicrystals, comparison with related approximant crystals is a basic strategy. In this study, we selected the ternary Al-Cu-Ru system because both icosahedral quasicrystalline (I-) and cubic approximant crystalline (C-) phases exist in this system [1]. Homogeneous specimens with no secondary phase were synthesized by arc-melting and spark plasma sintering. The thermoelectric properties were measured from 373K to 973K. To understand the experimental results, we performed an *ab initio* electronic band calculation and calculated the thermoelectric properties using the Boltzmann transport equation for C-phase.

In figure 1, the Seebeck coefficients (S) of I- and C-phases at 973K are plotted against the effective valence electron number per atom (e/a), where the effective valency of Al, Cu and Ru are +3, +1 and -2, respectively. S of both I- and C-phases strongly depends on the e/a , and the sign of S changes from positive to negative with increasing e/a , indicating that there exist a pseudo-gap near the Fermi energy. We confirmed the existence of pseudo-gap from the band calculation for C-phase. We note that the calculated S of C-phase is quantitatively in good agreement with the experiment. Detailed thermoelectric properties and a guiding principle for high-efficient thermoelectric material will be discussed in the presentation.

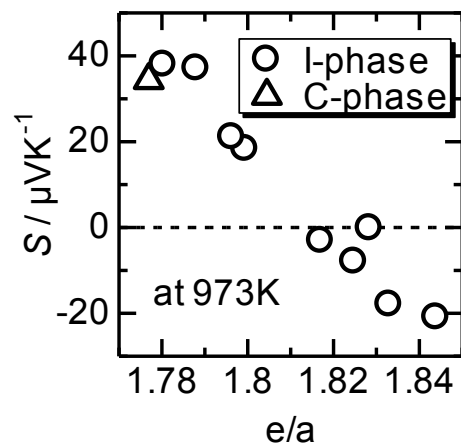


Figure 1

[1] S. Mi and B. Grushko, *Intermetallics* **12**, 425 (2004).

Development of Thermal-Rectifier Using Al-Based Quasicrystals

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Recently, thermal rectifiers, in which the heat-flow in one direction j_{q1} becomes much larger than j_{q2} that flows towards the opposite direction, have attracted considerable interest as a new solid device to control heat current. [1] We realized in our previous studies that quasicrystals and their corresponding approximants could be used as one of the materials in a thermal rectifier because of their characteristic thermal conductivity increasing with increasing temperature more dramatically than that expected from the Wiedemann-Franz law. This characteristic behavior is caused by the narrow pseudogap of a few hundred meV in width at Fermi energy under the influence of aperiodic structure. [2] By using two 1/1-cubic approximants of icosahedral quasicrystal, we developed a thermal rectifier working at temperatures above 300 K despite that the thermal rectification ratio ($TRR = j_{q1} / j_{q2}$) was limited less than 1.1.[3] In this study we attempted to develop a new thermal thermal-rectifier containing of Al-based icosahedral quasicrystal that possesses a very large increase of thermal conductivity with increasing temperature. It was estimated from the theoretical calculations using the experimentally determined thermal conductivity that the thermal rectifier consisting of the Al-Cu-Fe icosahedral quasicrystal and polycrystalline Si is capable of possessing TRR in excess of 1.5. Indeed, the large TRR value exceeding 1.4 was experimentally confirmed for the thermal-rectifier consisting of the Al-Cu-Fe icosahedral quasicrystal and polycrystalline Si placed between two heat reservoirs kept at 300 K and 550 K.

[1] M. Peyrard, *Europhysics Letters* **76**, 49 (2006).

[2] T. Takeuchi, *Zeitschrift fuer Kristallographie* **224**, 35 (2009).

[3] T. Takeuchi *et al.*, *Journal of Electronic Materials* **40**, 1129 (2011).

Diffuse scattering and phason modes in the Zn-Sc icosahedral quasicrystal

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Recently, a new binary icosahedral quasicrystal Zn-Sc has been obtained by Canfield *et. al.* [1]. Because of the chemical order and the x-ray contrast between Zn and Sc, this phase is a nice system for the structure refinement. On the other hand, a large amount of diffuse scattering can be seen on the x-ray diffraction pattern [1]. In this study, we carried out an absolute scale measurement of the x-ray diffuse scattering of i-ZnSc to study the possible presence of phason modes (phason diffuse scattering) and estimate phason elastic constants K_1 and K_2 .

Millimeter size single grain of i-ZnSc was obtained by slowly cooling from the melt. Systematic Q-scans and diffuse scattering maps have been measured on the D2AM beamline (ESRF) using an incoming x-ray energy equal to 9.3 keV.

Compared with i-ZnMgSc quasicrystal [2], we find that the amount of diffuse scattering is larger in i-ZnSc sample. Also, the maximal Q_{perp} value necessary for indexing the diffraction pattern was found to be less than 3 (r.l.u.) i.e. much smaller than for i-ZnMgSc for which it was found to be 7 [2]. In addition, as for other quasicrystals [3] a characteristic diffuse intensity distribution due to phason fluctuations around strong Bragg reflections is clearly visible on the systematic reciprocal space map. The ratio K_2/K_1 is found to be close to the three-fold instability limit, which results in the strong elongation of the diffuse scattering along directions parallel to a three-fold axis. Finally, the simulation is carried out based on the elastic theory and reproduces well the observed anisotropic shape of the diffuse scattering.

[1] P. C. Canfield, *et. al.*, Phys. Rev. B, 2010, 81, 020201.

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[3] T. Janssen, *et. al.*, Aperiodic Crystals. Oxford University Press, 2007.

Diffuse scattering resulting from macromolecular frustration.

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Distinctive diffuse scattering (see Fig. 1) in the form of diffuse rings around Bragg positions has been observed in the diffraction patterns of a crystal of the N-terminal fragment of the Gag protein from Feline Foamy Virus. It is shown that these are caused by geometric frustration as molecules try to pack on the triangular b - c mesh of the space group $P6_122$. In order to explain the strong diffuse scattering it is necessary for the crystal to contain occupational disorder such that each unit cell contains one or other of two different molecular arrangements, A and B. The

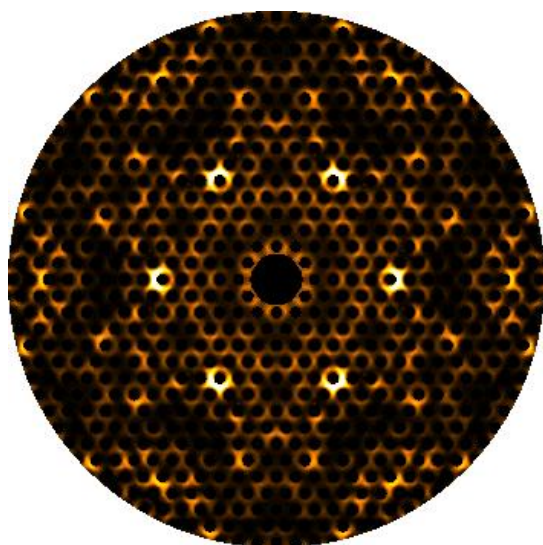


Fig. 1 The $hk2$ section of the Gag protein diffraction pattern.

frustration arises because the nearest neighbour packing prefers neighbouring cells to be AB or BA, which can't be achieved on all three sides of a triangle simultaneously. To explain the observation that reciprocal sections $hk\ 5n l$ where $n =$ integer, contain only Bragg peaks it is necessary that A and B are identical molecular arrangements differing only by a translation of $0.2c$. The implications of the disorder for solving the structure of the protein by conventional techniques as well as the possibility of using the diffuse scattering for this purpose are discussed.

A preliminary description of this has recently been published [1]. Here we describe some more recent developments.

- [1] T.R.Welberry, A.P. Heerdegen, D.C. Goldstone and Ian A. Taylor, *Acta Cryst.* **B67**, 516–524, (2011).

Diffuse scattering of decagonal Al-Cu-Co and Ni-rich Al-Ni-Co quasicrystals II Simulations

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Diffuse scattering of decagonal Al₆₄Cu₂₂Co₁₄ and Al₇₂Ni₂₀Co₈ quasicrystals (d-Al-Cu-Co and d-Al-Ni-Co) was measured by an imaging plate Weissenberg camera with synchrotron radiation x-ray. The diffuse scatterings on the Bragg reflection layers and diffuse layers at the middle in between two Bragg layers were observed. The diffuse scattering in the Bragg layers connects nearby Bragg reflections in both cases, while that in the diffuse layers is composed of many relatively sharp spots in the former and of very broad peaks in the latter. The diffuse intensities of both cases are simulated, based on the theory proposed recently [1] and superstructure models given in a previous paper of this series. Four kinds of columnar clusters can contribute to the diffuse scattering intensity. The correlation lengths of three clusters are different in d-Al-Cu-Co and d-Al-Ni-Co, leading to different diffuse scattering intensity distributions in the diffuse layers. The results of the simulation of diffuse scattering intensity will be presented.

[1] A. Yamamoto, *Acta Crystallogr.* **A66**, 372 (2011).

Diffuse scattering in $\text{KAlSiO}_4\text{-O1}$

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The monoclinic KAlSiO_4 polymorph O1 [1] exhibits an Al-Si-ordered $[\text{AlSiO}_4]$ -framework. Within this framework, layers of elliptically distorted six-membered (*sechser*) rings of alternating $[\text{AlO}_4]$ and $[\text{SiO}_4]$ tetrahedra can be identified. Vertices of the tetrahedra can either point up (U) or down (D) to connect with the adjacent layers. The framework topology of $\text{KAlSiO}_4\text{-O1}$ shows rings with UUDDUD and UUUDDD configurations [1].

Single crystals of $\text{KAlSiO}_4\text{-O1}$ have been synthesised using a flux-technique. X-ray diffraction experiments revealed multiple twinning, as well as two types of one-dimensional diffuse scattering (see Fig. 1). The dominant rods of diffuse scattering are oriented parallel to b^* . Every third (along a^*) streak exhibits higher intensities. This is consistent with stacking faults ($\perp b$) due to an $a/3$ -translation. The sequence of directedness of the tetrahedra in the rings across the translation plane is not changed, but the position of the sequence's starting point is, thus locally changing the framework topology. The other (weaker) system of diffuse streaks ($\parallel a^*+b^*$) is attributed to a second type of stacking faults.

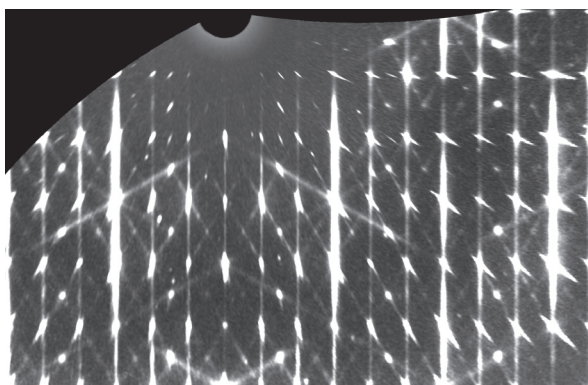


Fig. 1: Layer ($hk0$) of the reciprocal space of $\text{KAlSiO}_4\text{-O1}$, showing two types of one-dimensional diffuse scattering and their twin-related equivalents (X-ray data).

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Interpretation of diffuse scattering from single crystals with direct 3D PDF fitting

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X-ray diffuse scattering is a unique tool for analysis of disordered single crystals. Currently the most widely used method of the diffuse scattering interpretation is Monte Carlo modeling. Despite the fact that it gives enormous flexibility in the simulation of disordered crystals, refinement of diffuse scattering with MC techniques is usually very hard because model parameter refinements are computationally demanding.

In this contribution we present a new method for diffuse scattering interpretation. The method is based on direct fitting of the three-dimensional difference pair distribution function (3D- Δ PDF) of the crystal, which is the Fourier transform of diffuse scattering from a single crystal. It contains the information about interactions of pairs of atoms, ignoring such atoms, which are perfectly ordered as well fully uncorrelated atomic pairs. When the average structure of a crystal is known, 3D- Δ PDFs can be straightforwardly interpreted qualitatively, and by PDF fitting one can obtain quantitative information about local structure correlations.

The application of the method is demonstrated on a modeling of experimental diffuse scattering from single crystals. We also describe the impact of experimental problems like resolution function and background on the final result of diffuse scattering interpretation. These effects do not specifically apply to the results of PDF refinements, but should be considered for the quantitative interpretation of diffuse scattering with any method.

Incommensurately Modulated Protein Crystals

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Protein crystals can be modulated too. One of the earliest observed modulated protein crystals is a complex of profilin and actin. Actin filaments and filament formation are extremely important for a wide range of cellular processes. In solution, the protein complex disassociates as the pH of the system is lowered. This allows the free actin to assemble into filaments. When the complex crystallizes it undergoes an incommensurate modulation near the pH boundary where the disassociation has been observed for the soluble system. Initially, it was difficult just to get the complex in the modulated state. Over the last several years progress has been made towards solving the modulated structure. Currently, the area of focus is trying to get a good supercell approximation. This supercell could then be used as a starting point to refine the incommensurate data. Results from refinement of various supercell approximations will be discussed.

Parallel to the profilin:actin work, simulated data has been developed with the goal of using it to modify Jana for the purpose of processing incommensurate protein data. Details on this ongoing working with Jana will be presented.

As a side effect of trying to solve the incommensurate profilin:actin data, other protein crystallographers have from time to time sent in interesting diffraction data that they have collected and have asked for an opinion on or help with processing the data. Selected cases will be presented. Incommensurate modulated protein crystallography continues to be a very challenging problem.

New Challenges in Chemical Crystallography

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Until recently aperiodic molecular crystals have largely been ignored by molecular crystallographers. The first interest in solving and refining aperiodic molecular structures came from the pharmaceutical industry [1, 2]. However, Chemical crystallographers are now becoming increasingly aware of the Devil that can lurk in the details of the diffraction pattern [3], though the majority of chemical crystallographers still either close their eyes (solves the average structure) or throw the crystals away when faced with indications of an aperiodic structure.

With new higher intensity in-house X-ray sources and easier access to synchrotron radiation, more and more molecular structures are showing clear signs of being aperiodic. However, it is not necessarily the largest organic molecules that are aperiodic, but often the small, very symmetric molecules. Recently an incommensurately modulated polymorph of 1,3,5- tricarboxylate benzene (Trimesic acid, TMA) was discovered, but due to a combination of both twinning and the presence of multiple phases in the “single” crystals, the structure solution is a challenge [4]. We have also found a molecular compound that on lowering the temperature shows clear signs of an incommensurately modulated phase before the structure locks into a known ordered structure. These structures will be discussed including reasons for why chemical crystallographers often prefer to turn a blind eye to aperiodic structures.

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Poster Abstracts

Direct Imaging of Phason-Chains in Complex Boride Approximant by Angle-Resolved STEM

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There are various approximant crystalline phases available in B-Ti-Ru alloys [1], and the quasicrystalline phase indeed occurred when the relevant alloys is rapidly solidified [2]. Their structures can be systematically described based on the hexagon-boat-star (HBS) tiling, and the boride approximants reported are all constructed by H and B tiles. In these approximant borides, there occur many possible atomic sites in terms of local phason-flipping represented as bowtie flip, hence generating multiple variant structures with different phason-flip configurations. In the present paper, we attempt to determine such local phason-related flipping/displacement behaviors through the site-by-site analysis using angle-resolved scanning transmission electron microscopy (AR-STEM). From systematic imaging with low-angle to high-angle detectors, AR-STEM is able to show up directly the light atom position [3] (i.e., boron), atomic columnar distortions of Debye-Waller type [4] and heavy atom sites with chemical disorders (i.e., mixed occupations). We further tune the structure model based on first principles calculations and Rietveld refinement with synchrotron x-ray data set.

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Resonant Inelastic X-ray Scattering Study of Order-Disorder Phase Transition in $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ Decagonal Quasicrystal

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Energy spectrometer for inelastic X-ray scattering was installed on a six-circle diffractometer at beamline BL-4C (Photon Factory at the High Energy Accelerator Research Organization, Japan) [1]. The energy resolution is estimated to be 13 eV. By the combination of energy spectroscopy and diffraction, simultaneous real-time data acquisition of both the momentum and the energy transfer was applied into the diffraction anomalous fine structure measurements in $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ decagonal quasicrystal [2]. The $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ possesses an order-disorder phase transition at high temperature [3]. Also, short-range order (SRO) diffuse scattering was observed in the as-quenched sample.

At room temperature, resonant inelastic X-ray scattering (RIXS) in the as-quenched sample was observed only near the Co K-edge. RIXS vanishing near the Ni-K edge suggests that intrinsic excitation is induced by the local circumstance of Co atoms. We interpret that the anomaly in RIXS is connected with the Al-Co interaction, which was calculated using quantum-based pair potentials [4].

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The Optical Properties of Quasicrystals

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We will review our previous work, on the unusual optical conductivity of quasicrystals [1]. Although they are made up of well conducting metallic elements, their frequency dependent conductivity lacks a Drude peak that is the characteristic feature of a metal, nor is there evidence of incoherent hopping conductivity as seen in metallic glasses. Instead the conductivity rises linearly from a low value to saturate in the region of 1 eV. This applies to the icosahedral materials *i*-AlMnSi, *i*-AlCuFe, *i*-AlPdRe and their approximants. Decagonal quasicrystals such as *d*-AlCoCu, *d*-AlCoCuSi show a completely different behavior. In the decagonal plane they exhibit a constant conductivity, similar to what is seen in metallic glasses, while in the periodic direction they act like good metals. Models have been advanced to explain these phenomena in terms of a pseudogap at the Fermi surface. We also present preliminary data on the 3D diffraction patterns of *d*-AlCuCo and *d*-AlCuCoSi systems. As expected *d*-Al₆₅Co₁₇Cu₁₈ has a 0.4 nm lattice constant in the periodic direction, but also has very weak superlattice of 0.8 nm.

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Incommensurate-Commensurate Phase Transition in $\text{GdBaCo}_2\text{O}_{5+\delta}$

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The fundamental structure of $\text{GdBaCo}_2\text{O}_{5+\delta}$ (GBCO) is regarded as a stacking of $[\text{GdO}_\delta]$ - $[\text{CoO}_2]$ - $[\text{BaO}]$ - $[\text{CoO}_2]$ along the c axis [1]. GBCO shows the insulator-metal transition at $T_{\text{IM}} \sim 350$ K [1]. Here, we report structural phase transitions in GBCO ($\delta \sim 0.35$) around T_{IM} , examined by the electron diffraction. Two different types of transmission electron microscopes (TEM) are adopted for obtaining the electron diffraction patterns; the conventional and Lorentz TEMs, which enable us to obtain electron diffraction patterns in magnetic fields of ~ 2 T and 0 T, respectively. We observed satellite spots in the electron diffraction pattern commonly obtained by both electron microscopes at room temperature. The satellite spots reveal that the modulation wave vectors are $q_{\text{lt}1} = (\sim 1/3, 0, 0)$ and $q_{\text{lt}2} = (0, \sim 1/3, 0)$ with respect to the fundamental tetragonal (T) lattice. It was revealed that the modulation structure is attributed mainly to ordering of oxygen and vacancies in the GdO_δ layers by the single-crystal X-ray diffraction [2]. Upon heating in zero fields, additional superlattice spots with a commensurate modulation, $q_{\text{ht}} = (0, 1/2, 0)$, appear at ~ 400 K, while the satellite spots from the low-temperature T phase persist up to ~ 420 K. The high-temperature orthorhombic (O) phase has a different order of oxygen and vacancies from that in the low-temperature T phase [2]. Thus, this phase transition is characterized by the oxygen reordering. On the other hands, with increasing temperature under magnetic field, GBCO undergoes the distinct incommensurate-commensurate phase transition in which the q vectors in the low-temperature phase start to change toward $(1/2, 0, 0)$ or $(0, 1/2, 0)$ at ~ 400 K, and eventually, enters the high temperature phase above ~ 450 K. We discuss this oxygen reordering transition in terms of the coupling among the spin, charge, and lattice degrees of freedom.

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A₄(Cr,Fe): a structure survey

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The complex metallic alloy Al₄(Cr,Fe) is regarded an orthorhombic approximant to the decagonal AlCrFe phase with the *a*-axis corresponding to the periodic direction of the quasicrystal [1]. Large Al₄(Cr,Fe) single crystals have been grown using the Czochralski method [2].

A structure model of Al₄(Cr,Fe) has been published by Deng et al. [1]. The space group was determined from X-ray single crystal data to be *Immm* (Pearson symbol: *o*/366-59.56) [1]. In this structure model no distinction is made between Cr and Fe, because these transition metals are almost isoelectronic and can therefore not be discriminated using X-rays. To distinguish between Cr and Fe occupied sites a single crystal neutron diffraction experiment (sample size: (3 x 3 x 3) mm³, wave length: 1.5 Å) was performed at FRM II. The composition of the investigated crystal was measured by electron probe microanalysis to be Al_{79.1}Cr_{17.8}Fe_{3.1}. Axial as well as radial composition profiles were found to be almost uniform within the error of measurement.

As a result, using the neutron diffraction data the structure model of Deng et al. [3] could be refined further with respect to Cr and Fe positions. But additionally reflections *hkl* at *k* = *n*/2 (*n* = 1, 2, 3...) were found. From these additional reflections we conclude a superstructure, doubling the unit cell in *b*-direction. As these reflections at *k* = *n*/2 (*n* = 1, 2, 3...) are remarkably well defined ("sharp") the modulation exhibits long range order. The nature of these additional reflections will be discussed in more detail.

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A Modulated Protein Training Dataset

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The toolbox for computational protein crystallography is full of many rich and easy to use applications that make solving and refining data from typical diffraction datasets routine. There is a gap in the available software when it comes to more complex data. Current software cannot handle modulated diffraction data. To adapt software so that it can handle modulated data requires some kind of training data to test the software changes against. To help fill this void a comprehensive modulated training dataset has been created consisting of the atomic positions, atomic modulation functions and the structure factors packaged as both a supercell implementation and a 3+1 indexing. Two variations of the training data are available. One provides only first order satellites and the other provides first and second order satellites.

Constructing a dataset that can be processed using both approaches should make it easier to test and verify that phasing and the refinement methods are working as expected. The supercells each consist of an MTZ file and a PDB file which can be read in by all of the protein crystallography software. The modulated datasets consist of a single crystallographic information file (CIF) which can be read into Jana 2006.

X-ray diffraction study of TiPO_4 structure at low temperatures

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Low-dimensional systems have recently attracted much attention as objects for studying the complex interplay between spin, charge, orbital, and lattice degrees of freedom. Titanium phosphate is a quasi-one-dimensional quantum ($s = 1/2$) magnetic system which crystallizes in the orthorhombic space group $Cmcm$ [1]. In 2011 Law *et al.* [2] reported two magnetostructural phase transitions of TiPO_4 at 111 K and 74 K respectively. The low-temperature phase was described as a commensurate spin-Peierls state with Ti-Ti bond alternation along the Ti chains. Model calculations expect very weak superstructure reflections, which couldn't be resolved in an early neutron powder diffraction experiment. It was also proposed that the intermediate phase is the incommensurate phase which is similar to that found for TiOX [3]. The current work presents low-temperature single-crystal X-ray diffraction of titanium phosphate using synchrotron radiation. We have detected the development of commensurate and incommensurate phases of TiPO_4 at low temperatures. The weak satellites were found along $\mathbf{a}^*$ and could be indexed with the $\mathbf{q}$ -vector ($\sigma_1 00$). Below 70 K σ_1 is temperature independent and has a value of 0.5 and indicates the cell-doubling along $\mathbf{a}$. Above 70 K the $\mathbf{q}$ -vector becomes temperature-dependent incommensurate and disappears in the temperature range between 115 and 140 K.

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NON-UNIFORM Variation of the unit cell In A series of modular compounds: A stringent evidence of alternate cation/anion occupational modulations.

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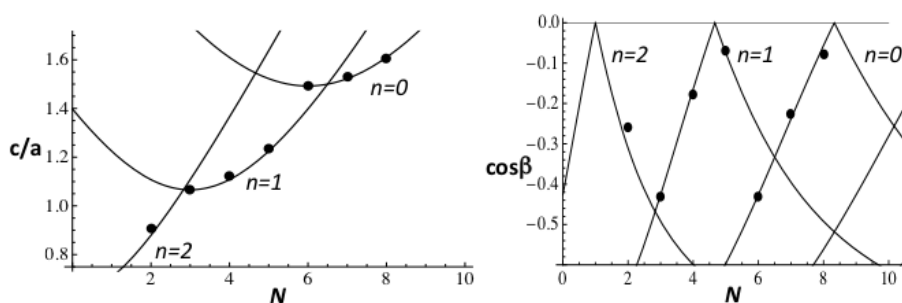
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Modular structures have by definition regions where one or several approximate subperiodicities can be defined associated with their modules. This property is the basis for their alternative description as modulated structures.¹ The approximate subperiodicity of a module can be taken as a reference average lattice, and the real structure is then described by means of a modulation with respect to this average sublattice. The modulation wave vector depends on the member of the series. This approach permits a unified description of a series, if the average subcell is essentially the same for all compounds.

In the simplest cases where the modules have similar orientations, a modular structure is expected to have as unit cell a supercell of an average unit cell directly related with the ideal periodicity of the modules. This means that the unit cells in a homologous series of modular structures are in principle constrained by the metrics of the idealized lattice of the underlying modules. This property is somehow trivial as long as it is taken as a very rough approximation, but we show here that strikingly this constraint is very severe in the pavonite homologous series.² The unit cell of each member of the series accommodates with high precision an integer number of a common subcell. This explains the conspicuous non-uniform variation of the unit cell of the members of the series (see Figure), and evidences that the interface between the modules is subject to very strong steric conditions. It implies also that cations and anions must alternatively occupy the nodes of the underlying average lattice, according to a surprising alternate cation/anion occupational modulation.



Values of c/a and $\cos\beta$ in the pavonite compounds $^N P$, compared with the theoretical values obtained as functions of N , assuming a perfect orthogonal subcell $\{a_b, c_b\}$ with $c_b/a_b = \sqrt{2}/2$.

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Random Tilings with Linear Phason Strain

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There are two kinds of phason disorders in quasicrystals, known as linear phason (LP) and random phason (RP), which are intrinsically correlated with each other. The aim of the present study is to elucidate how these two components are correlated with each other through case studies on random tilings that are constrained to have fixed LP strains. A periodic approximant to the decagonal HBS tiling is used as the initial state, and bow-tie flips are stochastically excited under periodic boundary conditions to generate a random tiling ensemble with the fixed LP strain. Due to the flips, another prototile, called E tile, occurs in the resulting tilings. From the calculated diffraction patterns, the intensities and the positions of the sharpest reflections are found to be insensitive to LP, except the corresponding peak shifts. The noticeable peaks, sharp or broad, also remain constant in the number, and they are mapped to a small region of the reciprocal perp-space near the origin. However, differences in the diffraction patterns are found in the diffuse components. Since peak shifts are determined by LP, diffuse components that are likely to develop between broad peaks lying close to each other can depend strongly on LP. It is therefore interesting to see how pronounced diffuse components are related with the LP strain. In the direct space, the diffuse components manifest in undulating arrays of tiles, which prior to randomization started as being a straight alignment of tiles.

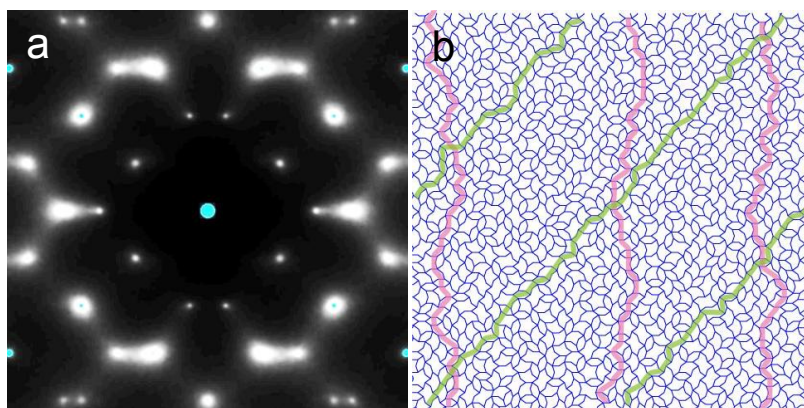


Figure: A random tiling with a linear phason strain corresponding to $1/1 \times 1/1$ approximant.

(a) The calculated diffraction pattern.

(b) The tiling with different degrees of undulation for two different orientations.

Substitution rules and topological invariants for the Robinson and Taylor Tilings

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A relatively simple substitution for the Robinson tilings [1] is presented, which requires only 56 tiles, up to translation. In this substitution, found by Joan Taylor, neighboring tiles are substituted by partially overlapping patches of tiles. We show that this overlapping substitution nevertheless gives rise to a normal primitive substitution tiling, implying that the Robinson tilings form a model set and have pure point diffraction. Moreover, the substitution can be used to compute the Čech cohomology of the Robinson tiling space via the Anderson-Putnam method [2]. The cohomology is computed, and some of its features are related to properties of the Robinson tilings. The overlapping substitution can replace a more complicated substitution found earlier [3].

In a very similar way, Taylor's hexagon tilings [4,5] are generated by an overlapping substitution, too. Also for these tilings, the cohomology of the associated tiling space is computed, and its features are related to properties of the tilings. We also discuss relations to other aperiodic hexagon and half-hexagon tilings showing up in the literature.

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Synthesis Optimization, Structural and Thermoelectric Properties of 1/1 Tsai-type Quasicrystal Approximants in A-Au-B System (A = Yb, Gd and B = Si, Ge)

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Abstract

Yb-Cd (Tsai-type^[1]) quasicrystals constitute the largest family of icosahedral quasicrystals where Yb can be replaced by other rare earth elements and Cd by p- and/or d-block elements. YbCd₆ is a prototype 1/1 Tsai-type approximant crystal which has similar local structure as Yb-Cd quasicrystal. In this study, the syntheses of Yb_{15.8}Au_{62.4}Ge_{21.8}, Gd_{13.5}Au_{69.3}Ge_{17.2} and Gd_{14.4}Au_{69.9}Si_{15.7} Tsai-type 1/1 quasicrystal approximants are optimized using the self-flux technique. The crystal structures of the compounds are refined by collecting single crystal x-ray diffraction data. The structural refinements indicate that the basic polyhedral cluster units in the compounds are symmetrically similar. The basic polyhedral units in all the three compounds can be described as concentric shells consisting of disordered tetrahedra, dodecahedra, icosahedra, icosi-dodecahedra and defect triacontahedra, from the inside and out. It is observed that the inner tetrahedra in GdAuGe_{1/1} and YbAuGe_{1/1} can be replaced by a rare earth atomic position at the center of the cluster which could have a damping effect on the lattice vibration, a property required for thermoelectric materials. Furthermore, the thermoelectric properties of the compounds are probed for the first time and their dimensionless figure of merit is calculated at different temperatures. This study is also intended to show the systematic effect of chemical substitution of structurally similar materials in their thermoelectric property. A significant difference is observed in the thermoelectric figure of merit values among these materials, which could arise due to their slight difference in their crystal structure and chemical composition, as we go from Si to Ge and/or Yb to Gd.

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Magnetic Properties of Cd_6R (R =rare-earth) Crystalline Approximants

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Since the discovery of an icosahedral quasicrystal (QC) by Shechtman et al [1], the behavior of spins on a quasi-periodic lattice has attracted a particular attention in solid state physics. Theoretical calculations suggest the existence of a long-range magnetic order, however, only spin-glass like freezing have been reported in the magnetic QCs such as Zn-Mg- R and Cd-Mg- R QCs [2]. Moreover, no long-range magnetic order has been reported in their crystalline approximants made of same icosahedral clusters. Recently, various long-range magnetic orders such as antiferromagnetic and ferrimagnetic ones have been found in quasicrystalline approximants, Cd_6Tb [3] and Cd_6Sm [4], respectively, which are made of an icosahedral rare-earth cluster. The magnetic susceptibilities of Cd_6R approximants are found to obey the Curie-Weiss law above 50 K except for $R = \text{Sm}$ and their Weiss temperatures are all negative indicating that R atoms at the vertices of an icosahedron are in a trivalent state and their $4f$ spins are well localized with antiferromagnetic interaction. Antiferromagnetic transition behaviors have been observed in a series of Cd_6R with meta-magnetic anomalies in M - H curves, the detail of which will be discussed in the presentation.

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Existence of Magic Numbers for the Determination of Convex Subsets of Cyclotomic Model Sets by Discrete Parallel X-Rays

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We report recent progress in the problem of distinguishing the collection of convex subsets of cyclotomic model sets Λ by (discrete parallel) X-rays in prescribed Λ -directions. Here, an X-ray of a finite planar point set in a fixed direction gives the number of points in the set on each line parallel to this direction and a Λ -direction is a direction parallel to a line through two different points of Λ . It turns out that for any of these model sets Λ there exists a “magic number” m_Λ such that any two convex subsets of Λ can be distinguished by their X-rays in *any* set of m_Λ prescribed Λ -directions [1]. In particular, for pentagonal, octagonal, decagonal and dodecagonal model sets, the least possible numbers are (in that very order) 11, 9, 11 and 13.

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Short-range Spin Fluctuation in the Zn-Mg-Tb Quasicrystal and the Relation to the Boson Peak

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Sato et al.[1] have measured the magnetic excitations in the Zn-Mg-Tb icosahedral quasicrystal by the inelastic neutron scattering. They found out very interesting results. That is, they observed the broad inelastic peak, which is attributed to the collective harmonic fluctuation of the short-range-ordered spins in the dodecahedral spin cluster. They also observed that the degree of freedom that freezes at the macroscopic freezing temperature T_f is the motion of entire spins, but not individual ones ; the freezing is very different from the canonical spin glasses. They suggested a possible close relation between the inelastic peak and the boson peak in the topological glasses. However it is unclear why the collective fluctuations do not propagate to adjacent clusters. In this study, we will propose the mechanism of localized spin fluctuation around the dodecahedral clusters, extending the previously theoretical formula [2,3]. One(I.K) of the present authors has discussed the origin of the boson peak by using the effective Lagrangian in the gauge-invariant formula with spontaneous symmetry breaking [4,5]. Furthermore, in this study, we will discuss the close relation between the inelastic peak and the mechanism of the boson peak, which is introduced by the present author.

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Physical property of icosahedral $\text{Zn}_{88}\text{Sc}_{12}$ quasicrystal

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Icosahedral (*i*) $\text{Zn}_{88}\text{Sc}_{12}$ quasicrystal (QC) discovered by Canfield et al^[1] in 2010 is another stable binary *i*QC following the discovery of Cd-based QCs^{[2][3]}. Because of the absence of chemical disorder, the *i*- $\text{Zn}_{88}\text{Sc}_{12}$ is also expected to exhibit physical properties intrinsic to *i*QCs. An interesting feature about the *i*QC is that two different morphologies, i.e., PD (Pentagonal Dodecahedron) and RT (Rhombic Triacontahedron), of single grains are obtained depending on the initial composition, the reason of which has not been understood. In this study, we have prepared $\text{Zn}_{88}\text{Sc}_{12}$ single grains having two different morphologies and investigated their electronic properties in detail. In this work, single-grained *i*- $\text{Zn}_{88}\text{Sc}_{12}$ were prepared by a self-flux method using high-purity Zn and Sc. The electrical resistivity $\rho(T)$ exhibits a negative temperature coefficient, which is a typical behavior of ternary *i*QCs, and its resistivity is $\sim 200 \mu\Omega\text{cm}$ at 290K. In addition, it shows a negative magnetoresistance. Both the behaviors are reminiscent of weak localization (WL) effect. The possible origins for the WL effect in the chemical disorder free *i*- $\text{Zn}_{88}\text{Sc}_{12}$ will be discussed in the presentation.

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Analysis of dislocations in quasicrystals composed of self-assembled spherical nanoparticles

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Talapin *et al.* [1] have recently shown that systems consisting of two types of spherical nanoparticles, such as Fe_2O_3 and Au with diameters of 13.4nm and 5.0nm, respectively, can self-assemble into dodecagonal quasicrystals. Naturally, such systems exhibit a certain degree of disorder, containing different structural defects including dislocations [2]. We analyze TEM images of such quasicrystals [3] using an automated procedure that identifies the positions of dislocations and determines their Burgers vectors. To achieve this we decompose the quasicrystal into its individual density modes, or Fourier components, thereby identifying the different components of the Burgers vectors, as described in [4]. We typically find a density of few dozen dislocations per μm^2 . The Burgers vectors that we find are all of lowest order, containing only zeros and ones as their components.

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Average Unit Cell in Fourier Space and Its Application to Decagonal Quasicrystals

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The paper describes a new technique for solving structure of quasicrystals. The technique is based on transformations between an average unit cell and an envelope of diffraction peaks [1-3]. An average unit cell approach describes a structure in terms of a distribution of atomic coordinates. An envelope is a continuous function that connects tops of peaks characterized by the same index of the modulated vector. It is possible to reduce positions of all available peaks into only few envelopes. This allows us to determine the best fitting curve of envelopes and thus obtain a pseudo-infinite set of diffraction peaks. A Fourier transform of envelopes, in general, leads to a self-convoluted distribution of atoms within an average unit cell. An iterative process enables us to restore phase of peaks and thus the straight distribution. Because the technique can be applied to many different average unit cells, a random noise is easily observable and removed. Additionally, in special cases when the underlying structure is highly symmetrical (like Penrose tiling or 1D Fibonacci chain), it is possible to obtain the distribution in one step without adjusting the phase. Apart from theoretical and modeling aspects of the technique the paper also presents the results of applying it to the well-known decagonal quasicrystal Al-Ni-Co [4-6].

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The Average Unit Cell concept for the Generalized Penrose Tiling

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The application of the Average Unit Cell (AUC) concept [1] to the Generalized Penrose Tiling (GPT) will be presented. The concept of the GPT was first introduced by Pavlovitch and Kleman [2]. As in the case of Regular Penrose Tiling (RPT) the GPT is built of two rhombuses (thick and thin). However, some new arrangements of tiles occur, which are not possible in the case of RPT. This could also be explained as introducing another pair of thick and thin rhombuses with different matching rules. In the 5D approach the RPT is generated as a projection of a 5D cubic lattice through a window of rhomb-icosahedron in the perpendicular space. The atomic surfaces are four equilateral, equidistant pentagons placed one above another and built from the vertices of the mentioned rhomb-icosahedron. In the case of the GPT, the window is shifted along the direction of its body diagonal [3]. Therefore there are five atomic surfaces: 2 pentagons and 3 decagons. In the AUC concept the probability distribution for rhombuses of RPT can be obtained as an oblique projection of the atomic surfaces on the physical space. This holds also for the GPT. We will present the derivation of the AUC distributions for a given type of rhomb in a given orientation for the arbitrarily chosen GPT (for any given shift of the projection window). In the RPT these distributions are triangular, whereas in the case of the GPT they are triangular (originating from the pentagonal atomic surfaces) or hexagonal (originating from the decagonal atomic surfaces). The derivation of the structure factor for any decoration of the unit tiles and any shift of the projection window will also be discussed.

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Hume-Rothery Stabilization Mechanism in Tsai-type Cd₆Ca Approximant and *e/a* Determination of Ca and Cd Elements in the Periodic Table

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The first-principles FLAPW-Fourier method can be used as a powerful tool to explore the Hume-Rothery stabilization mechanism in complex intermetallic compounds [1]. Mizutani and his coworkers recently demonstrated that *e/a*-dependent stabilization mechanism holds true not only for RT-type Al-Mg-Zn and Al-Li-Cu 1/1-1/1-1/1 approximants [2] but also for MI-type 1/1-1/1-1/1 approximants including Al-Mn, Al-Re-Si, Al-Cu-Fe-Si etc [3]. The aim of the present work is to extend the approach above to Tsai-type Cd₆Ca 1/1-1/1-1/1 approximant and to confirm if the Hume-Rothery stabilization mechanism universally holds for a whole series of 1/1-1/1-1/1 cubic approximants.

Nozawa and Ishii [4] have recently determined all atomic coordinates for Cd₆Ca 1/1-1/1-1/1 approximant by first-principles electronic structure calculations and studied the most stable configurations of its innermost tetrahedral shell. We have further refined the atomic coordinates and employed it for the FLAPW band calculations with subsequent FLAPW-Fourier analysis. The Cd₆Ca approximant contains 168 atoms per unit cell. The square of the Fermi diameter, *e/a* and *e/uc* and *critical* reciprocal lattice vector $|G|^2$ were determined. The present work is extended to determine *e/a* values of Ca and Cd elements in the periodic table.

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Stabilization of the High Temperature Phase of Cu-In at 100° C

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The η -phase field of the binary system Copper-Indium contains a variety of NiAs-Ni₂In superstructures with temperature (and composition) dependent modulation wave vectors. The high temperature *A* phase has been described as a near-commensurate lock-in phase earlier [1]. As a part of a general investigation of the η -phase field of the ternary system Copper-Indium-Tin it was found that the structural pattern of the *A* phase can be preserved at low temperatures by doping Cu₃In₂ with Tin. Although the Laue symmetry is *P6/mmm* the structure is not possible to refine in *P6₃/mmc* but the symmetry must be reduced. Reduction to orthorhombic symmetry in a twinned 3+1d model proved ineffective and only by the further reduction to monoclinic (*P2₁/m*, unique *c*) could the structure be refined to a satisfactory fit with data. The alternative route of reducing the symmetry within the 3+2d model was unsuccessful for *P6₃mc*, but worked well for the centrosymmetric *P6₃/m*. In fact the two models, twinned 3+1d *P2₁/m* and 3+2d *P6₃/m* turned out to be very similar in terms of fit, and so the high symmetry solution *P6₃/m* was chosen. The composition of the undoped phase is close to Cu₃In₂, but the homogeneity range is considerable. The modulation is driven by the sinusoidal distribution of one partially occupied Cu position over trigonal bipyramidal interstices and the resulting displacive relaxation of the surrounding atoms.

The effect of doping elements on η -phase field structures has been observed before for the structurally related compound Cu₆Sn₅ [2].

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Structure of 3/2-2/1 Orthorhombic Approximant to Decagonal Al-Cr-Cu Quasicrystal with 1.2 nm Periodicity

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We have analyzed the structure of a 3/2-2/1 orthorhombic approximant crystal ($Amm2$; $a = 1.2603(1)$ nm, $b = 3.2836(2)$ nm, $c = 2.3892(1)$ nm) to decagonal quasicrystals (DQCs) in the Al-Cr-Cu system, by means of single crystal x-ray diffraction for the first time. The crystals were grown by the self-flux method starting from molten metals with the composition of $Al_{80}Cr_4Cu_{16}$. The 3/2-2/1 approximant crystals were found in pentagonal-shaped plate crystals (Fig.1) which grew together with prismatic crystals (ζ phase, hexagonal, $a = 1.7634(1)$ nm, $c = 1.2514(1)$ nm). The composition of the 3/2-2/1 approximant determined by EPMA was $Al_{78.0}Cr_{16.1}Cu_{5.9}$ which was very close to that obtained for the ζ phase. The structure of the 3/2-2/1 approximant consists of six atomic layers perpendicular to the a -axis. The stacking sequence is $F_1P_1P_2F_2P_2P_1F_1$, where F_1 and F_2 mean flat layers, and P_1 and P_2 mean puckered layers, respectively. The projected structure along the a -axis can be described by a hexagon-and-star tiling (Fig.2) with an edge length of about 0.66 nm. Centers of pentagonal atom columns, whose diameters are 0.48 nm, coincide with the vertices of the tiling. Most of the transition metal atoms are situated at the vertices and the two positions on the edges. It is expected that the similar situation is realized in the corresponding DQC with 1.2 nm periodicity.

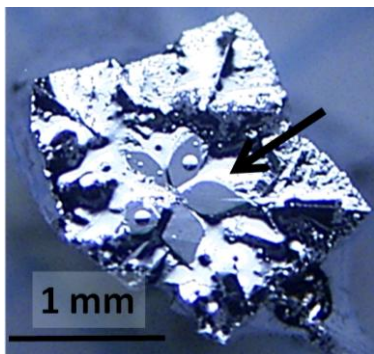


Fig. 1 Pentagonal-shaped plate crystal (thickness: ~ 0.5 mm), the arrow indicates domains of 3/2-2/1 approximant.

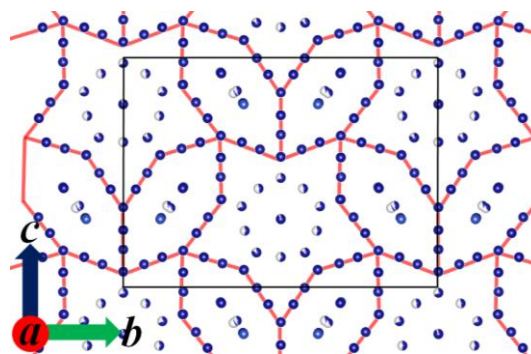


Fig. 2 Arrangement of the transition metal atoms and the tiling structure in the 3/2-2/1 approximant.

Physical properties of single-grained Ag-In-R(R = rare-earth) 1/1 approximants

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The Cd_6R (R=rare-earth) compounds which is a 1/1 approximant to the stable binary icosahedral Cd-Yb quasicrystal^[1] are known to exhibit structural and magnetic transitions at low temperatures. The structural phase transition is interpreted to be due to orientational ordering of a Cd_4 tetrahedron located at the center of the icosahedral cluster^[2] whereas the magnetic transition is attributed to an antiferromagnetic transition.^[3] On the other hand, such structural and magnetic transitions have not been reported in Ag-In-R 1/1 approximants which are isostructural to the Cd_6R 1/1 approximants. In order to gain insight into the occurrences of structural and magnetic transitions, the physical property has been investigated for single grains prepared by a self-flux method in a series of Ag-In-R 1/1 approximants. In the presentation, the temperature dependence of the electrical resistivity and the magnetic susceptibility will be reported.

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Structural investigation of the incommensurate modulated $\text{Ta}_2\text{O}_5\cdot\text{Al}_2\text{O}_3$ system

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The low temperature structure of tantalum pentoxide, L- Ta_2O_5 , has been the subject of repeated investigations. Although Ta_2O_5 has been widely utilised in tantalum capacitors the structure of this compound is still not completely understood. The addition of other metal oxides into Ta_2O_5 structure has been shown to form a stable high temperature phase isostructural to L- Ta_2O_5 . In this study, we investigated the addition of Al_2O_3 into Ta_2O_5 [1] to further determine the metal ion ordering and position of oxygen ion vacancies. $(1-x)\text{Ta}_2\text{O}_5\cdot x\text{Al}_2\text{O}_3$ ($x = 0.04, 0.06$ and 0.08) were synthesized, followed by structural characterization using synchrotron X-ray and neutron powder diffraction [2]. Refinements were performed using a [3+1] dimensional incommensurately modulated composite structure approach with a composition dependent modulation vector, q , in the orthorhombic superspace group $Xmmm(0\beta0)s00$. Atomic modulation functions across the $(1-x)\text{Ta}_2\text{O}_5\cdot x\text{Al}_2\text{O}_3$ series were found to be very similar not only to that of pure L- Ta_2O_5 , but also to the previously reported $\text{Ta}_2\text{O}_5\text{-WO}_3$ system [3]. Introduction of the modulation to the structural models resulted in more favourable bond valence sum values and bond distances compared to the basic structure. Additionally, Fourier difference map showed aluminium to preferentially occupy the octahedral sites. This contribution will also report on a variable temperature synchrotron X-ray diffraction study of the $x = 0.06$ member of the series.

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Effect of heat treatment on the electrical resistivity of icosahedral Al-Pd-Re quasicrystal prepared by the SPS method

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It is well known that icosahedral(*i*-) Al-Pd-Re quasicrystal exhibits the highest resistivity with a strong negative temperature coefficient among the quasicrystals that have been investigated to date. Insulating behaviors have been observed at low temperatures at the particular composition of $\text{Al}_{70.5}\text{Pd}_{21.0}\text{Re}_{8.5}$ [1]. However, polygrain samples prepared by conventional arc-melting method have a highly porous structure, which is not favorable for the study of the intrinsic nature of the electronic properties [2]. In this work, we have employed the spark plasma sintering (SPS) method which is capable of preparing dense uniform samples and investigated the role of the heat treatment condition in the electronic properties of *i*- $\text{Al}_{70.5}\text{Pd}_{21.0}\text{Re}_{8.5}$.

Polygrain *i*- $\text{Al}_{70.5}\text{Pd}_{21.0}\text{Re}_{8.5}$ quasicrystals were prepared using the SPS method. A mixture of pure element of Al(4N, < 20 μm), Pd(3N, < 50 μm) and Re(3N, < 50 μm) powders with the nominal composition of $\text{Al}_{70.5}\text{Pd}_{21.0}\text{Re}_{8.5}$ were sintered by the SPS method. The samples were then annealed at 823 ~ 1223K for 48 hrs. The characterization of the samples was performed by power X-ray diffraction and SEM. The electrical resistivity was measured by a four probe method between 290K and 17K. It is found that the electrical resistivity changes systematically with the annealing temperature: The highest resistivity ratio ($\rho_{17\text{K}}/\rho_{290\text{K}}$) is obtained when sample annealed at a lower temperature. The condition where the most insulating behavior occurs will be discussed in the presentation.

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***In-situ* high temperature TEM studies of Cd-based icosahedral quasicrystals.**

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An occurrence of an order-disorder phase transition related to the structure of the cluster, was discovered above ~100 K for a series of Cd₆M (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 possesses an orientationally disordered Cd₄ tetrahedron at the centre of the cluster. Also, the phase transition has been interpreted as involving orientational ordering of the Cd₄ tetrahedron at low temperature. In contrast, for Tsai-type icosahedral quasicrystals, there have been no reports of the phase transition. Although, Saitoh [3] reported that Cd-Yb and Cd-Mg-Yb icosahedral quasicrystals have no icosahedral symmetry at room temperature using convergent beam electron diffraction (CBED) method. This suggests that the tetrahedra at the center of the cluster are possibly oriented in the same direction. Therefore, we expect that an order-disorder transition occurs in the Cd-based quasicrystals at high temperature. In this work, we have studied the high temperature behavior of Cd-based quasicrystals using in-situ high temperature TEM.

Fig. 1 shows a CBED pattern of Cd-Mg-Yb quasicrystal taken with the incident beam parallel to the fivefold axis. The pattern shows the break of the fivefold symmetry, and no significant change is observed under 570K. Results of other TEM observations will be discussed in details.

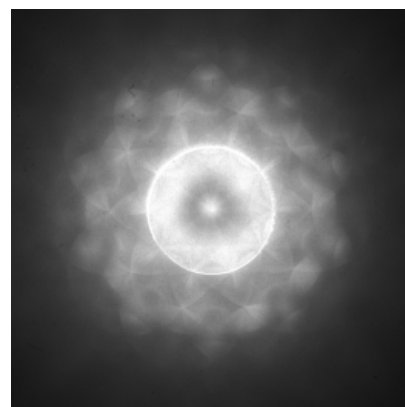


Fig. 1 CBED patterns of i-Cd-Mg-Yb along fivefold axis at 570K.

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Rotation of tetrahedral cores in Tsai-type approximants with various chemical combinations

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$\text{Cd}_{5.7}M$ ($M=\text{Yb, Ca}$) are the first thermodynamically stable binary quasicrystals (QCs) [1]. Structures of these QCs and its cubic approximant crystals Cd_6M and Zn_6Sc can be described using five-layered atomic clusters called Tsai-cluster as a building block. The innermost cluster of the Tsai-cluster is a Cd/Zn tetrahedron, and M/Sc atoms occupy an icosahedral third shell. Various phase transitions associated with change in orientational arrangements of the tetrahedral core are found experimentally [2, 3]. We performed first-principles electronic structure calculations for cubic Cd_6Ca [4] and Zn_6Sc [5], and found out in both systems that the tetrahedral cores are rotated around its twofold axis under pressure. A roughly evaluated transition pressure for Cd_6Ca [4] agrees well with the experimentally reported one for Cd_6Yb [3], whereas different pressure dependence is expected for Zn_6Sc [5].

We carried out further calculations for cubic approximants Cd_6Y , Cd_6Sc , Zn_6Ca and Zn_6Y to find out effects of chemical combinations. The calculations used here are based on the density functional theory with plane-wave basis sets. Cubic cells including 168 atoms with lattice constants determined to minimize the total energies are used as the unit cells.

Various potential energy curves for rotation of the tetrahedral core are obtained. In Cd-based compounds, the potential energy curves have a single minimum meaning parabolic shape, but double minima in Zn-based compounds. Furthermore, curvatures of the potential energy curves depend on the second elements (Ca/Y/Sc) in each Cd- and Zn-based system. We will discuss the origin of these differences.

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Synthesis of single-grained Ag-In-R (R = rare earth) 1/1 crystalline approximants

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(Ag,In)₆R (R = rare earth) compounds are 1/1 crystalline approximants (APs) composed of the Tsai-type icosahedral cluster with 168 atoms in the unit cell. The compounds are isostructural to the Cd₆R APs with Cd replaced by Ag and In[1]. The (Ag,In)₆R APs are of particular interest in view of comparison between the surface and bulk structures since they do not contain elements of high equilibrium vapor pressure such as Cd and thus they are more suitable for surface experiments. Moreover, it is also of interest to gain insight into the possible occurrence of structural and magnetic transitions which have been observed in isostructural Cd₆R APs[2] [3].

Up to date, there has been no report on synthesis of single grains in the Ag-In-R systems except for R=Yb and Eu[4] [5] where the rare-earth elements are divalent. Hence, we have conducted synthesis of single grains in the Ag-In-R systems where R is trivalent by the self-flux method. After thorough investigation of the phase constitution in a wide composition range in the Ag-In-Tb system, we have successfully obtained single-grains of Ag-In-Tb 1/1 APs with 2×2mm² size having clearly defined facets when slowly-cooled from the composition of Ag₅₀In₄₀Tb₁₀.

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Incommensurate structures occurring in the charge density wave states of $(PO_2)_4(WO_3)_{2m}$

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Mono Phosphate Tungsten Bronzes with pentagonal tunnels (MPTBp), $(PO_2)_4(WO_3)_{2m}$ with m ranging from 4 to 14, form a large family of compounds that can be described by the regular stacking of slices of tetrahedra PO_4 phosphates and slabs of corners sharing WO_6 polyhedra^[1] with a thickness depending on m . This family is of special interest since it provides a model system of quasi-two dimensional (2D) conductors in which the dimensionality can be driven by adjusting the parameter m . MPTBps exhibit successive temperature dependent Peierls-type phase transitions toward unusual charge density wave (CDW) states associated to the occurrence of satellite reflections of weak intensities and then to incommensurate or/and commensurate modulated structures^[2]. An analysis of the modulation observed in the CDW states for three members ($m=8, 9$ and 10) of the family is proposed. A global description of the diffraction patterns above the transition (showing pre transitional diffuse scattering) and below (with the occurrence of satellite reflexions) is done; a comparison of the symmetry and of the components of the modulated vector is given. A general description of the MPTBp using the superspace formalism shows that the symmetry of all the MPTBps is deriving from the super space group $Pn\bar{m}(00\gamma)0s0$, with $\gamma = 1/(m+2)$ ^[3]. The different phase transitions toward the CDW states have to be explained in light of this general model and the related hidden symmetry. The results of the structural analysis of the modulations for $m=8, 9$ and 10 are then discussed in regards with the CDW properties.

[1] P. Roussel, O. Pérez and Ph. Labbé, Acta Cryst. B57, 603-632 (2001)

[2] Foury, P. & Pouget, J. P. (1993). Int. J. Mod. Phys. B7, 3973-4003.

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Hume-Rothery Stabilization in Be and its Complex Alloys

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The Hume-Rothery stabilization mechanism refers to the e/a -dependent phase stabilization mechanism, in which energy of a given system is effectively lowered through the formation of an FsBz-induced pseudogap at the Fermi level [1]. The aim of the present work is to examine how different the stabilization mechanism in the hcp Be [2] is from that in its complex alloys (Be₁₃Mg, Be₁₃Ca, and Be₁₃Sb with N=112 in the unit cell [3] by using the approach described below.

We have performed FLAPW electronic structure calculations with subsequent FLAPW-Fourier analysis. The e/a values were calculated from the average of the $|2(k+G)|^2$ of the maximum Fourier coefficient $|C_{k+G}|^2$ at the Fermi level by making use of the tetrahedral method.

The analysis led us to conclude that the above Be based complex alloys are stabilized through the Fs-Bz interaction, while the hcp Be metal is stabilized due to mainly to the orbital hybridization effect.

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Extremely Long-Period 1D Stacking Polytypes in $\text{Al}_{13}\text{Co}_4$

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We report a new structure family of $\text{Al}_{13}\text{Co}_4$ which includes known approximants, $m\text{-Al}_{13}\text{Co}_4$, $o\text{-Al}_{13}\text{Co}_4$ and $o'\text{-Al}_{13}\text{Co}_4$ [1]. An ingot of about 10g with the nominal composition of $\text{Al}_{76.5}\text{Co}_{23.5}$ ($\text{Al}_{13}\text{Co}_4$) was prepared using arc melting technique under argon atmosphere and annealed at 980°C for 12h. In the sample many unknown electron diffraction patterns with streaks or superlattice reflections along specific direction are frequently observed. These patterns are basically explained as being structural polytypes constructed by a stack of the pentagonal-cluster chain (Fig.). On the basis of careful examinations of diffraction peak appearances, we find a striking feature that the stacking periods are extended into extremely long distances, typically being longer than $\sim 160\text{\AA}$. Furthermore, their stacking sequences can be uniquely determined with an aid of hyperspace crystallography. We are able to explain qualitatively these structural behaviors according to a modified axial next-nearest-neighbor Ising (ANNNI) model with essential infinite long-range interaction.

During the course of simulations based on ANNNI model without forced long-range interaction, we find that twining is a quite frequent event, since the twin variants generated by local exchanges of two basis vectors are equivalent in terms of free-energy. Despite this reasonable implication, surprisingly no twin crystals are observed in the present long-range modulation series. This is the reason why we claim that the infinite long-range interaction is essentially necessary to explain the occurrence of the $\text{Al}_{13}\text{Co}_4$ polytypes with extremely long-period modulations. Such unrealistic interactions might come from extra degree of freedom defined for hyperspace crystals; e.g., phason-mediated interactions.

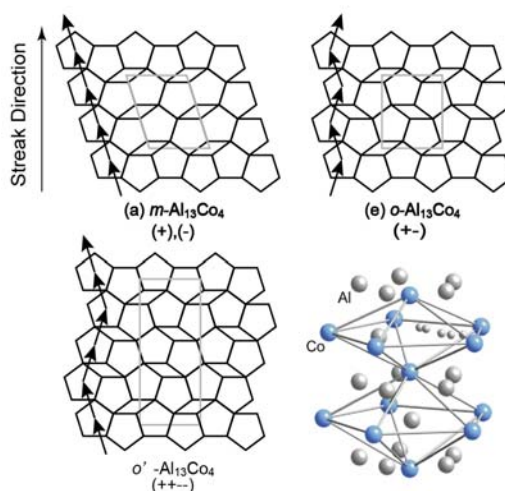


Fig. Stacking sequences of known approximants and pentagonal cluster [1].

[1] F. Fleischer et al., *J. Alloys and Comp.* **500** (2010) 153

Average Unit Cell concept for icosahedral quasicrystals

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Icosahedral quasicrystals (*i*-QCs) are structures with fully aperiodic arrangement of atoms in all 3 directions. It results in the occurrence of non-crystallographic 5-fold symmetry axes in a diffraction pattern. The Laue class for *i*-QCs is then $m\bar{3}5$. Most stable icosahedral phases are observed in ternary systems, however there exist also binary quasicrystalline structures too. First detailed structure solution for binaries (Cd-Yb) was given by Takakura et al. [1]. There is also the structure solution for ternaries Al-Pd-Mn [2] and Ti-Zr-Ni [3] known.

Here, the first results of the statistical approach to the structural solution of *i*-QCs will be presented. The method is based on the Average Unit Cell (AUC) concept [4] used for Ammann Tiling (AT, called also Ammann-Kramer-Neri Tiling [5]) with different decorating atoms. AT is defined by two structural units – prolate and oblate rhombohedron for which the volumes ratio is given by the golden ratio $\tau = 1.618...$ The atomic surface (within the higher dimensional description) and the AUC for AT have both the shape of rhombic triacontahedron. However the AUC concept allows the calculation in physical space only. The structure factor for empty and decorated AT lattice was calculated and numerical diffraction pattern was obtained.

The statistical method has been successfully used for complete structure solution of decagonal phases Al-Ni-Co and Al-Cu-(Co,Rh,Ir) by Kuczera [6].

- [1] H. Takakura et al., *Nature Materials* **6**, 58 - 63 (2007).
- [2] A. Fang et al., *J. Phys.: Condens. Matter* **15**, 4947-4960 (2003).
- [3] R.G. Henning et al., *Phys. Rev. B* **67**, 134202 (2003).
- [4] J. Wolny, *Phil. Mag.* **77**, 395-414 (1998).
- [5] P. Kramer, R. Neri, *Acta Crystallogr. A* **40**, 580-587 (1984).
- [6] P. Kuczera, J. Wolny, F. Fleischer, W. Steurer, *Philos. Mag.* **91**, 2500-2509 (2011); P. Kuczera, J. Wolny, W. Steurer (in prep).

Structure of τ^2 -Al₃Co, a monoclinic approximant of the Al-Co decagonal quasicrystal

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Decagonal quasicrystals (DQCs) with periodicities of about 0.4, 0.8 and 1.6nm were reported in rapidly solidified Al-Co alloys and a variety of corresponding approximant phases have been found in this binary system. Among them, (100) twins of the τ^2 -Al₃Co phase was realized by the annealing of DQC and the [010] electron diffraction pattern shows a strong resemblance to the 10-fold electron diffraction pattern of DQC. These facts readily suggest that τ^2 -Al₃Co is a good approximant for DQC. This study reports the single crystal structural analysis of τ^2 -Al₃Co. As shown in Fig.1, τ^2 -Al₃Co structure could be realized by a tessellation of pentagonal atomic columns with an edge length of 1.23nm. The column is τ^2 times larger than that found in the monoclinic Al₁₃Co₄, and this implies that *a* and *c* parameters of τ^2 -Al₃Co are about τ^2 times inflated from those of Al₁₃Co₄. The structure of τ^2 -Al₃Co also indicates the columnar structure similar to that found in W₂-(AlNiCo) approximant related to the Al-Ni-Co DQC. The present structural model was also studied by a Cs-corrected HAADF-STEM image, which has an enough resolution to reproduce separately individual transition-metal atoms in projected structures of the present approximant.

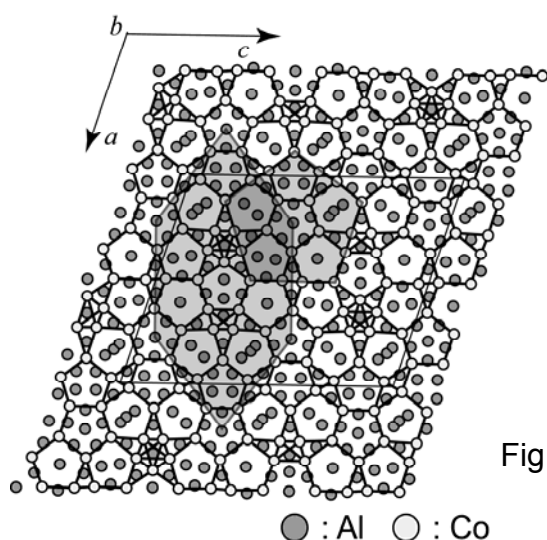


Fig. 1 The *b*-axis projection of τ^2 -Al₃Co.

Non-equilibrium Quasiperiodic Structure in Lamellar Structure of Al-Pd-Fe Complex Alloy Phases

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So far, almost all structural studies have been focused on quasicrystals with equilibrium and ordered structures, and therefore because of this, the structural information about those quasicrystals in state of growth or phase transition is still quite lacking. The Al-Pd-Fe alloy is a quasicrystal-forming system in which a decagonal quasicrystal with 1.6 nm periodicity (D_8 -phase) can be formed through a rapid solidification process. In this study, we have found that the formation of the as-grown Al-Pd-Fe D_8 -phase in non-equilibrium state can be localized in a kind of characteristic lamellar structure in the conventionally solidified $Al_{75}Pd_{15}Fe_{10}$ alloy. This provides a great opportunity to investigate the formation process of a quasiperiodic structure and to clarify its correlation with related crystalline structures as well. TEM observations show that the Al-Pd-Fe D_8 -phase, coexisting with its crystalline approximant ξ -phase, is sandwiched by monoclinic Al_3Fe (M- Al_3Fe) phase with definite boundaries and orientational relationships between them. High-resolution electron microscopy and high-angle annular dark-field imaging techniques have been applied to reveal structural details of various characteristic units in the lamellar structure. On the basis of this, characteristics of the imperfect Al-Pd-Fe quasiperiodic structure in non-equilibrium state will be presented and discussed in terms of atom cluster arrangement, and furthermore in terms of packing of intrinsic building units as well.

Growth Morphology of faceted AlCuCo and AlCuFe Single Quasicrystals

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Growth morphology 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 specimens of both alloys were obtained in a helium atmosphere using the Bridgman-Czochralski-Growth (BCG) apparatus equipped with an induction furnace. The nominal composition of an Al-Cu-Fe alloy, exhibiting polyhedral equilibrium single grains of the icosahedral ψ phase, was 65 at. % Al, 20 at.% Cu and 15 at.% Fe. For the decagonal Al-Cu-Co phase the initial chemical composition was 73.5 at. % Al, 17.5 at.% Cu and 9 at.% Co. Both types of single quasicrystals exhibited a decorations on their facets, however the character of decorations was totally different (fig.1).

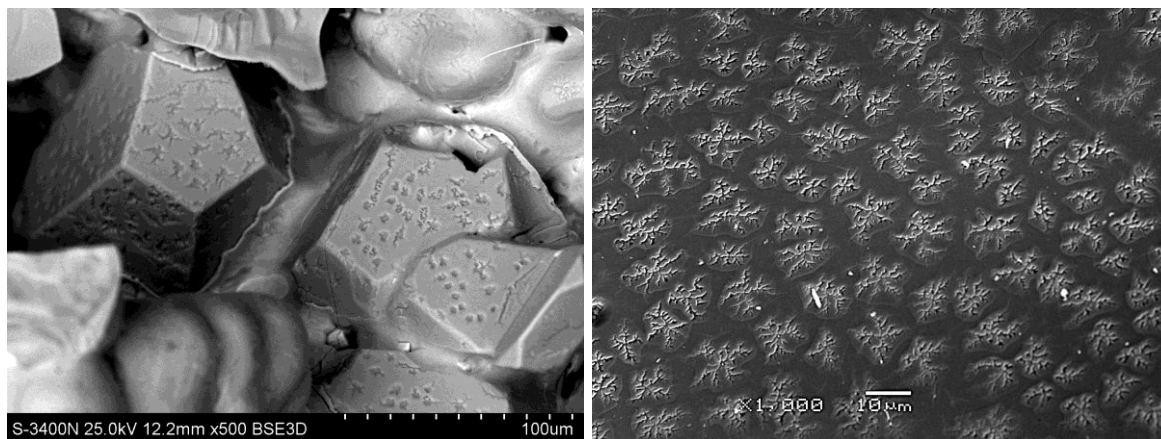


Fig. 1. Decorations on facets of icosahedral $\text{Al}_{60}\text{Cu}_{26}\text{Fe}_{14}$ (left) and on surface decagonal $\text{Al}_{73.5}\text{Cu}_{17.5}\text{Co}_9$ (right)

Two stages of decorations has been developed on icosahedral $\text{Al}_{60}\text{Cu}_{26}\text{Fe}_{14}$ quasicrystals: cellular primary decorations and secondary fractal like decoration. Surface decorations on decagonal $\text{Al}_{73.5}\text{Cu}_{17.5}\text{Co}_9$ quasicrystals formed a kind of irregular stars placed on the neighboring islands.

Some comments on the inverse problem of diffraction.

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In a recent paper [1], Lenz and Moody presented a method for constructing families of (real) solutions to the inverse problem for a given pure point diffraction measure. We give some examples of their technique, and discuss some possible adaptations. In particular, we present some derived examples of homometric structures.

- [1] Lenz, D. and Moody, R.V., *Stationary processes with pure point diffraction*.
arXiv:1111.3617

Surface Characterization of Gd₅Ge₄

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Gadolinium, and alloys of Gd with various post-transition elements, are considered promising materials for magnetic refrigeration near or below room temperature. Gd₅Ge₄, an orthorhombic system with 36 atoms per unit cell, is in this group. We have characterized the (010) surfaces of two different samples of Gd₅Ge₄ using scanning tunneling microscopy and x-ray photoelectron spectroscopy. Although there are differences between data from the two samples (notably in the progression of surface structure as a function of temperature), they have the following features in common: (1) Surface composition is the same as bulk composition to within + 5 atomic %, both after sputtering and after annealing at various temperatures; (2) The surface exhibits two main types of terraces, which have much different fine structures. The two types of terraces alternate across the surface. Under some conditions they have comparable areas and the alternation is visually striking. Under other conditions a single type dominates, but the second type is still discernible as small protrusions at step edges (i.e. as step bunches). Step heights between similar terraces correspond well to the spacing between similar layers along the <010> direction in the bulk structure, and step heights between dissimilar terraces correspond to the distances between dissimilar but dense layers. However, the fine structure on the terraces does not correlate with the bulk structure, and we suggest that there is significant surface reconstruction.

Pseudo Symmetry in Tungsten Bronze Type $\text{Sr}_3\text{TiNb}_4\text{O}_{15}$

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Many compounds with tungsten bronze type structures have been shown to display useful physical properties, including nonlinear optical behavior as well as ferroelectric properties.

This contribution focuses on the $\text{Sr}_3\text{TiNb}_4\text{O}_{15}$ tungsten bronze type compound. This composition has been reported a number of times but questions remain about the unit cell choice and the symmetry adopted by this compound [1-3]. We show that these discrepancies have arisen because of pseudosymmetry in the structure of $\text{Sr}_3\text{TiNb}_4\text{O}_{15}$. The parent structure of $\text{Sr}_3\text{TiNb}_4\text{O}_{15}$ can be considered to have tetragonal $P4bm$ symmetry with a $\sim 12 \times 12 \times 4$ Å cell, which is indeed adopted above 325 °C. The RT structure has been reported in the orthorhombic crystal system, however, with very similar a and b cell parameters resulting in a pseudo tetragonal structure ($17 \times 17 \times 4$ or $12 \times 12 \times 4$ and $Cmm2$ or $Pba2$, respectively [2, 3]). Further to this, and adding to the pseudo symmetry, synchrotron powder X-ray diffraction data indicated a doubling along the c -direction. In addition, electron diffraction data reveal that the symmetry may need to be lowered to $P222$ to be consistent with the observed extinction conditions. This high level of pseudo-symmetry makes refinements from powder data very difficult unless appropriate constraints are applied. Symmetry-mode analysis of the distortions in the structure and their direct refinement may be the answer to the problems encountered and will be discussed [4].

[1] F. W. Ainger, W. P. Brickley, G. V. Smith, *Proceedings of the British Ceramics Society* **18** (1970) 221.

[2] R. R. Neurgaonkar, J. G. Nelson, J. R. Oliver, *Materials Research Bulletin* **27** (1992) 677.

[3] E. O. Chi, A. Gandini, K. M. Ok, L. Zhang, P. S. Halasyamani, *Chemistry of Materials* **16** (2004) 3616.

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Anomalous properties and the electronic glass-like state in Al-based stable quasicrystals

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The thermodynamically stable Al-based quasicrystals have the anomalous electrical-conductivities, such as semiconductor-like properties [1]. It has been suggested that the semiconductor-like properties are due to the combination of a Hume-Rothery pseudogap and the presence of localized states at the Fermi level. In addition, Homes et al.[2] have reported the anomalous property of photo-conductivity in quasicrystal Al-Cu-Fe. Okada et al.[3] observed the fine structure of electron state of a few meV near Fermi level in stable Al-based quasicrystals. The present authors have considered the anomalous transport properties of Al-based stable quasicrystals with the quasicrystal-like model[4,5]. In this study, we will introduce the electronic glass-like states, and discuss the mechanism of anomalous photo-conductivity in Al-based stable quasicrystals.

- [1] S. J. Poon, *Adv. Phys.* **41**, 302 (1992).
- [2] C. C. Homes et al., *Phys. Rev. Lett.* **67**, 2699 (1991).
- [3] J. T. Okada et al., *J. Phys. Soc. Jpn.* **76**, 033707 (2007).
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- [5] K. Yamada et al. *Physics Procedia*, 2012, in press.

Diffuse scattering of decagonal Al-Cu-Co and Ni-rich Al-Ni-Co quasicrystals I Superstructure models

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Five dimensional models of decagonal Al-Cu-Co and Ni rich Al-Ni-Co quasicrystals are proposed for their diffuse scattering analyses. They have the lattice constants of $a \sim 2.7$ and $c \sim 8.1$ Å. These structures are 2-fold superstructures (with a doubled c) of the average structure obtained from the Bragg reflections. Their occupation domains are obtained from those in the basic Ni-rich phase of decagonal Al-Ni-Co by introducing the phason flip [1].

Four kinds of clusters included in the models and their disordered arrangement give the diffuse scattering on even and odd layers normal to the 10-fold axis in the reciprocal space. One of the four is quite similar to the cluster used in the diffuse scattering analysis in d-Al₇₀Cu₂₀Co₁₅ [2]. The existence of shifted clusters for three of them and the orientational disorder of another cluster provide the source of the diffuse scattering.

[1] A. Yamamoto, *Phys. Rev.* **B83** 184203 (2011).

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Arrangements of transition-metal atoms in ideal structures of Al-Ni-Co decagonal quasicrystals

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The Most of decagonal quasicrystals represented by Al-Ni-Co ones have been considered to be composed of atom columnar clusters with a diameter of 2 nm, and so their structures have been discussed by the structures of the atom clusters and their arrangements [1]. Also, the cluster structures have been used for initial models for X-ray structure refinements. However, structures of W-(AlNiCo) [2] and τ^2 -Al₁₃Co₄ [3] crystalline phases, which have been known to be important approximants for understanding structures of Al-Ni-Co decagonal quasicrystals, don't show the existence of the 2 nm clusters, but transition-metal (TM) atoms in the structures are systematically arranged with a bond-orientational order. On the other hand, recent Cs-corrected STEM (scanning transmission electron microscopy) has an enough resolution to reproduce individual TM atoms in projected structures of decagonal quasicrystals along the periodic axis, and so enables us to determine directly arrangements of TM atoms [4]. In the present paper, from the arrangements of TM atoms in pentagonal and rhombic tiles with an edge length of 2 nm, determined from HAADF (high-angle annular detector dark-field) images with the Cs-corrected STEM, we aim to derive arrangements of TM atoms in ideal structures of two kinds of decagonal quasicrystals in Al_{71.5}Co_{25.5}Ni₃ and Al_{72.5}Co_{17.5}Ni₁₀ alloys. The TM atoms on A and B planes stacking along the periodic axis are located at lattice points of pentagonal lattices with bond lengths of 0.47 nm and 0.76 nm, respectively. Those arrangements in the ideal structures are also obtained from special windows in the internal space.

[1] K. Hiraga, *Advances in Imaging and Electron Physics*. Vol.122 (Elsevier Science (USA) 2002).

[2] K. Sugiyama, S. Nishimura and K. Hiraga, *Alloys & Comp.* **342**, 65 (2002).

[3] K. Sugiyama, A. Yasuhara and K. Hiraga, *in the Aperiodic 2012 Conf.*

[4] A. Yasuhara, K. Saito and K. Hiraga, *in the Aperiodic 2012 Conf.*

Direct observations of aperiodic arrangements of transition-metal atoms in Al-Ni-Co decagonal quasicrystals by HAADF imaging with a Cs-corrected STEM

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Structures of decagonal quasicrystals found in Al-Ni-Co alloys have been characterized as two-dimensional aperiodic arrangement of columnar atom clusters with a decagonal cross-section of 2 nm in diameter [1]. On the other hands, the structure of a W-(AlNiCo) crystalline phase, related to the Al-Ni-Co decagonal quasicrystals, shows that transition-metal atoms of Ni/Co are arranged with a bond orientational order [2]. Therefore, our aim is that the structures of the Al-Ni-Co decagonal quasicrystals are to be characterized as aperiodic arrangements of Ni/Co atoms from direct observations of individual transition-metal atoms by HAADF imaging, which enables us to observe individual transition-metal atoms directly. The experiments were performed with a Cs-corrected STEM (JEM-ARM200F).

Figure 1 shows a HAADF-STEM image of a decagonal quasicrystal in an $\text{Al}_{71.5}\text{Co}_{25.5}\text{Ni}_3$ alloy. In the image, bright dots, corresponding to Ni/Co atoms, connected by solid and dotted lines are on A and B planes stacked along the periodic axis, respectively; Ni/Co atoms on the A and B planes are located at lattice points of pentagonal lattices with bond lengths of 0.47 nm and $0.47\tau=0.76$ nm, respectively.

[1] K. Hiraga: *Advances in Imaging and Electron Physics*. (Elsevier Science, 2002).

[2] K. Sugiyama, S. Nishimura and K. Hiraga: *Alloys & Comp.* **342**, 65 (2002).

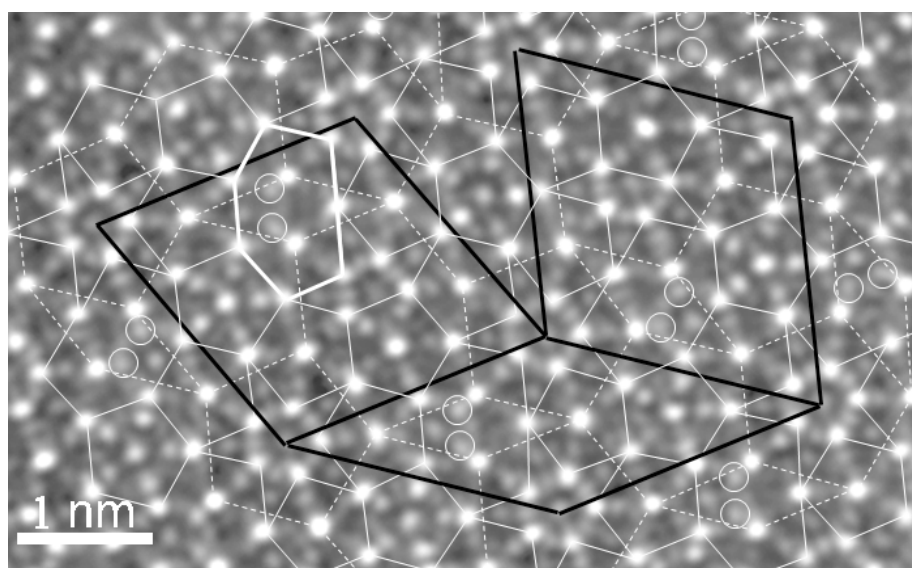


Fig.1

Arrangement of transition-metal atoms in an approximant crystal related to Al-Cu-Co decagonal quasicrystals studied by Cs-corrected HAADF-STEM

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The structures of approximant crystalline phases are important for understanding those of quasicrystals. Recent Cs-corrected STEM (scanning transmission electron microscopy) has an enough resolution to reproduce separately individual transition-metal atoms in projected structures of decagonal quasicrystals along the periodic axis, and so arrangements of transition-metal atoms can be directly determined from observed HAADF (high-angle annular detector dark-field)-STEM images. In this paper, we aim to determine an atomic arrangement of Cu/Co in a crystalline approximant in an $\text{Al}_{66}\text{Cu}_{15}\text{Co}_{19}$ alloy annealed at 900 °C for 36 h from HAADF-STEM observations with a Cs-corrected electron microscope (JEM-ARM200F). Figure 1 shows a HAADF-STEM image of the approximant crystal. In the image, atom columnar clusters, which are composed of a pentagon of bright dots and surrounding ten bright dots, are arranged with pentagonal and rhombic tiles with an edge length (thin line) of 2 nm, as indicated by circles. Two-types of the atom clusters, which are distinguished by circles of solid and dotted lines, have different directions of the central pentagons of bright dots and are orderly arranged in a rectangular unit cell with side lengths of 6.68 nm and 10.14 nm. From the close examination of Fig. 1, we can derive arrangements of Cu/Co atoms on two planes.

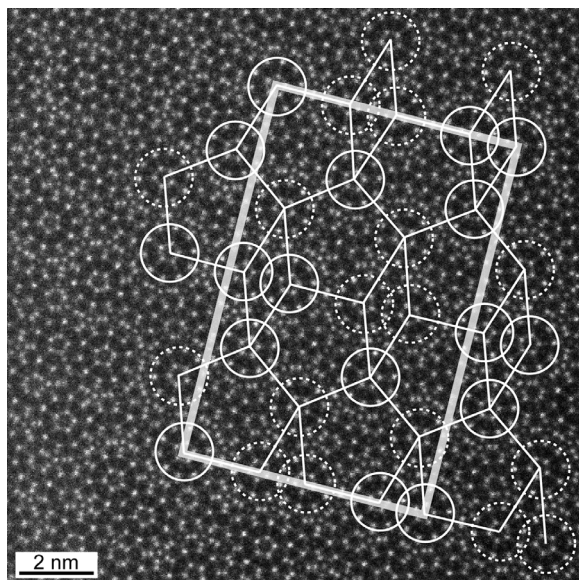


Fig. 1 Cs-corrected HAADF-STEM image of the approximant crystal.

Structure of ϵ_{16} phase in Al-Pd-Co system studied by HREM and X-ray diffraction

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A variety of orthorhombic phases related to the Al_3Pd approximant phase [1] were found in Al-Pd-(Fe, Mn, Co) systems. Their lattice parameters of $a = 2.35$ and b (pseudo-10 fold axis) = 1.68 nm are essentially similar to each other, nevertheless the corresponding c parameter are $\sim 1.2, 3.2, 4.5$ and 5.7 nm for ϵ_6 (Al_3Pd phase), ϵ_{16} , ϵ_{22} and ϵ_{28} , respectively [2,3]. Although their structures could be described by the tiling of pentagonal atomic columns with a periodicity of 1.68 nm, the atomic positions for a series of ϵ_n ($n=16, 22$ and 28)-phases are not determined quantitatively by single-crystal X-ray diffraction. In this study, the crystal structure of the ϵ_{16} phase in an annealed $\text{Al}_{72}\text{Pd}_{10}\text{Co}_{18}$ alloy was investigated on the basis of the combination between HREM and single crystal X-ray diffraction. Figure 1 shows an HREM image and the corresponding electron diffraction pattern from the ϵ_{16} phase in the Al-Pd-Co system. An edge length of a solid line in the image is 0.77 nm. A rectangle with a dotted line indicates a unit cell of the ϵ_{16} phase.

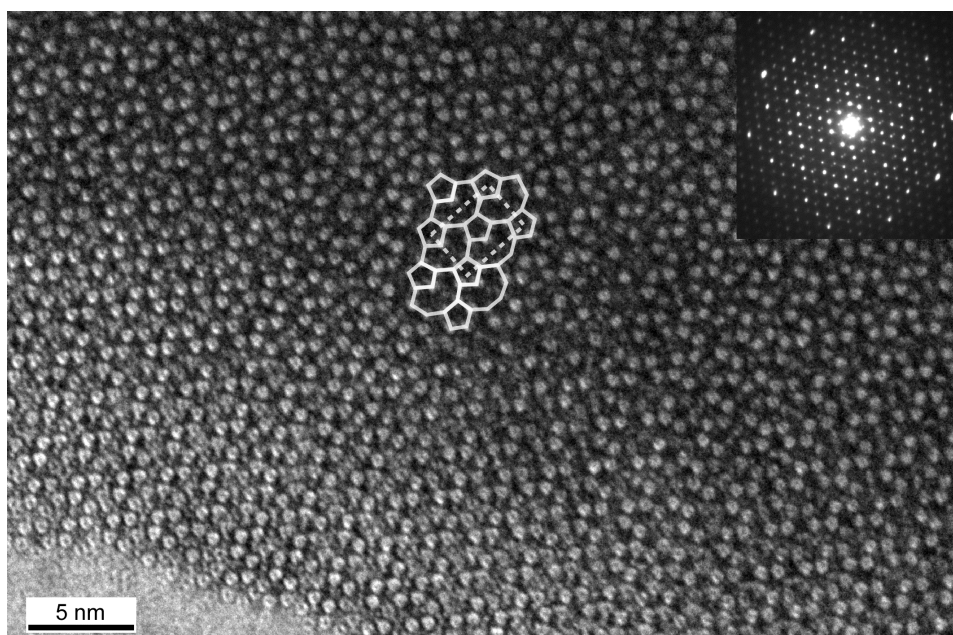


Fig. 1 HREM image and electron diffraction pattern of $\text{Al}_{72}\text{Pd}_{10}\text{Co}_{18}$ alloy.

- [1] Y. Matsuo et al., *Phi. Mag. Lett.* **70**, 155 (1994).
- [2] S. Balanetsky et al., *Z. Kristallogr.* **219**, 548 (2004).
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A transmission electron microscope study into the microstructure of the perovskite $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$

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Perovskite sodium bismuth titanate (NBT) doped with barium titanate (BT) is an attractive material for research due to its excellent piezoelectric properties [1]. Previous research [2] has shown that the room temperature phase of NBT belongs to the polar R3c space group. However, many experiments (in situ neutron scattering of NBT single crystal) have revealed deviations from the ideal R3c structure. Since the loss of symmetry compared to the average structure is critical in understanding NBT's ferroelectric properties, studying the local microstructure of NBT is essential.

In this work subtle changes in symmetry and structure were detected and characterised at the nanoscale using a variety of transmission electron microscopy (TEM) techniques, including selected-area electron diffraction, high-resolution (scanning) transmission electron microscopy and x-ray energy dispersive spectroscopy (EDS).

During the course of this work, evidence for local structure modulations was observed in both high-angle annular dark field (HAADF) images and a series of diffraction patterns taken along several reciprocal zone axes. These observations and their interpretation will be discussed during the conference. Meanwhile, bismuth nanoparticles were also observed when NBT-BT was exposed to the electron beam in the TEM at room temperature. The irradiation effects were investigated using selected area diffraction, EDS and their growth was studied in situ with time-resolved high resolution images. These observations will also be discussed at this conference.

[1] Y. Guo et al. *Chemistry of Materials* **23**, 219 (2011)

[2] G. Jones et al. *Acta Crystallographica B* **58**, 168 (2002)

Description of phase equilibria in complex metallic alloys of Al-Pd-Co system at 700°C

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Five complex metallic alloys $\text{Al}_{68}\text{Pd}_{14.6}\text{Co}_{17.4}$, $\text{Al}_{69.8}\text{Pd}_{13.8}\text{Co}_{16.4}$, $\text{Al}_{72}\text{Pd}_{12.8}\text{Co}_{15.2}$, $\text{Al}_{73.8}\text{Pd}_{11.9}\text{Co}_{14.3}$, and $\text{Al}_{76}\text{Pd}_{11}\text{Co}_{13}$ annealed at 700°C for 2000 h were investigated. After annealing the samples were rapidly cooled in water to fix their high-temperature microstructure. In the investigation, scanning electron microscopy including energy dispersive X-ray spectroscopy, transmission electron microscopy, X-ray diffraction, and electron backscatter diffraction were used. Binary phases Al_5Co_2 , Al_9Co_2 , $\beta\text{-Al}(\text{Co}, \text{Pd})$ and ϵ_{16} , as well as the ternary U-phase were identified in the analyzed samples. The ϵ_{16} was considered as quasicrystalline approximant. New lattice parameters of U, β and ϵ_{16} were determined. The above experimental results were used to construct the partial isothermal section of the Al-Pd-Co system at 700°C. It is an original result, because isothermal sections for temperatures lower than 790°C were not published yet. The thermodynamic modeling using Thermo-Calc software was done to create the thermodynamic database of the Al-Pd-Co system. The thermodynamic databases of Al-Pd, Al-Co and Pd-Co systems were compiled and extrapolated to ternary system. The further work related to assessment of thermodynamic parameters of ternary phases and solubilities of the third element in binary phases is in progress.

